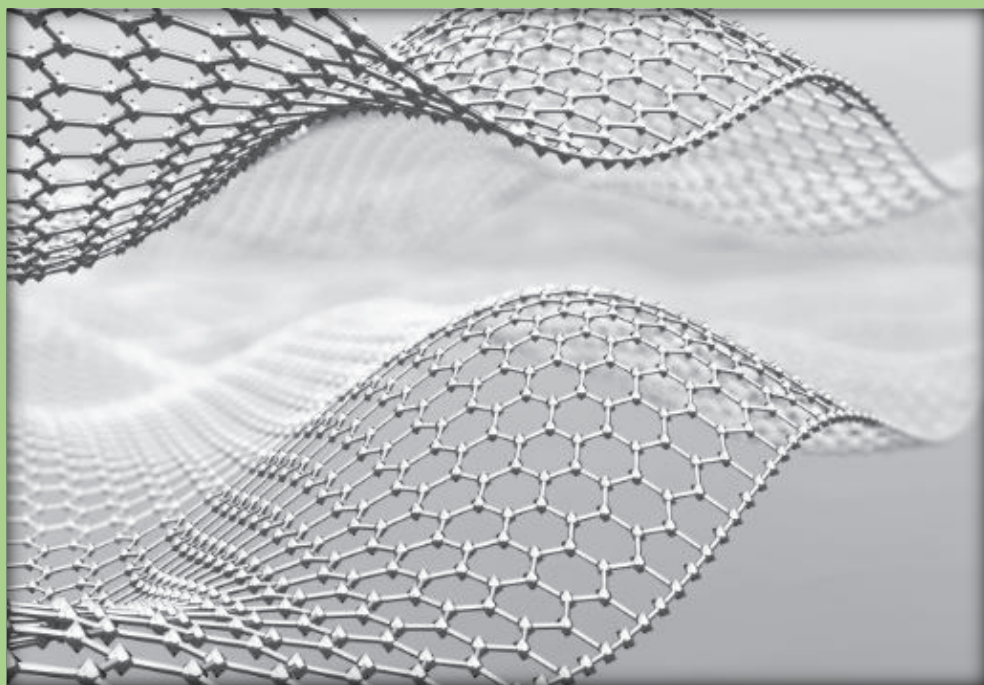


Nanocomposites: modeling and optimization



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Nanocomposites: modeling and optimization



BULGARIAN ACADEMY OF SCIENCES
INSTITUTE OF CHEMICAL
ENGINEERING

Nanocomposites: modeling and optimization

Edited by
Wilfried Becker and Tatyana Petrova

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Prof. Marin Drinov Publishing House
of Bulgarian Academy of Sciences

This book presents the results obtained under the project "Optimal safe loading and geometry for layered nanocomposites under thermo-mechanical loading". It consists of 6 chapters, divided into two parts - Modeling of nanocomposites (4 chapters) and Optimization of nanocomposites (2 chapters). The first two chapters are devoted to analytical modeling methods and ways for identifying the key factors affecting delamination in nanocomposite structures under mechanical loading and temperature differences. The third and fourth chapters discuss methods for numerical modeling of structures with nano-heterogeneities such as inclusions, pores or cracks under dynamic loading; the factors affecting their dynamic behavior are also determined. The final two chapters provide a review and analysis of the methods for optimizing nanocomposite structures, as well as the results for the optimal safe values of the geometry and loads of nanocomposite structures through multi-parameter optimization.

Acknowledgements

The authors express their gratitude to the National Science Foundation of the Republic of Bulgaria for financial support under contract No. КП-06-H57/3/15.11.2021, for the publication of this book.

This book is dedicated to the light memory of our colleague Assoc. prof. PhD Boyan Christov Boyadjiev.

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INTRODUCTION

With the emergence of graphene and other 2D nanomaterials, research interest in nanocomposites has increased sharply due to their numerous applications, including aviation engineering, electronics, automotive industries, nanoconcretes, adhesives, bio-nanocomposites, and more. Given the wide range of external conditions and impacts that nanocomposites are exposed to in industrial applications—such as mechanical loading (tension, compression, bending) and environmental factors (temperature, humidity, etc.)—it is crucial to understand how these materials respond to various stresses. Most importantly, it is essential to determine the optimal “architecture” of a nanocomposite and the technological load limits within which it remains functional and effective while preserving its structural integrity.

This book aims to provide a comprehensive overview of modeling and optimization methods for studying the behavior of nanocomposite structures under various loads. The theoretical methods are extensively illustrated with examples from both the literature and the results obtained during the implementation of the project "Optimal Safe Loading and Geometry for Layered Nanocomposites under Thermo-Mechanical Loading", under contract No. KII-06-H57/3/15.11.2021 with the Bulgarian National Science Fund. The fundamental research on theoretical prediction and the determination of the factors influencing nanocomposite behavior under static and dynamic loading, as well as the results presented here, will complement and assist other researchers in the field who are involved in the design, modeling, and optimization of new and existing nanocomposite structures.

The book contains six chapters, grouped into two parts: Modeling of Nanocomposites (four chapters) and Optimization of Nanocomposites (two chapters). Each of the six chapters includes results obtained from the aforementioned project.

Chapter I. Analytical modeling of nanocomposites behaviour

This chapter aims to analyse and summarize the achievements to date, in the field of analytical modeling of stresses and strains in nanocomposite structures (1-D and 2-D analytical models), in the elastic and plastic zones. It

is organized as follows: Review on papers for analytical modeling of nanocomposites, Examples of analytical solutions applications to the nanocomposites, and 2D analytical solutions for nanocomposites, including some authors' results from 2-D stress –function variational model and their validation by experimental/model data from the literature.

Chapter 2. Theoretical analysis of factors, influencing delamination and failure in nanocomposites

Here, the methods and findings about determination of the essential factors affecting delamination in the nanocomposite structures under static mechanical loading and temperature differences, are presented and discussed. First, a review on the available data in the current literature for the interface/interphase properties and their thickness/width in distinct nanocomposites is raked up. Then, the literature results obtained by parametric/sensitivity analysis for the main factors, affecting interface shear stress and generally influence on the mechanical characteristics of nanocomposites, are summarized. Finally, the authors' results from the performed parametrical analyses for distinct nanocomposite structures have been described, based on the 2-D model solutions from Chapter 1 for interface shear stress.

Chapter 3. Numerical modelling of functionally graded piezoelectric cracked nanocomposites subjected to dynamic loads by boundary element method

This chapter deals with modelling of time-harmonic shear wave (SH) scattering in infinite, semi-infinite and finite functionally graded cracked piezoelectric nanocomposite 2D solids. The computational tool is a non-hypersingular traction boundary integral equation method (TBIEM) based on an analytically derived fundamental solution or half-plane Green's function for functional graded piezoelectric material (PEM) combined with the boundary conditions derived in surface elasticity theory. The proposed numerical schemes are verified in respect to their accuracy and convergence. The simulation results illustrate the sensitivity of the fracture state of the cracked nanocomposites to the type and properties of the material gradient, to the surface elasticity properties, to the nanocracks existence and their

dynamic interaction, to the coupled properties of the PEM and to the type of the dynamic load.

Chapter 4. Numerical modelling of elastic nanocomposites with nanoholes and nanoinclusions subjected to dynamic loads by boundary element method

This chapter presents a systematic boundary element method (BEM) study on the dynamic response of infinite, semi-infinite, and finite isotropic/anisotropic nanocomposite solids with nanocavities, nanoinclusions, or nanorelief under time-harmonic or rapidly applied transient stress pulses along the existing boundaries. The mechanical models developed here are based on the classical elastodynamic theory for the elastic isotropic/anisotropic bulk solid and the non-classical boundary conditions along its boundary derived in surface elasticity theory by Gurtin and Murdoch (1975). The computational tool is an efficient direct displacement BEM based on the frequency-dependent elastodynamic fundamental solution for elastic isotropic or generally anisotropic material. The numerical scheme verification is discussed. The performed parametric analyses illustrate the dependence of the wave field in nanocomposites on the material anisotropy, on the surface elasticity properties, on the nanorelief peculiarities, on the nanocavities/nanoinclusions existence and their dynamic interaction, and on the type of the dynamic load.

Chapter 5. Methods for optimization of nanocomposites

This chapter explores, summarizes, and analysing various optimization methods used to enhance the design, properties, and manufacturing processes of nanocomposite structures (NCs). It examines different types of nanocomposites and the key factors subject to optimization, including NC geometry, loading conditions, environmental influences, and manufacturing techniques. A detailed discussion is provided on the numerical techniques and optimization methods, along with examples of their application to NCs. These methods include the response surface method, decision tree method, machine learning algorithms, artificial neural networks, differential evolution algorithms, the finite element analysis, genetic and evolutionary algorithms, topological optimization, adaptive optimization, and more. Additionally, the

chapter presents the authors' contributions to the performed optimization approaches for nanocomposites.

Chapter 6. Optimal safety intervals for geometry and loads in polymer nanocomposites by multi-parameter optimization

Here, the authors' results for defining and solving the optimization problem for obtaining the optimal design (geometrical dimensions) and the optimal loading (mechanical and/or thermo-mechanical) for layered nanocomposite structures without delamination in them, are presented. The implementation of multi-parametric optimization problem (MOP) is done by authors' developed programs, using metaheuristic Genetic Algorithm in Mathcad and in some cases, by alternative deterministic algorithm in Mathematica. The developed MOPs are applied successfully on 5 distinct nanocomposites structures, and the optimal values (or intervals of values) for the parameters are obtained for all considered case studies. It is checked that at these optimal values, the model interfacial shear stress (ISS) maximal value does not exceed the ultimate shear stress (USS) in the interfacial layer. Where it is possible, the results are compared with the available literature data.

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Prof. Wilfried Becker

Prof. Tatyana Petrova

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As editors of this book, we would like to express our sincere gratitude to the authors of the individual chapters for their hard work and dedication in contributing to this book, namely:

Chapter 1. Analytical modeling of nanocomposites behaviour

Prof. Tatyana Petrova, Assoc. prof. Elisaveta Kirilova, Asst. Apostol Apostolov, Assoc. prof. Rayka Vladova, Prof. Wilfried Becker

Chapter 2. Theoretical analysis of factors, influencing delamination and failure in nanocomposites

Asst. Apostol Apostolov, Prof. Tatyana Petrova, Assoc. prof. Elisaveta Kirilova, Assoc. prof. Rayka Vladova, Prof. Wilfried Becker

Chapter 3. Numerical modelling of functionally graded piezoelectric cracked nanocomposites subjected to dynamic loads by boundary element method

Prof. Tsviatko Rangelov, Prof. Petia Dineva

Chapter 4. Numerical modelling of elastic nanocomposites with nanoholes and nanoinclusions subjected to dynamic loads by boundary element method

Assoc. prof. Sonia Parvanova, Prof. Petia Dineva

Chapter 5. Methods for optimization of nanocomposites

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Chapter 6. Optimal safety intervals for geometry and loads in polymer nanocomposites by multi-parameter optimization

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PART I. MODELING OF NANOCOMPOSITES

Chapter 1. Analytical modeling of nanocomposites behaviour

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Annotation

This chapter aims to analyze and summarize the achievements to date, including some authors' results, in the field of analytical modeling of stresses and strains in nanocomposite structures, as well as the conditions under which delamination is observed in such structures. It is organized as follows: Section 1: Brief review on papers for analytical modeling of nanocomposites, Section 2: Examples of analytical solutions applications to nanocomposites, Section 3: 2D analytical solutions for nanocomposites, and Conclusions.

Keywords: nanocomposites, modeling, analytical solution, stress, strain, delamination

1. Brief review on papers about analytical modeling of nanocomposites

During the last two decades a boom in publications - 1,006,958 publications selected from Scopus, dedicated to the keyword “nanocomposites” (Scopus search 1, 2024) (Fig. 1 (a)) has been seen. It can easily be verified that the largest share is occupied by the works that are mainly experimental and investigate the methods of synthesis of new, mainly polymer nanocomposites. A significant part is devoted to the study of their properties and characteristics (mechanical, optical, electrical and thermal conductivity, etc.). Another reference shows that only 62,722 out of 160,223 articles include modeling in addition to the experiment (Scopus search 2, 2024). Given the increasingly wide application of nanocomposites in various industrial areas, the number of publications concerning modeling of the

behavior of nanocomposites is also increasing - 45,777 according to Scopus, 8,414 of which are review articles (Scopus search 3, 2024). In most cases, commercial software products such as ANSYS, Abaqus, COSMOS, etc., are used in the modeling of nanocomposites, as complex geometries can be simulated under different types of loads on the nanocomposite; the disadvantages of this type of modeling are the time for mesh preparation and execution, sometimes the convergence of the chosen numerical method in the software; modeling a so-called "jump" in any of the sought-after quantities in a given cell/s of the mesh also creates a problem. From a total of 5,859 published articles matching the keywords "nanocomposites" and "finite element modeling" (Scopus search 4, 2024), 797 are review articles.

In contrast to numerical methods, analytical methods for obtaining solutions for stresses, strains and other characteristics in nanocomposites are much faster, easier and convenient to use. Their disadvantages are usually the low dimensionality of the solutions, as well as the simplification of the geometry of the considered nanocomposite and the types of loads.

As far as the authors of the present work know, there is no published survey specifically dedicated to analytical methods for stress/strain modeling in nanocomposite structures, especially those in which the nanomaterial is considered as a separate layer. Given the rapid pace of research in the field and the ever-widening application of nanocomposites in industry, such a summary, accompanied by relevant analysis, would be helpful in future applications of layered nanocomposite structures, especially under specific loads.

A search was made in the available literature sources on the internet with the keywords "analytical solution+nanocomposite" and "shear-lag+nanocomposites". The result after 2004 to the present (by year) is graphically displayed in Fig. 1 (b) – totally 79 results found.

In Fig. 1 (b) the articles with results of the author of the present work (co-authored with colleagues) during the considered period are also included. From the figure it can be seen that the interest in this type of modeling systematically increased from the discovery of graphene until 2016, followed by a slight decline and the interest resumed again in the last 4-5 years. Along with graphene and the created nanocomposite structures based on graphene, whose applications are numerous and in various fields such as electronics, medicine, automotive, construction, energy, optics, etc., new 2D nanomaterials are also entering the scene - such as MXene ($\text{Ti}_3\text{C}_2\text{T}_x$) (2011), black phosphorus (2014), hBN (2014), borophene (2015), MoS_2 , WS_2 , as well

as hybrid combinations thereof like graphene/MoS₂ (Du *et al.* 2022), which have yet to be extensively studied and modeled.

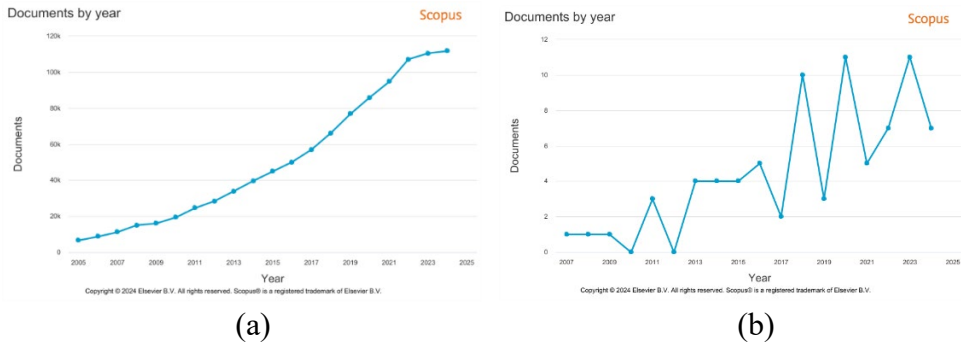


Figure 1: Number of articles during 2005-2024 found by keywords: (a) “nanocomposites”, (b) “analytical solution+nanocomposites+shear-lag”.

The classification of the types of analytical models covered in the reference can be done in several ways. If they are grouped by the dimensionality of the model, one-dimensional, two-dimensional and three-dimensional models can be distinguished. If they are grouped according to the applicability in different zones –elastic and plastic for changes in stresses and deformations - the models can be divided into linear-elastic and cohesive (plastic).

According to the dimensionality classification of the models covered in the reference, one-dimensional analytical models occupy a major share, and they are also those that refer to modelling primarily in the field of elasticity. A previous publication asset with the participation of the authors of the present work contributes to this by using analytical one-dimensional model solutions to describe the behavior of two-layer composites subjected to static/dynamic loads under conditions of varying temperature, humidity and electric field (Valeva *et al.* 2012; Ivanova *et al.* 2013, 2015, 2016, 2017; Becker *et al.* 2014; Kirilova *et al.* 2017, 2018; Petrova *et al.* 2015, 2016, 2017, 2018). Especially for nanocomposites, the developments with the authors’ participation cover one-dimensional solutions of a cohesion model for statically loaded graphene nanocomposites (Kirilova *et al.*, 2018; Petrova *et al.*, 2018), as well as two-dimensional solutions obtained by the 2D stress-function variational method as it seen from (Kirilova *et al.*, 2019, 2023; Petrova *et al.* 2022a, 2022b, 2023; Petrova, 2023; Apostolov *et al.* 2022, 2024; Vladova *et al.*, 2022, 2024) for statically loaded nanocomposites incorporating graphene, WS₂, MoS₂ to

different polymer matrices. The obtained solutions were studied by parametric analysis regarding the influence of different factors on delamination in the different types of composites and nanocomposites. Recently, except our proposed model, the new 2D shear-lag model, combined with bilinear cohesive zone model are presented by (Bai and Guo, 2020), for description of bidirectional interfacial shear stress transfer problems in graphene/flexible substrate structures subjected to uniaxial tension. The 2D shear-lag model is constructed soon by (Guo and Hu, 2024) for patch-layer reinforced composites

The models that give an analytical solution for higher dimensionality and/or outside the elastic region are very few, which is explainable due to the complexity in the formulation of the boundary value problems and in the computations in deriving the solutions, for example from (Zhang *et al.*, 2013; Amirpour *et al.* 2016; Askari and Ghasemi-Nejhad, 2020; Tapia *et al.* 2021). Except the Banarouei (2021) and Yang *et al.* (2024), no other publications were found offering analytical solutions for the stresses/strains in nanocomposites under combined (mechanical and temperature) loading. Examples of the joint use of analytical and/or numerical solutions for more than 1D in elastodynamics can be seen in (Rangelov *et al.* 2022 ; Rangelov and Dineva, 2023; Parvanova and Dineva, 2023; Manolis *et al.*, 2023).

In the present review, the emphasis is placed on the one- and two-dimensional analytical solutions derived for the stresses and strains in statically loaded nanocomposites. In the following sections, various examples of the available analytical models – 1D and 2D, in both the elastic and cohesive domains – will be reviewed and discussed.

2. Examples of analytical solutions applied to nanocomposites

The most commonly used one-dimensional and linear elastic model for both composite and nanocomposite structures is the so-called shear-lag model or method. Its first appearance in the literature was the work of Volkersen (1938), who gave an analytical description of the stress transfer σ in a joint-type structure (single-lap joint) loaded on both sides as follows (Fig. 2a).

Here, the main idea is that the connecting adhesion layer serves to transfer the load between the individual parts (adherents) of the structure, and this happens at the expense of the shear stresses τ , which distribute the load along the overlap length of the adherent connecting part l (Fig. 2a).

In the scheme of Fig. 2a, (a) and (b), it is graphically shown how the predictions of this model look analytically for the stress σ in the two arms of

the structure, as well as the interfacial shear stress τ in the cases of materials with different elastic stiffness. Volkersen offers the following analytical solution for the interphase shear stress τ for the joint structure (Fig. 2a):

$$\tau(x) = \frac{P\omega}{2 \sinh(\omega l/2)} \cosh \omega l + \frac{P\omega}{2 \cosh(\omega l/2)} \left(\frac{E_2 t_2 - E_1 t_1}{E_1 t_1 + E_2 t_2} \right) \sinh \omega l \quad (1)$$

where $\omega = \sqrt{\frac{G}{h} \left(\frac{E_2 t_2 - E_1 t_1}{E_1 t_1 + E_2 t_2} \right)}$

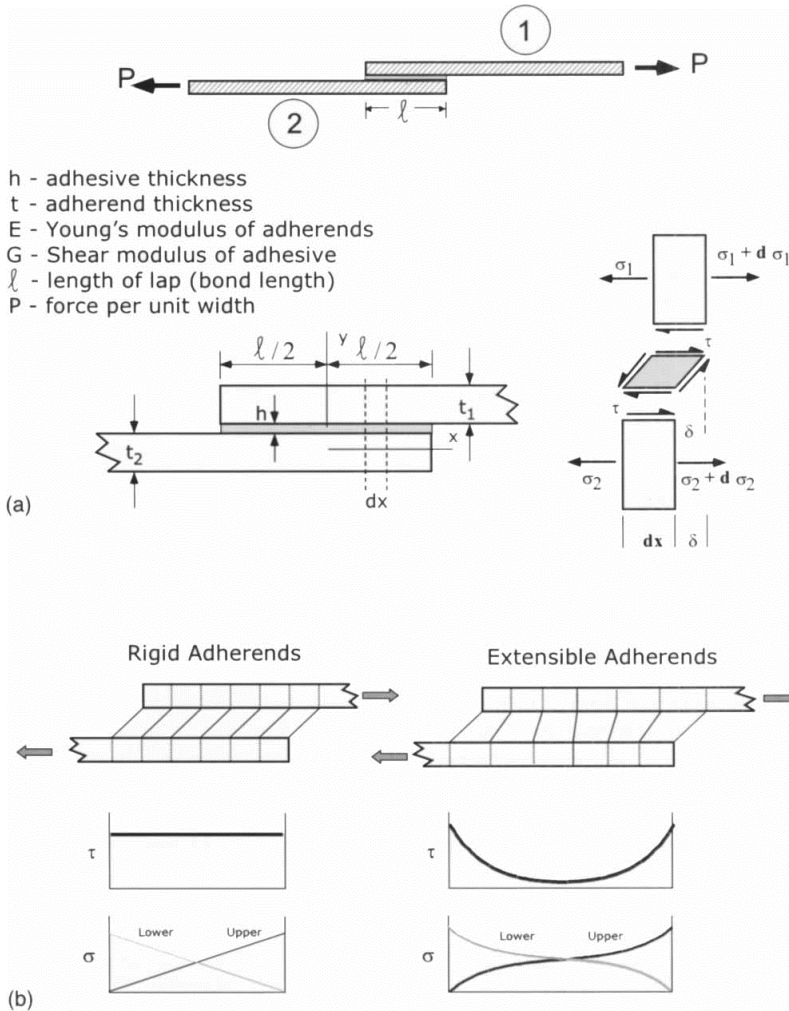


Figure 2a: Illustrative scheme of (a, b) Volkersen's shear-lag model (Dillard, 2002).

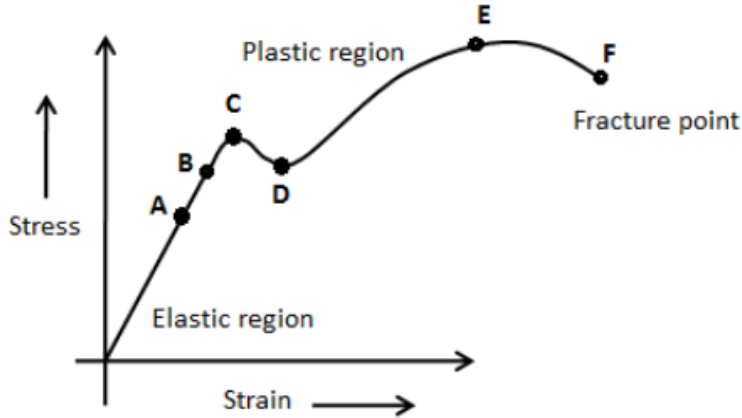


Figure 2b: Illustrative scheme the stress-strain diagram (Dillard, 2002).

As can be seen, the one-dimensional analytical solution (1) depends only on x , but it also depends nonlinearly on the material characteristics of the structure - Young's modulus E , the shear modulus G , and also on the geometry of the structure - the thicknesses of the two adherents t_1 , t_2 and the connecting part h , the length of the connecting (total) part l , as well as on the magnitude of the applied force P . *This solution is derived under specific assumptions – neglecting torsion and bending, as well as normal stresses in the structure, also the effects of shrinkage due to different values of Poisson's number, as well as assuming perfect fit in l and linear-elastic properties for the materials in the structure.* Despite the idealized formulation, this solution has its place in hundreds of publications and has been successfully validated with other models and, most notably, with experimental data in the elastic domain of applied loads (Dillard, 2002). The separate stages of the real behaviour of solids when an external strain is applied, are shown in Fig.2b.

Later, Cox, based on Volkersen's solution, revised and derived the shear-lag model and, accordingly, an analytical solution for σ and τ for fiber-matrix composite structures (composite materials containing threads or fibers, to increase their resistance and strength) (Teklal *et al.* 2018). From Fig. 3 it can be seen that the solutions for σ and τ again depend on the applied external deformation ε_1 , on the material properties of the thread and the matrix (substrate) E_f , G_m , as well as on the geometry of the object – length L , radius of the thread a and the substrate R (a cylindrical representative volume of the composite was considered), the thread size ratio $s=L/a$. This model obeys the

same assumptions as the previous one and has been used just as widely, especially in composite structures (Dillard, 2002).

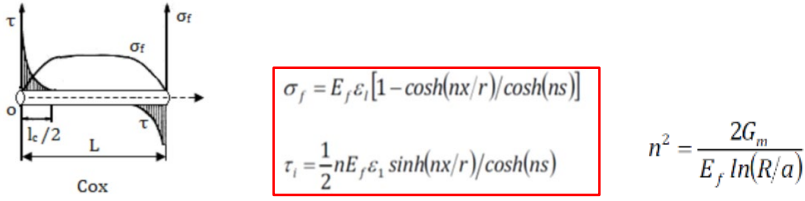


Figure 3: Cox model and solution for fiber/filament-incorporated composites (Teklal *et al.* 2018).

After the emergence of nanocomposites with embedded nano-threads/fibers, especially the embedding of carbon nano-tubes in various matrices, we can trace the use of the Cox model in the following several works from (Gao and Li, 2005; Ang and Ahmed, 2013; Kundalwal *et al.* 2014; Hu *et al.* 2019). In (Gao and Li, 2005), Fig. 4, left, the solutions for the stresses σ and τ are in cylindrical coordinates and in exponents, regarding the carbon nanotube length (along the z -axis), which is mathematically similar to Cox (Fig. 3), since hyperbolic sines and cosines are expressed with exponents, which is also confirmed by the graphical representation of σ and τ in both figures. In the work (Ang and Ahmed, 2013), to the analytical solution for the interfacial shear stress $\tau = \mu(q_0 - q_1 + q_2)$ the effects of additional residual stresses q_0 , q_1 and q_2 , arising respectively due to the different coefficients of thermal expansion of the two materials, are added, from the difference in Poisson numbers, and from the action of cohesive Van der Waals (vdW) forces (Fig. 4, right). In both examples, the solutions contain the geometric and material characteristics of the materials making up the nanocomposites, as well as the external load, and in (Ang and Ahmed, 2013) other characteristics such as thermal expansion coefficients, Poisson's ratios and cohesive forces are also considered. It is worth to note, that in (Ang and Ahmed, 2013) an external influence other than mechanical is considered and accounted for in the model solution. The use of a simpler basic model to which analytical solutions can be added/quantifying additional effects is a well-known mathematical approach that gives great results, but is unfortunately too rarely used, mostly due to difficulties in finding data on additional effects and quantifying them. Kundalwal *et al.* (2014) presented a three-phase (three types of materials) shear-lag model for a polyamide nanocomposite containing a carbon filament to which carbon nanotubes were

attached in a brush-like manner; the nanocomposite is subjected to a three-dimensional static load (Fig. 5, left).

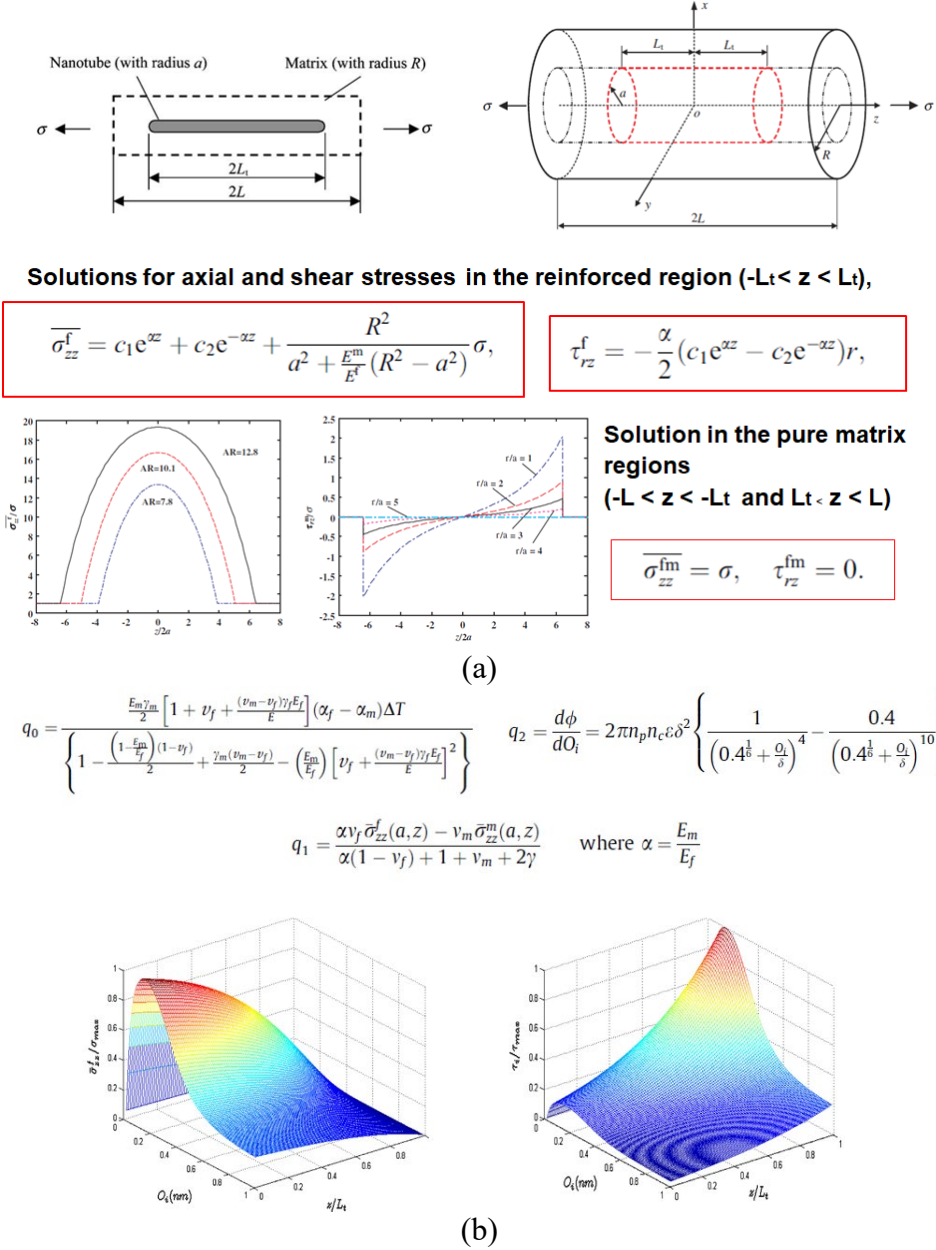


Figure 4: Application of the Cox model to fiber nanocomposites: (a)-(Gao and Li, 2005), (b) -(Ang and Ahmed, 2013).

Here the solutions for the stresses σ and τ are again expressed as a combination of hyperbolic sines and cosines and integration constants. In the same work, a comparison of the results obtained by the authors with results of the finite element method (FEM) is made; the agreement is more than good, confirming the use of analytical solutions in modeling even for three-phase nanotube/matrix nanocomposites.

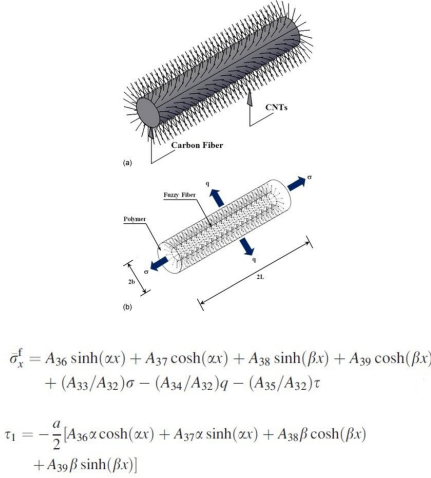


Figure 5: Application of the Cox model to fiber nanocomposites: left (Kundalwal *et al.* 2014), right (Hu *et al.* 2019).

In the publication of Hu *et al.* (2019), one can again observe the benefit of additional modeling of the interfacial shear stress τ to the basic shear-lag solutions. In particular, the interphase boundary is modeled by a spring layer model with its own stiffness coefficient K , which is reflected in the coefficient α of the exponents in the solutions (Fig. 5, right). In practice, this means that the interphase shear stress does not transmit the applied external stress directly and proportionally, but is limited by the value of the coefficient K .

After the discovery of the stable two-dimensional form of graphene (2004, although its existence is known since 1930), attempts were made to model the behavior of graphene nanocomposites, where the nanomaterial is a two-dimensional (2D) lattice/flake with an atomic thickness of 0.35 nm, incorporated or deposited in/on other material/s. The beginning of the modeling of graphene and other nanocomposites by the application of the shear-lag model to analytically describe the behavior of σ and τ was laid with the pioneering works of the Nobel Prize winners Novoselov and Geim. In their works (Gong *et al.* 2010; Gong, 2012), shear-lag modeling was applied

$$(w_i^m - w_i^f) K = \tau_i^f,$$

$$\overline{\sigma_{zz}^f} = c_1 e^{\alpha z} + c_2 e^{-\alpha z} + \frac{R^2}{a^2 + (R^2 - a^2) \frac{E^m}{E^f}} \sigma,$$

$$\sigma_{zz}^m = \frac{R^2}{R^2 + a^2 \left(\frac{E^f}{E^m} - 1 \right)} \sigma + (c_1 e^{\alpha z} + c_2 e^{-\alpha z}) \times \left\{ [1 - \beta (R^2 - a^2)] \left(\frac{E^m}{E^f} - \frac{a E^m}{2K} \alpha^2 \right) - \beta a^2 \right\}$$

$$\tau_{rz}^m = -\frac{a^2 \alpha}{2 (R^2 - a^2)} \left(\frac{R^2}{r} - r \right) (c_1 e^{\alpha z} - c_2 e^{-\alpha z})$$

$$\tau_{rz}^f = -\frac{\alpha}{2} r (c_1 e^{\alpha z} - c_2 e^{-\alpha z}),$$

for the first time to a Graphene/SU-8/PMMA nanocomposite subjected to static axial external deformation (Fig. 6).

The solutions for the interfacial tension τ and for the strain in the graphene layer e_f are again described by hyperbolic sines and cosines for external loading up to 0.4% successfully with the shear-lag model. At an external strain of 0.6%, however, the graphene begins to wrinkle, that is, the behavior becomes non-linear and the model cannot correctly describe the experimental data.

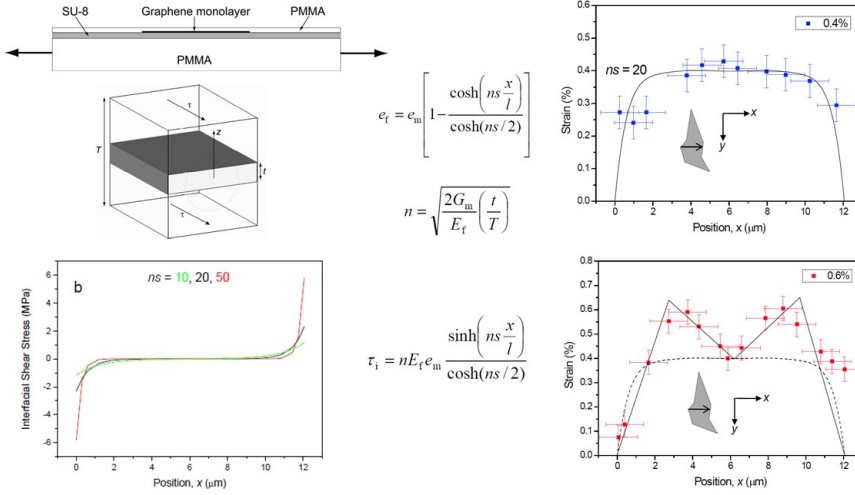


Figure 6: Illustrative scheme of σ and τ solutions and nanocomposite–shear-lag (Gong *et al.* 2010; Gong, 2012).

Shortly thereafter, Xu *et al.* (2016) investigated the influence of the length of the graphene flake/layer on the value of the interfacial shear stress and on the strain in the layer, again with shear-lag (Fig. 7). With parametric analysis they found that the length of the graphene layer significantly affects the stress transfer between the layers of the nanocomposite and specifically, τ and the strain in graphene ε . As the loading in the PET substrate increases, the strain ε in the graphene linearly increases until reaching a sliding mode and a retention plateau, after which exfoliation of the graphene flake/layer follows. As the length of the graphene flake/layer increases from 20 to 10000 μm , the interfacial tension τ decreases until complete exfoliation occurs. The interfacial mechanical properties of graphene less than 20 μm long are extremely sensitive to its length, while for graphene longer than 1000 μm they are no longer size dependent.

As can be seen from the figures, the solutions of the shear-lag model for the deformations in the nanomaterial layer successfully describe the experimentally measured data in the elastic region of the externally applied mechanical loads. Given the different mechanical properties of the investigated nanocomposites, and in particular, the choice of materials in the nanocomposite, the applicability limits of the model will also depend on this. It also turns out that the thickness of the nanomaterial layer is significant – for example, in (Wang, 2017) for the same applied external strain of 0.55%, the model solution for the strain in the WS_2 monolayer well describes the experimental data, but with several WS_2 layers this is no longer so, as a tendency to form wrinkles in the middle of the layer appears (Fig. 8, right, (d)), because of the interactions between the nanomaterial layers.

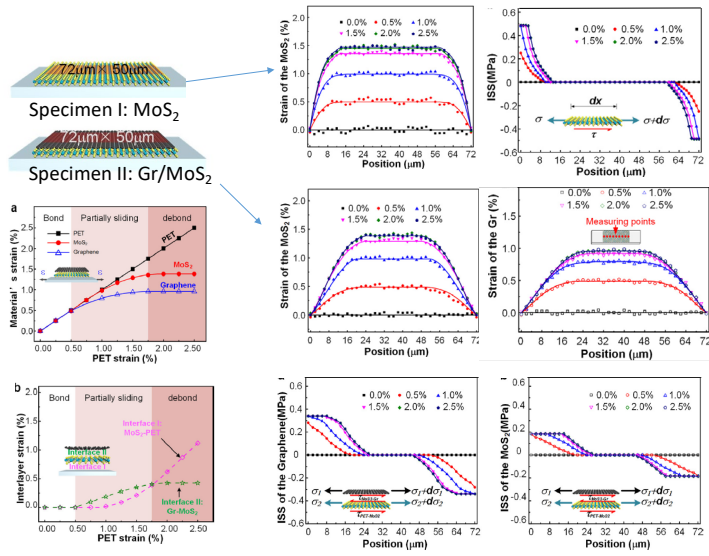


Figure 9: Illustrative scheme of ε and τ solutions and graphics - shear-lag (Du *et al.* 2022).

In Fig. 9 the effect of the interaction of two different nanomaterials (graphene and molybdenum disulfide) on the transfer of stress from the PET polymer layer to the upper two layers, is observed. It can be seen that in sample I of Fig. 9 the transfer is 100% from polymer to MoS_2 for loadings up to 1.2%, while in sample II with two nanolayers, the transfer drops to 75% from MoS_2 to graphene even at 1% external loading; as the external load increases, the stress transfer between the layers continues to decrease. This

effect, found experimentally, is due to the presence of a second interphase layer in sample II (Du *et al.* 2022). The conformation came from Du *et al.* 2022 and their experimental observations with a simple model, based on the force balance equations and superposition of solutions.

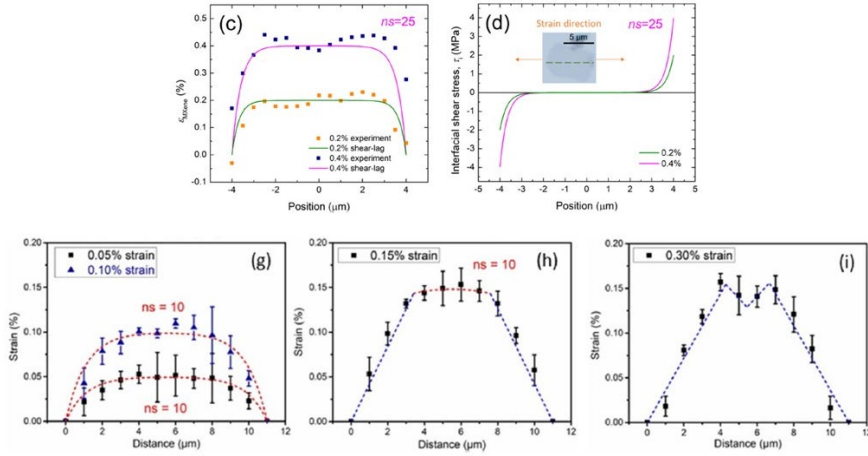


Figure 10: Illustrative scheme of ε and τ solutions and graphics - shear-lag, (top - (c) and (d) from (Liu *et al.* 2022), bottom, (g)÷(h) from (Wang *et al.* 2021a).

In Fig. 10, top, it can be seen for the $\text{Ti}_3\text{C}_2\text{Mxene/PMMA}$ nanocomposite that the model deformation in the Ti_3C_2 layer matches well with the experimental data for 0.2% external loading; at 0.4%, however, more substantial differences begin to appear in the plateau region for ε (Liu *et al.* 2022). When modeling the deformation in a 50-layer (17 nm) boron nitride nanocomposite hBN/PMMA (Fig. 10, bottom), the limits of the external load, up to which the model well describes the experiment, are even lower - up to 0.15% external load (Wang *et al.* 2021a).

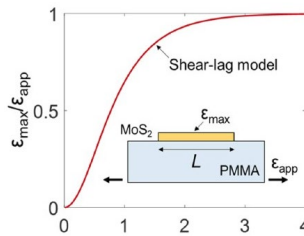


Figure 11: Illustrative scheme of ε solution, shear-lag (Chae *et al.* 2022).

As mentioned, the shear-lag model and its variations considered so far give solutions valid in the elastic region of external loads. When loading above this zone (up to $0.2 \div 0.4\%$, depending on the material) a different behavior is observed - the materials begin to slip and slide and the relationship between stresses and deformations is no longer linear (Fig. 2 (c), stress-strain diagram (Milkov, 2008). After this yield point, the stresses again non-linearly increase until the so-called fracture mode of the respective material/structure is reached. In order to analytically describe the stresses and strains outside the elastic zone, one-dimensional models operating in the yield zone were created. These are the so-called *partial debonding model* and *total debonding model* (Lacroix *et al.* 1992). These models were developed to describe the stresses in fiber/matrix reinforced composites and were later used for MoS₂ nanocomposites (Dong *et al.* 2023). In the *partial debonding model*, debonding is assumed to start at a distance $m.l/2$ from the matrix ends, where m is a number between 0 and 1, and represents the dimensionless length of the debonded portion. Perfect adhesion is assumed in the central part of the thread. The stresses - axial σ_f and shear τ , are determined by equations (2), and are graphically presented in Fig. 12.

$$\sigma_f = 4\tau_i \left(\frac{l}{2} - x \right) / d, \quad \tau = \tau_i \quad m = \frac{E_f \varepsilon - 2 \frac{\tau_{deb}}{n} \coth(ns(1-m))}{2\tau_i s} \quad (2)$$

In the *total debonding model*, when the fiber is detached from the supporting matrix along its entire length, i.e., $m=1$, and if s is the quotient of the length and diameter of the fiber, we will have the following expressions for σ and τ , and respectively the graphs (Fig. 12):

$$\sigma_{f,max} = 2\tau_i s \quad (3)$$

In cases where we are between the yield and failure limits, other models are applied to predict the stresses and strains in nanocomposites - the so-called *cohesive* or plastic models, also *nonlinear shear lag* type models, which also provide analytical solutions in these areas as it seen from (Jiang *et al.* 2014; Bronsgeest *et al.* 2015; Guo *et al.* 2015; Wang *et al.* 2016; Shao *et al.* 2023; Ciu *et al.* 2022; Ren *et al.* 2023; Liu *et al.* 2022a). The next few figures illustrate the results obtained by the aforementioned researchers. Given the rather voluminous output of solutions for these models, they are presented only schematically here.

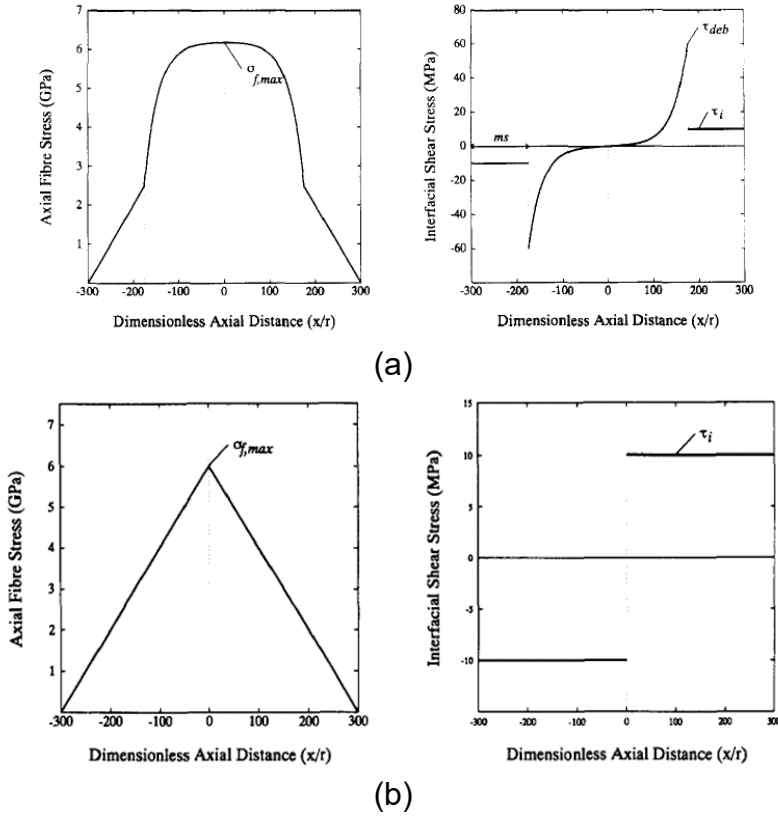


Figure 12: Illustrative scheme of σ and τ solutions for: (a) the partial debonding and (b) total debonding models (Lacroix *et al.* 1992).

As can be seen from Fig. 13, the solutions for ε and τ closely resemble those of ordinary shear-lag as combinations of hyperbolic sines and cosines. The difference is in the value of the β parameter in the x argument. Here, an additional constant k_m is also included in the parameter, which represents the effective stiffness of the polymer surface. The analogous parameter ns in shear-lag (see Fig. 6) does not take into account this effect, and here the sliding of the interfacial boundary is also taken into account when the interfacial tension exceeds a certain critical value (for the considered nanocomposite it is at 1.2% external load). The graphs for the deformations in the graphene layer above the elastic zone are described very well by the nonlinear shear-lag model at values of the external strain up to 3%.

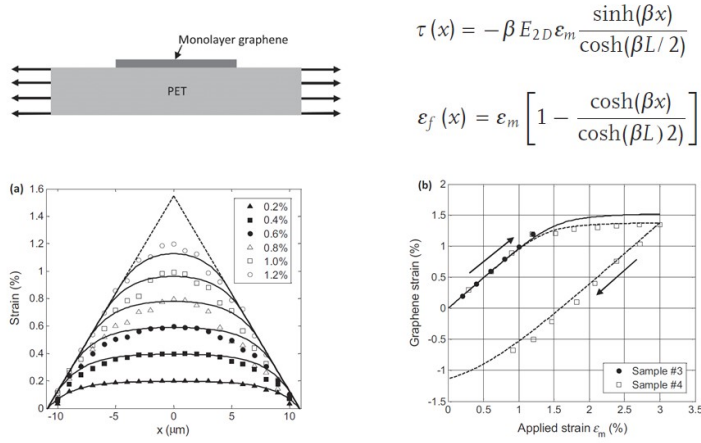


Figure 13: Illustrative scheme of ϵ and τ solutions and graphics – non-linear shear-lag analysis for graphene/PET (Jiang *et al.* 2014).

A similar result was achieved with the same nonlinear model in (Bronsgeest *et al.* 2015) for a graphene/cobalt nanocomposite (Fig. 14). In this work, the parameter β is again used, but in it, in addition to the k_m -like constant C , the material characteristics of the substrate (cobalt) are also included. This model accounts for the onset of sliding and, accordingly, the formation of wrinkles in graphene after a rather low level of external loading of 0.2%, due to the poor adhesion between graphene and cobalt.

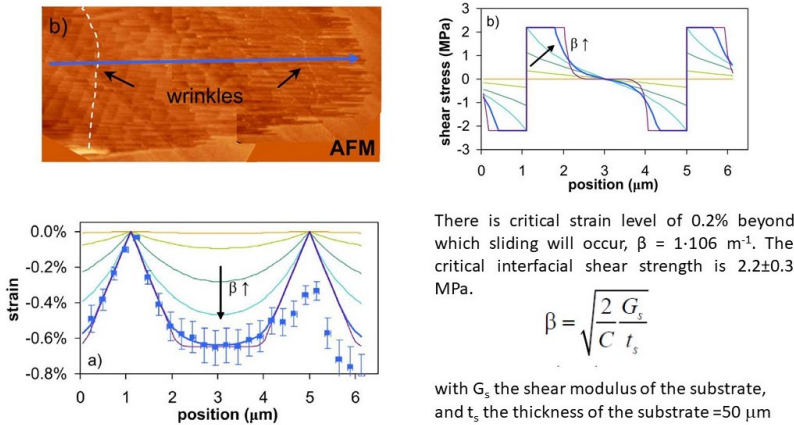


Figure 14: Illustrative scheme of ϵ and τ solutions and graphics: non-linear shear-lag analysis for graphene/cobalt (Bronsgeest *et al.* 2015).

An application of two nonlinear models, as well as the finite element method to describe the deformations in graphene above the yield zone can be seen in the work (Guo and Zhu, 2015) (Fig. 15). A cohesive model with shear-lag analysis was combined, and five behavior modes were established for the strain distribution for an external load of up to 3.3%. Applying this modeling approach allows determining important characteristics for the nanocomposite above the elastic limit such as interface stiffness, shear strength, and fracture toughness. A parametric analysis was also performed, which showed that higher interface stiffness and/or shear strength lead to higher stress transfer efficiency, while higher fracture toughness can delay debonding (delamination).

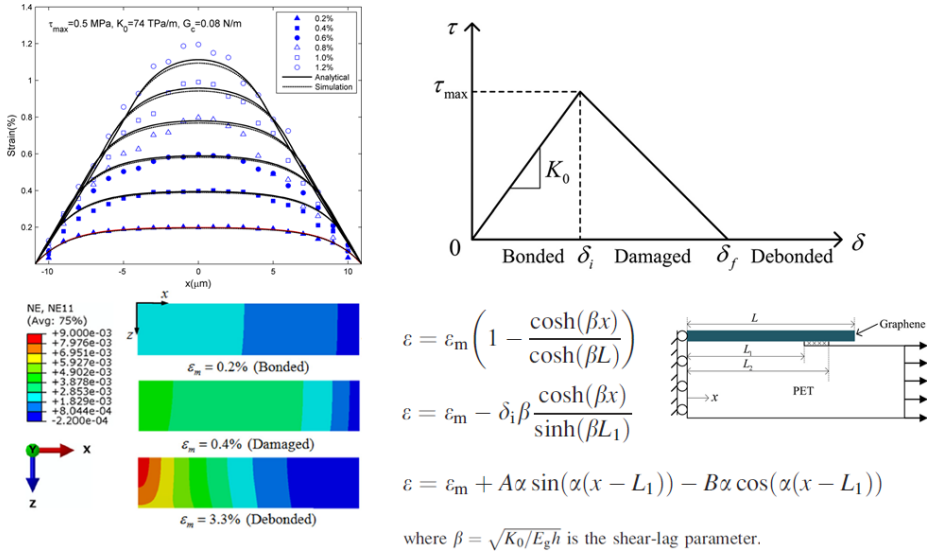


Figure 15: Illustrative scheme of ϵ solutions and graphics – cohesive model, shear-lag analysis and FE analysis for graphene/PET (Guo and Zhu, 2015).

As can be seen from the graphical comparison of the solutions in Figs. 16 and 17 with the experimental data or with the FEM, the non-linear shear-lag analytical solutions created to model the deformations and interfacial stresses in different types of nanocomposites outside the elastic zone do very well. In the available literature sources from (Cui *et al.* 2022; Ren *et al.* 2023; Liu *et al.* 2022a; Peng *et al.* 2024; Yang *et al.* 2024) the modeled nanocomposites are graphene-polymer combinations, with and without adhesive between two

materials; mostly non-linear shear-lag models are applied with simultaneously performed FE analysis or molecular modelling/dynamics approaches (Ren *et al.* 2023; Yang *et al.* 2024). In the work of Ren *et al.* (2023) a new *re-adhesive shear-lag model* is proposed (Fig. 18) to describe the interface damage of bi-layer graphene (BLG) by using the cohesive zone theory.

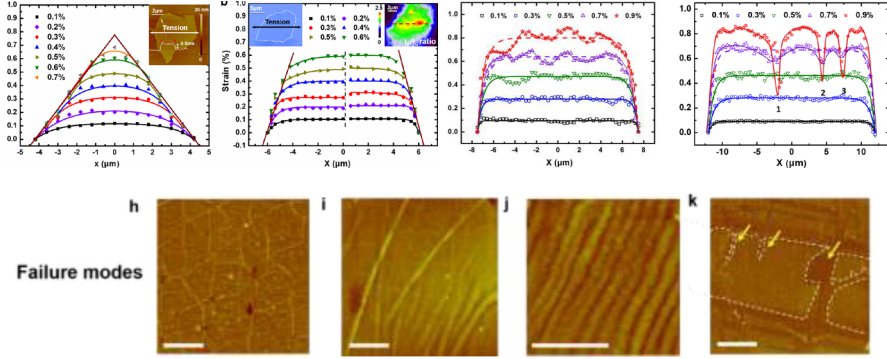


Figure 16: Illustrative scheme of ε solutions and graphics – non-linear shear-lag analysis for Graphene/PMMA (Wang *et al.* 2016).

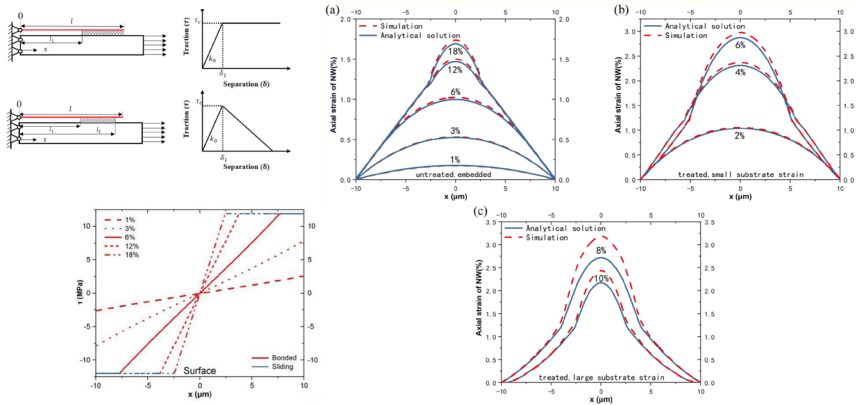


Figure 17: Illustrative scheme of ε and τ solutions and graphics: non-linear shear-lag analysis, bi-linear shear-lag analysis and FE analysis, for elastoplastic nano-fiber AgNW/PDMS (Shao *et al.* 2023).

It is assumed, that after the transferred stress exceeds the interfacial shear strength of BLG, the vdW interface between the two graphene layers will be damaged in the form of debonding, but if the two surfaces are flat enough, a new vdW interface will be formed again to re-bond the graphene layers, and start the new straining process with an external load and the same interfacial stiffness K_I . For the interface between the stretchable substrate (PDMS) and the bottom graphene layer, a cohesive shear-lag model is adopted as well to describe the interfacial shear stress with K_2 .

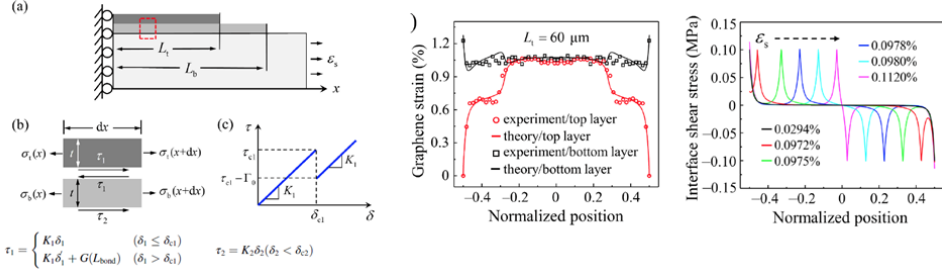


Figure 18: Results from *re-adhesive shear-lag model* of Ren *et al.* (2023).

In (Liu *et al.* 2022a; Peng *et al.* 2024) again stress transfer in graphene/PDMS is considered (Fig. 19, 20); in (Liu *et al.* 2022a) by molecular dynamic simulations (MD), and by *decohesive shear-lag model* in (Peng *et al.* 2024). The results from (Liu *et al.* 2022a) show that under uniaxial tensile strain, the interface shear coupling between two graphene layers evolves sequentially with bonding, sliding and debonding process, and the corresponding interfacial shear strength is inversely proportional to the sample size. MD simulations demonstrate the origin of this inverse proportionality as stronger interlayer vdW interaction induced by the edge lattices and atoms of bi-layer graphene that have more degrees of freedom.

Peng *et al.* 2024 proposed an improved shear-lag model with a trapezoidal-shaped cohesive zone to derive an analytical solution for the decohesion behavior. This theoretical model reveals that the decohesion behavior of the frictional adhesive interface is governed by three dimensionless parameters. Particularly, the dimensionless length of the film essentially determines the decohesion rate; while the other two parameters affect the critical substrate strain to initiate debonding. Adding a formvar (adhesive) layer leads to rapid

debonding process in contrast to the case without it, where the progressive crack propagation is observed.

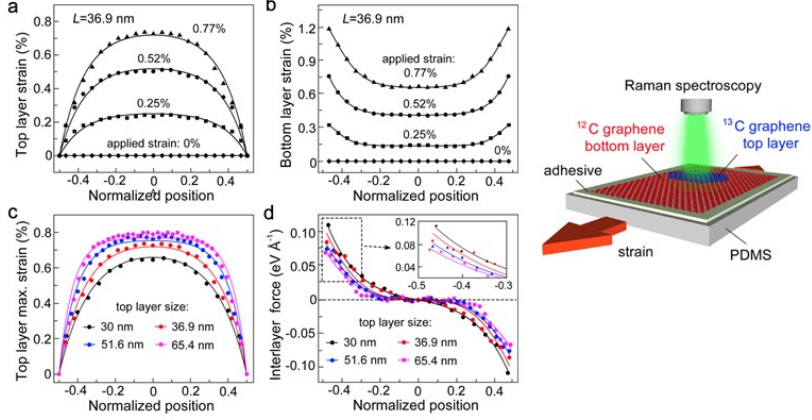


Figure 19: MD results of (Liu *et al.* 2022a).

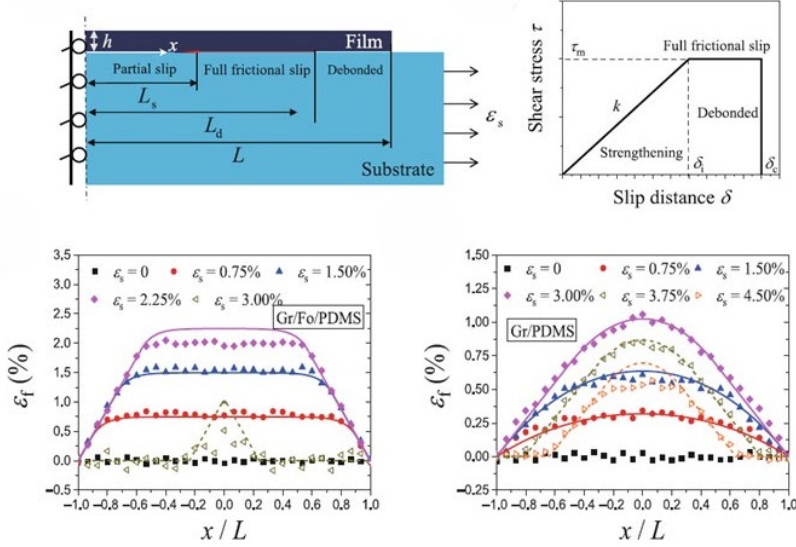


Figure 20: Improved shear-lag analysis with trapezoidal cohesive zone for graphene/PDMS, with and without adhesive layer formvar (Peng *et al.* 2024).

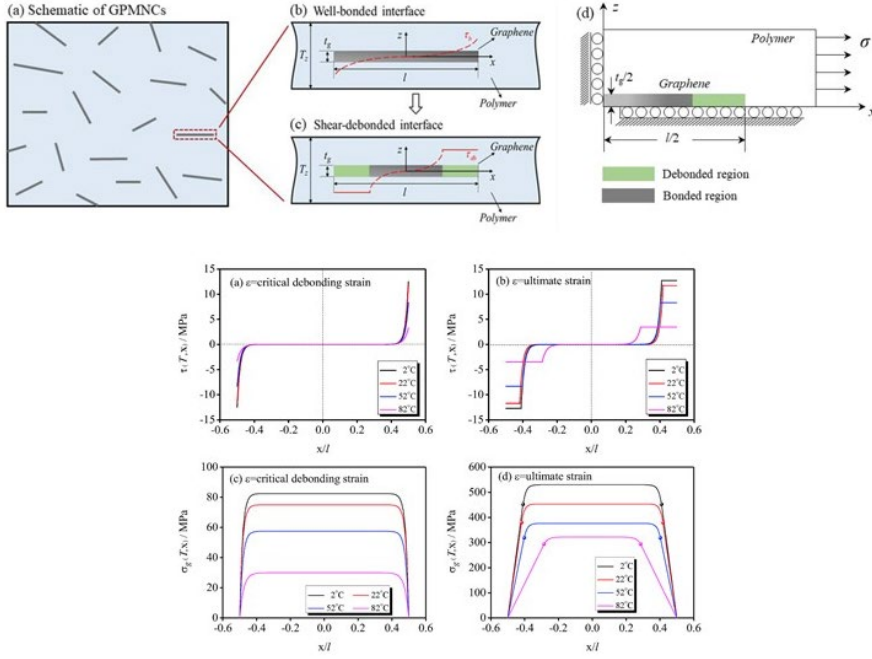


Figure 21: Results for non-linear shear-lag analysis with temperature accounting for ISS and stress in graphene (Yang *et al.* 2024).

The distributions of the axial stress in graphene nanoplatelets (GNPs), the interfacial shear stress and the strains at different temperatures are first quantified analytically (Fig. 21) by (Yang *et al.* 2024). Also, the evolution of interfacial debonding with external strain, the specific values of the critical debonding strain of the interface, and the maximum debonding ratio at different temperatures, are calculated. These quantitative results indicate that the interface is easy to debond and the debonding phenomenon is more significant at elevated temperatures.

Xing *et al.* (2023) performed experimental and theoretical investigations on a MoS₂/graphene heterostructure assembled on a formvar/polydimethylsiloxane (PDMS) substrate under biaxial tensile loading. They proposed a phenomenological strain transfer model of the finitely elastic interface, by simplifying the interfacial connection of the 2D NM film and the substrate as numerous shear springs, like in (Gong *et al.* 2010). The strain transfer mechanism from the substrate to the 2D material was described, and the strain transfer coefficient was introduced to qualify the strain transfer efficiency before interfacial slipping.

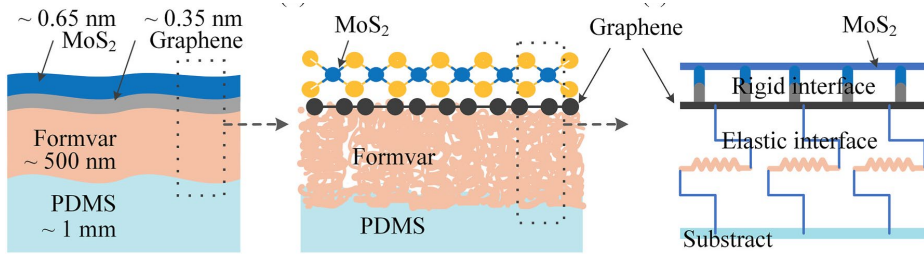


Figure 22: Scheme of strain transfer model in heterostructure Gr/MoS₂/formvar/PDMS (Xing *et al.* 2023).

In the past few years, an increase in theoretical studies of NC through molecular dynamics /atomistic simulations has been seen in the literature from (Lu *et al.* 2021; Baimova and Shcherbinin, 2023; Dahiya *et al.* 2024; Wu *et al.* 2024), especially for graphene-polymer NC. In the review articles (Baimova and Shcherbinin, 2023; Dahiya *et al.* 2024) the use of these methods is discussed and commented. In Baimova and Shcherbinin (2023) the advances in the MD simulation of fabrication and the study of mechanical properties of metal/graphene composites of various morphology, are presented. The thickness of the metal layer should be taken into account since, after some critical thickness, the strength of the composite is lower; the thickness of the graphene layers also affects the composite properties. If multilayer graphene is chosen as the reinforcement, it can be delaminated during tension, and this results in a decrease in the mechanical properties of the composite. Dahiya *et al.* (2024) in their review distinguished and commented a few approaches and techniques that are commonly used for modelling and analysis of graphene NC: Molecular dynamics simulations; Finite element analysis; Continuum mechanics; Analytical modelling and Experimental analysis. They recommended, that it is essential to emphasize the utilization of multi-scale modelling methodologies that effectively connect atomistic simulations with macroscopic phenomena, thereby bridging the disparity of these two levels of analysis.

Wu *et al.* (2024) by using MD simulations, investigated the mechanical properties of double layer WS₂ nanosheets (DLNS), graphene/WS₂(layer) composites and graphene/WS₂ nanotube (NT) composites. Their results reveal that the mechanical properties of DLNS degrade when compared to those of monolayer WS₂. The mechanical properties of graphene/WS₂ (layer) composite with both layers deformed are superior than those of WS₂, even

though inferior than those of bare graphene. The composite of graphene and WS₂ nanosheet shows a better mechanical performance in comparison to graphene and WS₂ NT composite with only graphene deformed.

3. 2D analytical solutions for nanocomposites

In contrast to the variety of 1D models and analytical solutions, described in the preceding section, the 2D models offering analytical solutions for layered nanocomposite structures are counted on the fingers. There are a lot of two-dimensional analytical solutions, offered by continuum mechanics, plate theory, etc., used for describing the behavior in layered composite structures (single lap-joint, double lap-joint) as it foreseen from (Zhang *et al.* 2019; Zhao and Lu, 2009; Zhao *et al.* 2014; Guo and Hu, 2024) at mechanical and/or temperature loading.

Guo and Hu, (2024) just proposed a modified 2-D shear-lag model based on trilinear cohesive zone model, considering unidirectional or bidirectional interfacial damage to analyze the stress transfer mechanism of rectangular patch-reinforced composites under tensile load (Fig.23, top). The bonding behavior of the composite interface can be described by cohesive theory. As depicted in Fig. 23, the trilinear cohesive zone model illustrates the bonding, damage, and debonding behaviors of the interface. It is assumed, that when the interface shear stress reaches the maximum value τ_{max} , the interface enters the damage stage I, and the interface transitions to the damage stage II after the interface shear stress decreases to the value of τ_b . The quantities δ_0 and δ_b are the critical failure displacements for the two kinds of failure cases, respectively. $K1$, $K2$ and $K3$ represent the interface initial stiffness of the cohesive unit, the interface stiffness for damage I, and the interface stiffness in the damage stage II of the cohesive unit.

The comparative analysis of the computational results from the 2-D, 1-D, and FEM models, done in (Guo and Hu, 2024) demonstrates the superior effectiveness of the 2-D model, especially in predicting the stress distributions in the damage stage. It is found that differences in Poisson's ratios between the substrate and the patch significantly affect the stress distribution within the composite. The increase in the thickness ratio between the substrate and the patch can lead to decrease in the normal stress in the patch. If the aspect ratio of the patch increases this leads to an increase in the normal stress in the patch. Additionally, as the Poisson's ratio difference and bidirectional stress ratio increase, the interface becomes less prone to damage.

Conversely, as the thickness ratio and aspect ratio increase, the interface becomes more prone to damage.

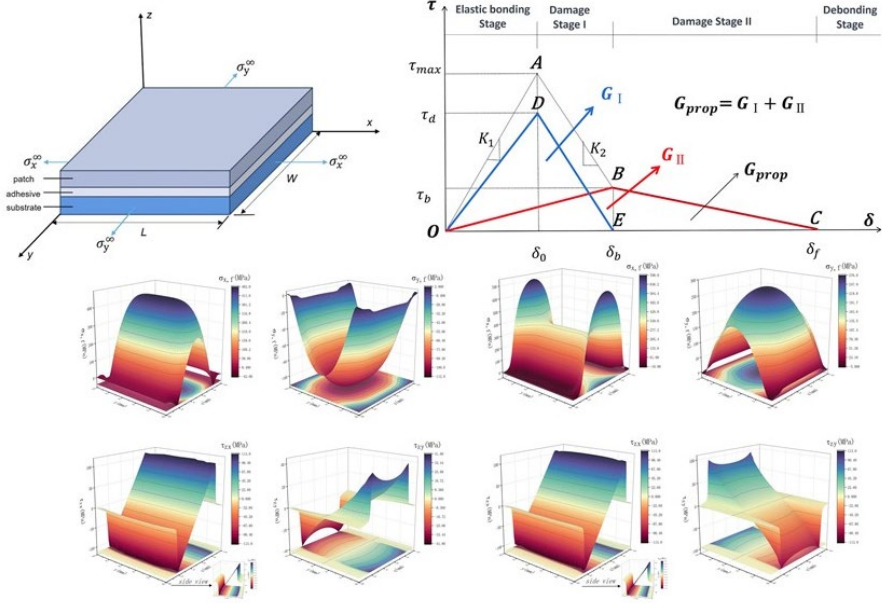


Figure 23: Scheme of the composite and modified 2D shear-lag analysis (top) and solutions for 2D stresses at axial (left, bottom); at bi-axial tension loading (right, bottom), in carbon/epoxy resin with an aluminum substrate (Guo and Hu, 2024).

Several works were also found on so-called nano-adhesives (nanoclays), nano-additions of graphene and other 2D nanomaterials to various adhesives, in order to strengthen single-lap joint structures as included in (Lu *et al.* 2021; Gupta *et al.* 2017; Akpınar *et al.* 2017; Jojibabu *et al.* 2020; Liu *et al.* 2011; Wang *et al.* 2021; Huang *et al.* 2022). For some biological materials such as bone or nacre (generic nanocomposite structure with staggered alignment of mineral platelets in protein matrix) (Liu *et al.* 2011), a perturbation method was applied for analytically solving the 2D displacement and stress fields of such type of nanocomposite structure under uniaxial tension. The disadvantage of all these models is that the interface layers between matrix and nano-layer are not taken into account. In 1D models like shear-lag the interface is represented as a line without considering its thickness and material properties. Meanwhile, it is proved that this interface layer exists and should not be ignored when modeling layered nanocomposites, analytically

or numerically (Lu *et al.* 2021; Wang *et al.* 2021; Huang *et al.* 2022). In the next chapter special attention is paid to the interface/interphases modeling in NC.

***Our contribution to 2D analytical models for NCs (under the project
KП-06-H57/3/15.11.2021)***

From 2019, our team started to work trying to fill the abovementioned gap; our contribution to the 2D analytical modeling of stresses and strain fields in layered nanocomposites with interface layer is expressed by the publications (Kirilova *et al.* 2019, 2023; Petrova *et al.* 2022a, 2022b, 2023; Petrova, 2023; Apostolov *et al.* 2022, 2024; Vladova *et al.* 2022, 2024). A detailed description of the 2D method (***stress-function variational method***) used to obtain analytical solutions for the two-dimensional stresses and strains in three-layer nanocomposite structures (Fig. 24) is given therein. In short, the applied method allows to obtain and solve analytically an ordinary differential equation with constant coefficients D_i of 4th order (eq. (4)) with respect to the unknown axial stress $\sigma_1 = \sigma_1(x)$ in the first layer (nanolayer):

$$2D_2\sigma_1^{IV} + (2D_3 - 2D_4)\sigma_1'' + 2D_1\sigma_1 + D_5 = 0 \quad (4)$$

The coefficients $D_i, (i=1...5)$ are calculated as:

$$D_1 = \frac{h_1}{E^{(1)}} + \frac{h_2\rho^2}{E^{(2)}}; \quad (4a)$$

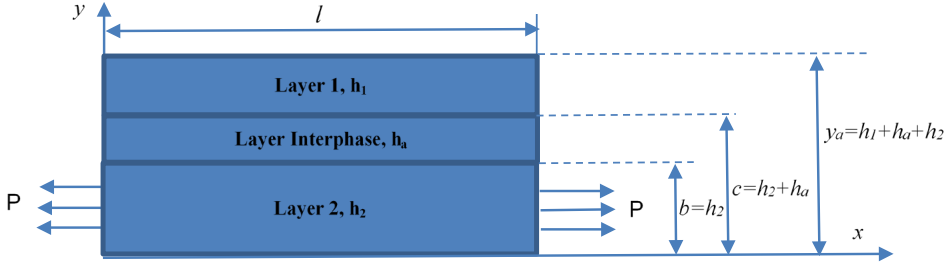
$$D_2 = \frac{h_1^5}{20E^{(1)}} + \frac{h_1^2 h_2}{120E^{(2)}} \left[6h_2^2 - 15h_2(y_t + h_a) + 10(y_t + h_a)^2 \right] + \frac{h_1^2 h_a}{12E^{(2)}} \left[3h_1^2 + 6h_1 h_a + 4h_a^2 \right]$$

$$D_3 = -\frac{\nu^{(1)}h_1^3}{3E^{(1)}} - \frac{\rho\nu^{(2)}h_1 h_2 \left[2h_2 - 3(y_t + h_a) \right]}{6E^{(2)}};$$

$$D_4 = \frac{2(1+\nu^{(1)})h_1^3}{3E^{(1)}} + \frac{2(1+\nu^{(2)})}{3E^{(2)}} h_1^2 h_2 + \frac{2(1+\nu^{(a)})h_1^2 h_a}{E^{(2)}}$$

$$D_5 = (\alpha^{(1)} - \alpha^{(2)})\Delta T \cdot h_1 - \frac{2h_2\rho\sigma_0}{E^{(2)}}$$

It should be noted, that for applied mechanical load only, $\Delta T = 0$ in coefficient D_5 . These coefficients are functions of Young's moduli and Poisson's ratios of the NC layers, NC length, layers' thicknesses, magnitude of mechanical load and temperature difference, if any, and layers' coefficients of thermal expansion (see eq. (4a)).



(a)

Layer (1):

$$\sigma_{xx}^{(1)} = \begin{cases} 0 & \text{if } x = 0 \\ 0 & \text{if } x = l \end{cases}; \quad \sigma_{xy}^{(1)} = \begin{cases} 0 & \text{if } x = 0 \\ 0 & \text{if } x = l \end{cases}; \quad y \in [h_2 + h_a, h_1 + h_2 + h_a]$$

$$\sigma_{yy}^{(1)} = \begin{cases} 0 & \text{if } y = h_1 + h_2 + h_a \\ \sigma_{yy}^{(a)} & \text{if } y = h_2 + h_a \end{cases}; \quad \sigma_{xy}^{(1)} = \begin{cases} 0 & \text{if } y = h_1 + h_2 + h_a \\ \sigma_{xy}^{(a)} & \text{if } y = h_2 + h_a \end{cases}; \quad x \in [0, l]$$

Layer (a):

$$\sigma_{xx}^{(a)} = \begin{cases} 0 & \text{if } x = 0 \\ 0 & \text{if } x = l \end{cases}; \quad \sigma_{xy}^{(a)} = \begin{cases} 0 & \text{if } x = 0 \\ 0 & \text{if } x = l \end{cases}; \quad y \in [h_2, h_2 + h_a]$$

$$\sigma_{yy}^{(a)} = \begin{cases} \sigma_{yy}^{(1)}(x, h_2 + h_a) & \text{if } y = h_2 + h_a \\ \sigma_{yy}^{(2)}(x, h_2) & \text{if } y = h_2 \end{cases}; \quad \sigma_{xy}^{(a)} = \begin{cases} \sigma_{xy}^{(1)}(x, h_2 + h_a) & \text{if } y = h_2 + h_a \\ \sigma_{xy}^{(2)}(x, h_2) & \text{if } y = h_2 \end{cases}; \quad x \in [0, l]$$

Layer (2):

$$\sigma_{xx}^{(2)} = \begin{cases} \sigma_0 & \text{if } x = 0 \\ \sigma_0 & \text{if } x = l \end{cases}; \quad \sigma_{xy}^{(2)} = \begin{cases} 0 & \text{if } x = 0 \\ 0 & \text{if } x = l \end{cases}; \quad y \in [0, h_2]$$

$$\sigma_{yy}^{(2)} = \begin{cases} \sigma_{yy}^{(a)}(x, h_2) & \text{if } y = h_2 \\ 0 & \text{if } y = 0 \end{cases}; \quad \sigma_{xy}^{(2)} = \begin{cases} \sigma_{xy}^{(a)}(x, h_2) & \text{if } y = h_2 \\ 0 & \text{if } y = 0 \end{cases}; \quad x \in [0, l]$$

where $\sigma_{xx}^{(i)}$, $\sigma_{xy}^{(i)}$, $\sigma_{yy}^{(i)}$ are the stresses for the three layers $i=1, a, 2$.

(b)

Figure 24: Representative volume element (RVE) of three-layered nanocomposite structure - (a), and boundary and contact conditions - (b).

The following model assumptions are set:

1. The axial stresses in the layers are assumed to be functions of the axial coordinate x only.
2. In the interface layer the axial stress is negligible in comparison to the stresses in the other two layers.
3. All stresses in the layers (axial, normal (peel) and shear stresses) are determined under the assumption of the plane-stress formulation.
4. The effect of bending on the stress field is also neglected.

Two types of model solutions for the axial stress σ_1 in the nanolayer are derived, depending on the geometry of the three-layer nanocomposite and its material properties:

$$\sigma_1 = C_1 \exp(\lambda_1 x) + C_2 \exp(\lambda_2 x) + C_3 \exp(\lambda_3 x) + C_4 \exp(\lambda_4 x) - A \quad (5)$$

$$\begin{aligned} \sigma_1 = & \exp(-\alpha x)[M_1 \cos(\beta x) + M_2 \sin(\beta x)] + \\ & + \exp(\alpha x)[(M_3 \cos(\beta x) + M_4 \sin(\beta x))] - A \end{aligned} \quad (6)$$

All other stresses in the layers are expressed by this solution/s and its derivatives as a functions of x , y and layers' thicknesses, as:

$$\begin{aligned} \sigma_x^{(1)} &= \sigma_1; & \sigma_y^{(1)} &= \frac{1}{2}(y - (h_1 + h_2 + h_a))^2 \sigma_1''; & \sigma_{xy}^{(1)} &= (y - (h_1 + h_2 + h_a)) \sigma_1' \\ \sigma_x^{(a)} &\equiv 0; & \sigma_y^{(a)} &= \left[\frac{h_1^2}{2} + h_1(h_2 + h_a - y) \right] \sigma_1''; & \sigma_{xy}^{(a)} &= h_1 \sigma_1'; & \rho &= \frac{h_1}{h_2} \\ \sigma_x^{(2)} &= \sigma_0 - \rho \sigma_1; & \sigma_y^{(2)} &= \frac{-h_1}{2h_2} [y^2 - y(h_1 + h_2 + 2h_a)] \sigma_1''; & \sigma_{xy}^{(2)} &= \frac{h_1}{h_2} y \sigma_1' \end{aligned} \quad (7)$$

The 2D strains in each layer are expressed by equations (8) in the general case of thermo-mechanical loading of the NC structure:

$$\begin{aligned} \varepsilon_{xx}^{(i)} &= \frac{1}{E_i} \sigma_{xx}^{(i)} - \frac{\nu_i}{E_i} \sigma_{yy}^{(i)} + \varepsilon_{Txx}^{(i)}; & \varepsilon_{yy}^{(i)} &= -\frac{\nu_i}{E_i} \sigma_{xx}^{(i)} + \frac{1}{E_i} \sigma_{yy}^{(i)} + \varepsilon_{Tyy}^{(i)}; \\ \varepsilon_{xy}^{(i)} &= \frac{1 + \nu_i}{E_i} \sigma_{xy}^{(i)}, & \varepsilon_{Txx}^{(i)} &= \alpha_x^{(i)} \Delta T, & \varepsilon_{Tyy}^{(i)} &= \alpha_y^{(i)} \Delta T \end{aligned} \quad (8)$$

where $\alpha^i, \beta^i, i = 1, a, 2$ are the coefficients of thermal expansion of the layers, T and ΔT are the temperature and temperature difference, respectively. In the solutions for the stresses (Eqs. 5-7) the temperature influence is accounted by the constant A ($A = D_5/2D_I$), which depends on the value of the external static load σ_0 and ΔT ; practically, it is a partial solution of the non-homogeneous ODE for axial stress (Eq. 4) (Vladova *et al.* 2022). The coefficients M_i, C_i are integration constants in the model solution, determined from the boundary conditions.

For convenience, only the main results and the validation of our model solutions with literature experimental and model data will be given below. The results of the parametric analysis are also presented in the next chapter. The sensitivity of the model solutions, makes it possible to determine the main factors affecting the delamination in the investigated nanocomposite structures, giving them wide application in various industrial sectors.

Validation of 2D model (stress-function variational method)

The validation of the model results obtained by us for the stresses and strains, with data found from the literature, is performed for the following nanocomposite structures: graphene/SU-8/PMMA (Gong, 2012), WS₂/SU-8/PMMA (Wang, 2017), 3-layered graphene/SU-8/PMMA (Androulidakis *et al.* 2017) and (Du *et al.* 2022) for MoS₂/interface/PET and graphene/MoS₂/PET. The results of the comparison of the obtained solutions can be seen below in Figs. 25-31.

The validity of the proposed method and analytical solutions is only within the elastic region. It is worth mentioning that this region varies for different types of 2D nanomaterial used. At 0.6% external load (Fig. 25 (b)) both model solutions - ours and the shear-lag one used in (Gong, 2012) cannot describe Gong's experimental data for graphene strain sufficiently accurately. The explanation for this is Gong's experimental observation that when the external load varies in the range of 0.4% to 0.7%, a creep and relaxation zone is recorded in the graphene, which is the cause of the drop (approximately in the middle of the flake, to 0.4%) in the distribution of the measured axial strain in graphene. According to Gong, it seems that the interface between the graphene and the polymer is not efficient enough and the transfer of the applied external load occurs through interfacial friction in this range. The strain in the graphene does not drop to zero in the middle of the flake, however, indicating that the flake remains unbounded. Further evidence to

support this claim can be found in (Polyzos *et al.* 2015). They experimentally investigated the behavior of stresses and strains in a suspended graphene flake between two PMMA layers subjected to an axial external load. It is reported that up to 0.8% external load "*there is evidence that axial loading of graphene is always accompanied by the formation of orthogonal wrinkles/folds, similar to what is observed in a thin macroscopic membrane subjected to axial tension*". Polyzos *et al.* (2015) also emphasized that the limitations in their research method require a linear relationship between stress and strain, that is, within the elastic zone.

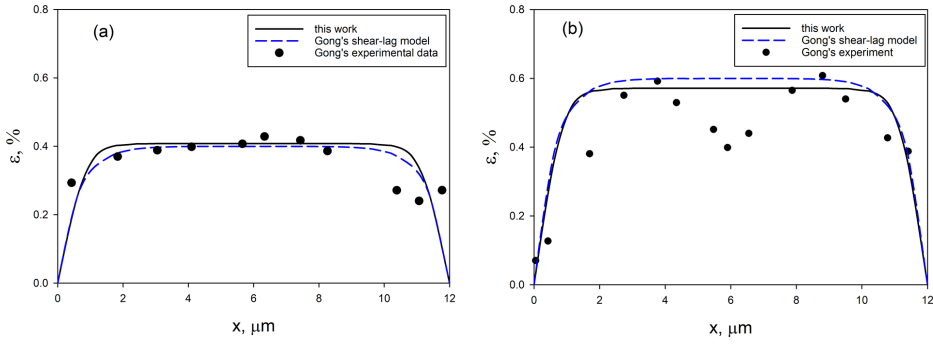


Figure 25: Comparison of model predictions (Petrova *et al.* 2022b) for the ε in graphene with shear-lag model data and experimental data (Gong, 2012); (a) at external load 0.4%, (b) – at 0.6%.

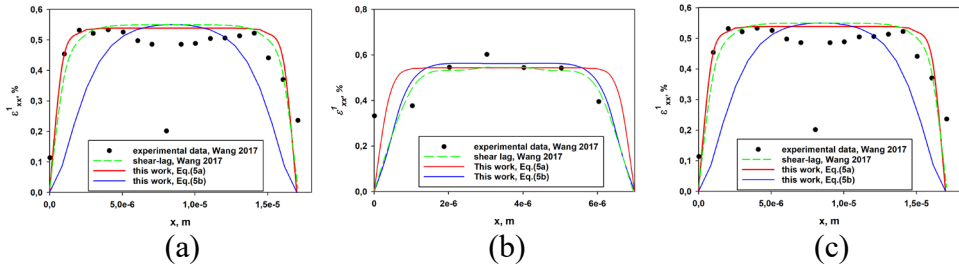


Figure 26: Comparison of the two model solutions for ε in monolayer WS_2 , according to equations (5) and (6) and (8) (Petrova *et al.* 2022a), with experimental and model shear-lag data of (Wang, 2017) at (a) external load 0.35%, (b) same at 0.55%, (c) multilayer WS_2 at 0.55%.

From Fig. 26 it is seen, that for WS_2 this description in the elastic zone depends not only on the external load magnitude, but on the thickness of the nano layer, too. As is illustrated in Fig. 27, both solutions for axial stress in WS_2 are in good agreement with the shear-lag predictions, especially Case 2 (Eq. (6)), may be because both shear-lag and Case 2 are expressed by hyperbolic sines and cosines.

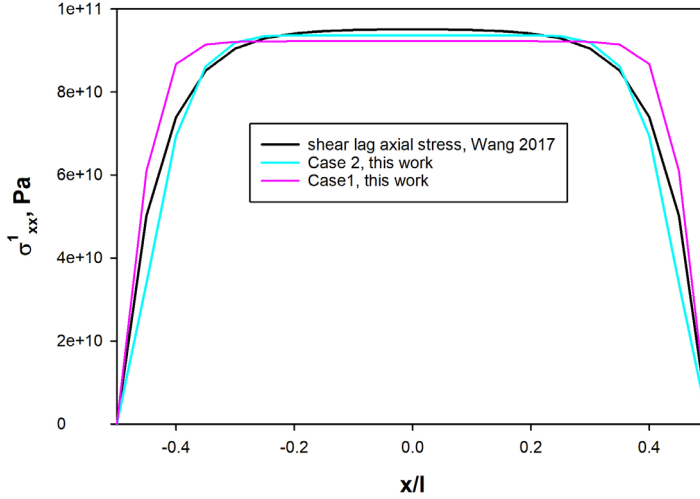


Figure 27: Comparison of model axial stress σ_l solutions (Petrova *et al.* 2023) in layer WS_2 , with shear-lag model results of (Wang, 2017), for 0.35% external load.

The similar dependence is observed for multi-layer graphene when the external load is out of the elastic range (Fig. 28). Here the main deviations are in the right end of the flakes for both external loads considered. Probably, this is due to the defect in the flake itself or to an error in the measurement method in (Androulidakis *et al.* 2017). The other main emphasis in (Vladova *et al.* 2022) is the comparison between the model solutions for the deformations (strains) in the layers of the considered 3-layered graphene/SU-8/PMMA nanocomposite, under different types of external loads, as can be seen from Fig. 29. In the case of a purely thermal effect (the red line), the deformations are nearly three times smaller than in the case of a purely mechanical effect (the black line). In the case of thermomechanical loading (green line), a superposition effect is observed in the amplitudes of the two loads, or in other words, the behavior is the same as in the mechanical load, but stronger, with

the addition of the temperature effect, and this is best seen in the axial and the normal stress. Also, the effect of temperature is more clearly visible for deformations in the polymer layer than in graphene. It has to be noted, that a similar observation is also found in the model results of Banarouei (2021), obtained with finite elements. The master thesis of Banarouei (2021) is the first (to the best of our knowledge) to report results related to the distribution of stresses and longitudinal strains in graphene at different external temperatures. Since the simulation used in (Banarouei, 2021) is FEM, no direct quantitative comparison is possible, only a qualitative assessment.

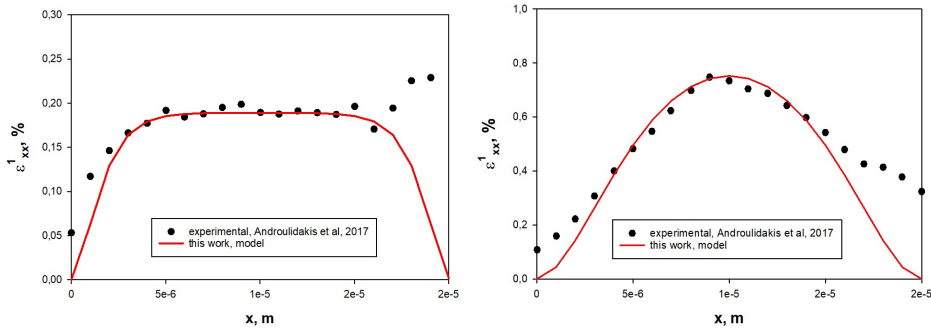


Figure 28: Comparison of the model axial deformations (Vladova *et al.* 2022) in 3-layer graphene with experimental data of (Androulidakis *et al.* 2017), at external mechanical loading of 0.3% and 0.8 %.

Our model strain predictions (Boyadjiev *et al.* 2023) for a hybrid nanocomposite structure with 2 interfaces (graphene/MoS₂/PET) at external load 0.5% are in good accordance with experimental data (Fig. 30 (b)). For the nanocomposite sample with one interface (MoS₂/interface/PET) the coincidence is quite good (Fig. 30 (a)); probably, the existence of two interfaces in the first sample between both nanomaterials (graphene and MoS₂) and (MoS₂ and PET) did not positively influence the stress transfer efficiency in this sample. Our model results for critical lengths in 2 specimens MoS₂/PET and Gr/MoS₂/PET, estimated from the model strain distribution data in Fig. 30 confirm experimental, as well as theoretical results of (Du *et al.* 2022) – 24 μ m.

The 2D stress-function method is applied also in modelling analytically the axial strain and interface shear stress distributions in a two-

phase hBN/PMMA nanocomposite under axial tension load (Petrova *et al.* 2023a). The novelty here is the introduction in the model of an interface layer between the hBN layer and the polymer. The existence of this interlayer has been experimentally observed in many nanocomposites, but up to now its properties and dimensions are difficult to measure. The interface layer properties – Young’s modulus, Poisson’s ratio and thickness are simulated and modeled, based on the approach proposed in the work of Zhu and Narh, (2004).

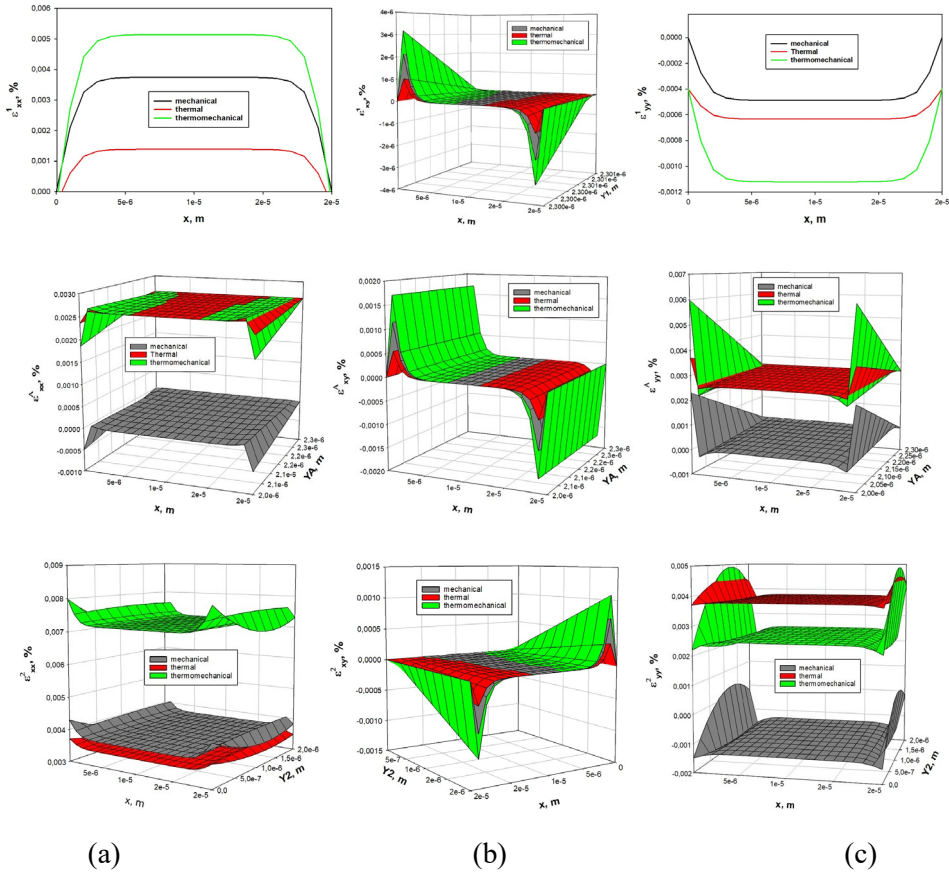


Figure 29: Comparison of axial (a), shear (b) and peel strains (c) in graphene/SU-8/PMMA layers, under different types of loading (Vladova *et al.* 2022).

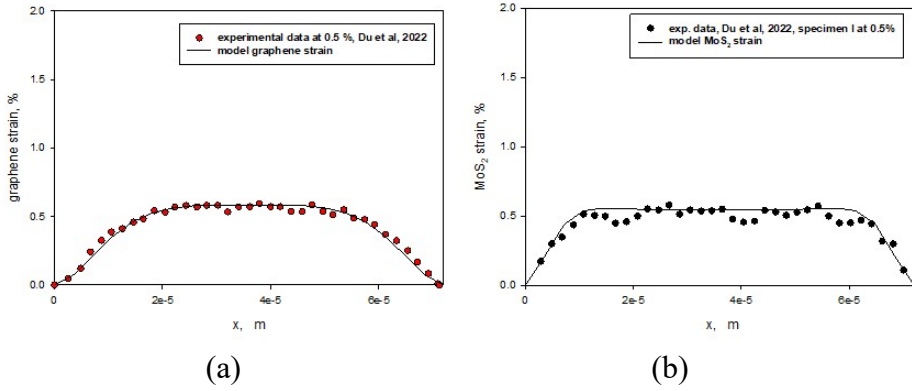


Figure 30: Comparison of the model axial strain ε in the graphene layer (a), and in the MoS₂ layer (b), with experimental data of (Du *et al.* 2022) at an external mechanical load of 0.5% (Boyadjiev *et al.* 2023).

The model axial strain in the hBN layer, as well as the interfacial shear stress have been calculated and compared with both experimental data and shear-lag model results of Wang *et al.* (2021a), at three different mechanical external strains - 0.05%, 0.1% and 0.15% (Fig. 31). The obtained results coincided very well with literature data. They could be used for a fast prediction of the strain and interfacial shear stress distributions in nano-electronic devices, in elastic zone of external loadings.

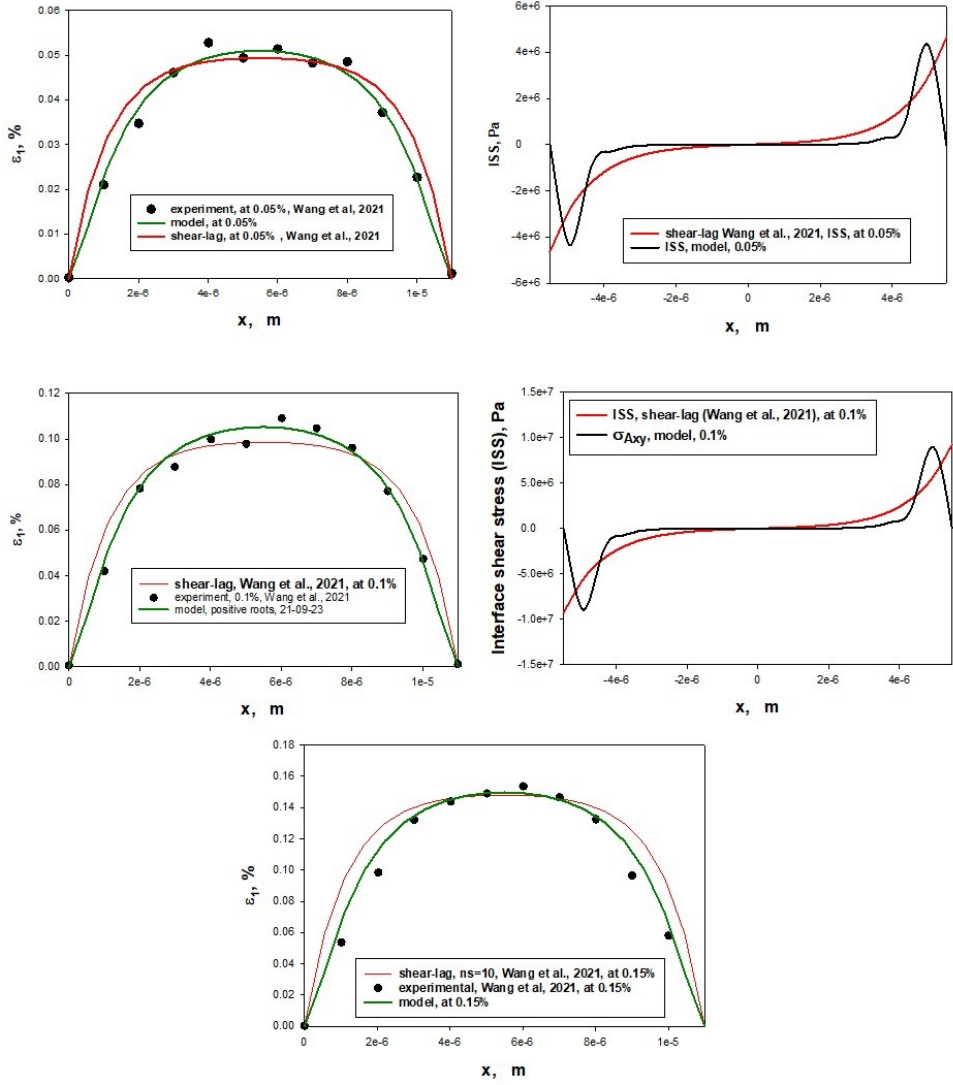


Figure 31: Comparison of the model axial strain in the hBN flake at 0.05%, 0.1% and 0.15 % external load, with experimental and shear-lag data of Wang *et al.* (2021a) in (Petrova *et al.* 2023a), for Case 1 (eq.(5)).

4. Conclusions

The following conclusions and remarks after this chapter could be proposed:

Analytical “shear-lag” type models give simple 1D solutions, validated by experiments and FEM, for the prediction of stresses and strains in composite and nanocomposites structures, subjected generally in tension loading. Analytical models allow adding of different effects to the stresses, especially to ISS, like interface spring stiffness constant, effects of residual stresses, due to the thermal and Poisson contraction, effect of wdW forces, effect of sliding, etc. They also allow to obtain analytical solutions to describe a complex combination of external and internal factors, acting on the stress transfer in nanocomposites. The correct application of shear-lag models for matrix-fiber nanocomposites is constrained - firstly in the elastic zone only, secondly by the volume of added fibers, and also, by the fiber length and interaction between fibers. Different models are derived to cover these gaps. Partial and total debonding models, as well as non-linear shear-lag models create the “bridge” between predictions of stress transfer in the elastic and plastic zone (cohesive shear-lag models and FEM simulations).

The new “fashion” in NC modeling is multi-scale modeling, allowing the combination of different model approaches in different scales. The newly developed 2D analytical stress-function method allows deriving 2D solutions for a three-layer nanocomposite structure, subjected to mechanical (axial tension) and thermo-mechanical static loading. These solutions are successfully validated in the elastic zone by experimental and shear lag data for different nanocomposite structures.

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Notations list

Notation	Meaning
σ	Stress, Pa
τ	Interfacial shear stress, Pa
ε	Strain (deformation) in nanomaterial, -
l	Length of the arm connecting part or length/length of the structure/flake, m
x, y, z	Cartesian coordinate system, m
E	Young's modulus, Pa
G	Interface/adhesive shear modulus, Pa
t_1, t_2	Thicknesses of the two arms (adherends) of the joint, m
h	Joint connecting part/adhesive, m
P	Magnitude of the applied force to the joint (force per unit width), N/m
ε_1	Applied external deformation, -
a	Radius of the thread, m
R	Radius of the substrate, m
$s=L/a$	Thread size ratio/Aspect ratio, length to diameter, -
q_1, q_2, q_3	Additional residual stresses, Pa
K, K_1, K_2	Interface spring stiffness coefficient/ interfacial stiffness, TPa/nm
m	Dimensionless length of the debonded portion, -
k_m	Parameters, represents the effective stiffness of the polymer surface (constant), -
n	Parameter in shear-lag model, -

β, C	Parameters in non-linear shear lag models, m^{-1}
k_0	Constant stiffness, TPa/m
δ_0, δ_b	Critical failure displacements for the two kinds of failure cases, m
$\alpha^i, \beta^i, i=1, a, 2$	Coefficients of thermal expansion of the layers, $1/\text{K}$
$T, \Delta T$	Temperature and temperature difference, K
A	Constant, solution of non-homogeneous ODE (4), Pa
M_i, C_i	Integration constants in the model solutions (5) and (6), -

Chapter 2. Theoretical analysis of factors, influencing delamination and failure in nanocomposites

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Annotation

Here, the methods and findings about determination of the essential factors affecting delamination in the nanocomposite structures under static mechanical loading and temperature differences, are presented and discussed. First, a review on the available data in the current literature for the interface/interphase properties and their thickness/width in distinct nanocomposites is raked up. Then, the literature results obtained by parametric/sensitivity analysis for the main factors, affecting interface shear stress and generally influence on the mechanical characteristics of nanocomposites, are summarized. Finally, the authors' results from the performed parametrical analyses for distinct nanocomposite structures have been described, based on the 2-D model solutions from Chapter 1 for interface shear stress.

1. Review on the studies for interface/interphase properties in nanocomposites

The delamination and fracture in nanocomposites (NC) and especially, in their applications as parts of electronic and sensor devices, are still the main problems which have to be avoided in their design, testing and manufacturing. According to (Tian *et al.* 2024), this could be due to different reasons: the presence of defects in the fabricated NC materials, or manufacturing defects, external factors like temperature, humidity, etc., as well as to the low stress transfer efficiency between the substrate (matrix) and the nanomaterial (NM).

Part of the listed reasons causing delamination in NC can be prevented by a more precise selection of the materials in NC, a proper choice of NC processing methods and control over obtaining NC (Georgieva *et al.* 2019; Georgieva *et al.* 2023a, 2023b). As for the low degree of efficiency in stress transfer in NC, according to the available literature (Tian *et al.* 2024; Zare *et al.* 2017; Elmasry *et al.*, 2023; Wang *et al.*, 2023) it can be due to many factors: type, size, shape, arrangement, % content of nanoparticles/nanomaterials in the volume of the matrix/substrate in NC, various external influences (mechanical, physical and others) on NC, etc. Some researchers (Wang *et al.*, 2023; Wang and Liu, 2023) have emphasized the interface or even the intermediate phase (layer) between NM and the substrate as well as the main reason for the low degree of stress transfer in NC.

Here is the place to comment in more detail on the difference between the two concepts - "interface" and "interphase", used both in the experimental (Tian *et al.*, 2024; Wang *et al.* 2023; Liu *et al.* 2016) and in the theoretical (Elmasry *et al.* 2023; Wang and Liu, 2023; Petrova, 2023; Lu *et al.*, 2021; Deng and Vliet, 2011) studies for NC in the literature. From a search in the Scopus database with the keywords "nanocomposites" AND "interphase" AND "modeling", the results obtained are 437 documents (Fig.1, (a)÷(d)), in the period 2000-2024; the distribution is presented graphically by year – (a), by region (b), by type of publication (c) and by country (d).

Other results (784 found) are obtained, if the keyword “interphase” in the previous search is replaced by “interface”; it is presented in Fig.1 for the same 4 categories. When comparing the two Figs: 1 and 2, in the corresponding 4 categories, it can be seen that the trend in the increase in the number of publications on the selected keywords is general; in the second variant of the search, with "interface", it seems being more stable over the years. The distribution of publications by subject area, as well as by types of publications in both search options, is almost identical. Most of the publications in both searches are articles, followed by conference papers and book chapters or review articles. The main subject areas for both searches are Material science, Engineering, Physics, Chemistry, Mathematics and Chemical engineering. There are major differences in the ranking of the distribution by country (Fig.1, (d) and Fig.2, (d)). When a filter "experiment" is added to each of both primary searches, about ¼ of results are concerned with both modeling and experimental studies (100 of the results with “interphase” remain, and 219 of those with “interface”). If the new keyword

“analytical modeling” is replaced in the primary searches, the result for the first one (with “interphase”) is only 12 documents found, respectively, for the second (“interface”) search the result is only 11 documents found. The latter outcome reflects only constrained use of the analytical models for simulating the interphase/interface in NC.

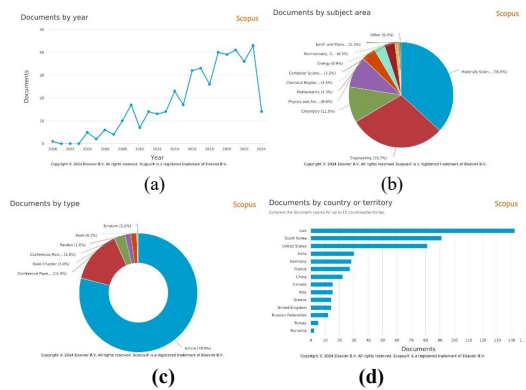


Figure 1: Scopus search by keywords: “nanocomposites” and “interphase” and “modeling”.

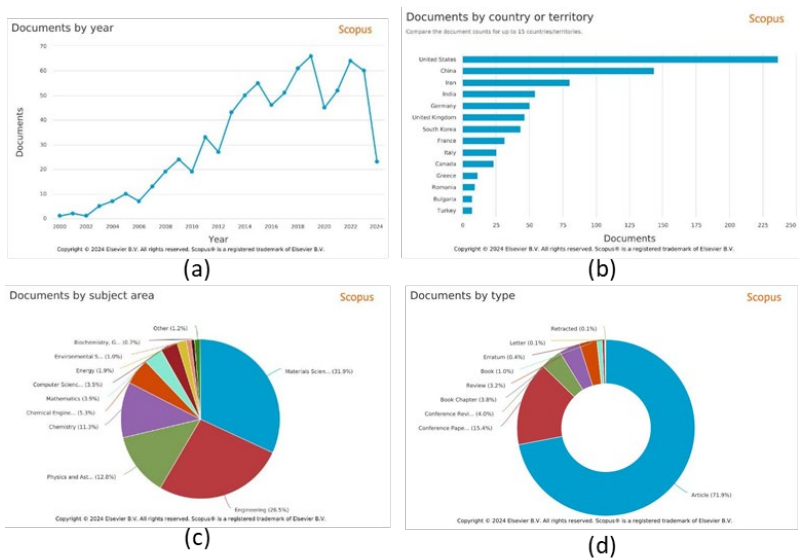


Figure 2: Scopus search by keywords: “nanocomposites” AND “interface” AND “modeling”.

The definitions of the two concepts "interface" and "interphase" in NC studies have been discussed and continue to intrigue the researchers (Elmasry *et al.* 2023; Liu *et al.* 2016; Lu *et al.* 2021; Deng and Vliet, 2011; Pukánszky, 2005; Jesson and Watts, 2012; Mishnaevsky, 2012; Netravali and Mittal, 2016; Schadler, 2018; Pant and Mehra, 2021; Villeneuve-Faure *et al.* 2022). In the review of Jesson and Watts (2012) the interphase is defined as: *"a region, called the interphase, being the volume of material affected by the interaction at the interface. The term interphase, a three-dimensional zone, as distinct from a two dimensional interface, was first coined by Sharpe (1974)¹ and the term is now widely used in the adhesion community to indicate the presence of a chemically or mechanically altered zone between adjacent phases.....interphase zone will lead to a gradation of properties from one phase to another, rather than the abrupt change necessitated by the acceptance of a two-dimensional interface"*. This version of definition is widely used also in the Chemical engineering and in multi-phase transfer processes (Doichinova and Popova-Krumova, 2013; Boyadjiev *et al.*, 2016, 2018; Popova and Boyadjiev, 2008). Recently, Pant and Mehra (2021) have proposed to model the gradation of interphase properties in NC (E – Young's modulus and ν - Poisson's ratio) by an exponential and parabolic variation, separating the interphase in 3 layers for spherical nanoparticle (NP) inclusions in the matrix. Earlier, in his review Pukánszky (2005) also commented that a distinction should be made between the two concepts, analyzing the techniques for identifying the properties and geometry (width/thickness) of the interphase, in different types of composites and NC. Villeneuve-Faure *et al.*(2022) have mentioned, that *"interphase presents different mechanical (among others) properties from both the matrix and the nanoparticles"*; for example, Mishnaevsky (2012) has ascertained that the Young's modulus of interphase is 2.9÷8 times higher than that of the epoxy matrix. A review on the experimental identification of the interphase in 2D nanomaterials is also presented by (Wang *et al.* 2023), with data on the interphase adhesion energy studies for NCs, both between two adjacent layers of nanomaterials, and in their adhesion to different substrates. In the later, significant advances in the understanding of the elastic properties, in-plane failures, fatigue performance, interfacial shear/friction, and adhesion behavior of 2D materials, are presented.

From the modeling point of view, in particular at multiscale modeling, in (Elmasry *et al.* 2023) it is concluded that *„Interfaces could be treated as*

¹ In 1972, Sharpe proposed the interphase concept to describe the transition region at the interface between two phases of different materials.

regions of distinct atomic structure or merely as a thin layer of interphase material near the interface as in the framework of continuum mechanics..the interphase zone includes the interface layer between the fibre and the matrix and a region of a finite thickness extending on both sides across the interface“. In the review of (Elmasry *et al.* 2023) also an overview of the most important approaches in multiscale modeling is made - analytical, semi-analytical and numerical, where in the latter also finite element modeling (FEM) and molecular dynamics (MD) are covered. In the modeling of interfacial interactions, a group of models is distinguished, which are divided in the review into “*interphase models, for representing a second phase between the inclusion and the matrix and interface models*” (see Fig.3). These authors have also made a comparison between the Young modulus results predicted by the different types of models both with each other and with experimental data.

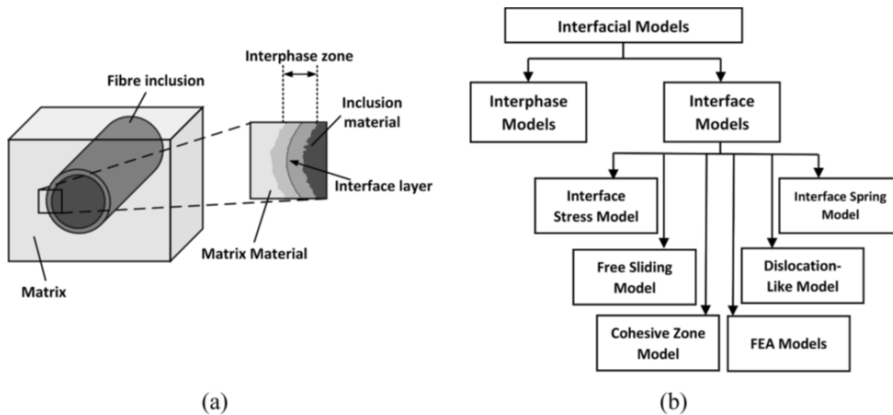


Figure 3: Types of modeling of interfacial interactions by interface and interphase models (Elmasry *et al.*, 2023).

In the book of Netravali and Mittal (2016), as well as in the other book chapters (Wang and Liu, 2023; Schadler, 2018), all devoted to the Interface/Interphase in polymer NCs, different methods for their identification and modeling of their geometry and properties, as well as which factors influence them, are discussed in detail, since „*by better understanding of interface and interphase characteristics it should be possible to predict as well as design polymer nanocomposites with desired properties and performance*“. Wang and Liu (2023) also indicated from the experimental techniques/models addressed in their chapter, that the physico-chemical factors – functional groups, extended chain morphology, aggregations,

wrinkles, as well as a few model parameters (for example, shear-lag parameter β and interfacial shear strength, aspect ratio, thickness and properties etc.) can serve as quantitative indicators of the efficiency of the transfer of stress through the interfacial region of NC. In (Schadler, 2018) it is revealed that for polymer NC *“there are both intrinsic and extrinsic interfacial regions. The intrinsic interphase develops as a result of the polymer matrix interacting with the nanofiller surface. The extrinsic interphase is the result of carefully placed molecules on the nanofiller surface”*. Also, it is postulated, that the properties of the intrinsic interphase region can be broadly characterized by: (1) changes in the relaxation time/mobility of the polymer and (2) changes in mechanical, electrical, dielectric, or optical properties of polymer NC.

To be more comprehensive, in *Table 1* the available data in the current literature data for the interphase properties and their thickness/width in distinct NC are raked up. When attempting to summarize and analyze the data, for example for interface zone width/thickness, it is seen that they are spread over too wide a range to distinguish any quantitative relationship. In older types of NCs where NPs such as nanoclay, Si, Al, Ti, and other types of oxide nano-additives in combination with different substrates, the width of the interface zone is fluctuating from 0.5 nm to fractions of a millimeter. When graphene is also combined with different polymers, it varies from 10.5 Å to 90 nm. Both 12.5 nm and 87 nm interphase thicknesses are observed for graphene oxide/substrates; the situation is similar for hBN and MoS₂ with polymer matrices – respectively 23 or 80 nm for hBN and so far, only one value found for MoS₂ – 67 nm. As can be seen from both Table 1 and literature studies, the data obtained for the width (thickness) of the interface zone are either experimental or theoretical, or a combination of both. The scatter in the data is due both to the way it was obtained and to the differences and accuracy of the measurement methods, and distinct geometry and loading conditions for the considered NC structures. Also, in the model predictions we have simplifications and assumptions that do not accurately account for the width (thickness) and properties of the interfacial zone, and the models may not always correctly simulate the contact and boundary conditions in this transition region. In other words, there are too many factors that influence the dimensions and properties of the interface/interphase zone. Regardless of the above, the interfacial zone at NCs exists and should be considered in the modeling of design and stress transfer efficiency of both existing and newly created NCs, especially in terms of their ever-increasing number of industrial applications.

A similar situation happened to the data of elastic properties of the interphase zone like elastic modulus E and Poisson ratio ν – simulated or measured in papers, included in *Table 1*. In most of works, the scientists still step on the presumption for spherical/cylindrical NP inclusions and respectively, the spherical (shell) interphase zone between the NP and substrate matrix (Deng and Vliet, 2011; Villeneuve-Faure *et al.* 2022; Zhu and Narh, 2004; Saber-Samandari and Khatibi, 2006; Heydari-Meybodi *et al.* 2015; Hosseini *et al.* 2017; Zahedi *et al.* 2019). Usually, the interphase properties are assumed (and modeled) as a % or mean of the properties of the matrix (Zhu and Narh, 2004; Heydari-Meybodi *et al.* 2015; Manta, 2018). More complex relationships and methods for determining elastic properties of the interphase are proposed in (Hosseini *et al.* 2017; Lahoud-Dignat *et al.* 2016; Cremonuzzi *et al.* 2023; Mehdipour *et al.* 2024). Recently, in the paper of Mehdipour *et al.* (2024) it is postulated, that “*the interphase zone surrounding the Graphene NPs is assumedto be an empty rectangular cube in nanocomposite materials, and its properties are typically considered to be functionally graded, with intermediate characteristics between those of the GNPs and the matrix*”. In fact, the idea a graded interphase has been reported earlier by Pukánszky (2005) for nanoparticles – SiO₂, Graphite, Mica, glass, CaCO₃ in polymer matrix, i.e., for older type of NC before graphene. Mehdipour *et al.* (2024) revealed that the chosen thickness of the interphase, the amount of aggregation of NP and the optimal percentage of graphene NPs can be combined in such a way as to achieve the maximal value of the reinforcement and optimal effective Young's modulus of the considered graphene NC. In this paper, the stiffness of the interphase is modeled by an integral power law relation between the stiffness of graphene nanoplatelets (GNPs) and matrix as well as their thicknesses; the predicted results coincided very well with experimental data for creep strain, total strain response and E of NC.

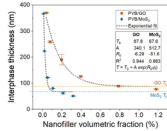
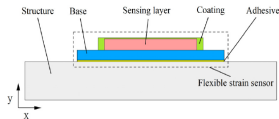
Table 1: Literature data for interphase properties and structure geometry in NC (measured /modeled).

Properties of interphase/interface in NC – E , ν	Thickness of interphase/ interface in NC	NC type	Method of determining, source
$E_{\text{interphase}}=10\div 100\%(E_{\text{matrix}})$	The thickness of the interlayer was assumed to be	montmorillonite (MMT)/PA	FEM, (Zhu and Narh, 2004)

	0.5 or 1.0 nm around the nanoclay particle		
NA	Between 0.0036 – 0.16 μm	Polymer/nanoparticles: SiO ₂ , Graphite, Mica, glass, polymer CaCO ₃	Experimental & model, (Pukánszky, 2005)
The average (over the thickness of the interphase) elastic modulus of the interphase, E_i: $E_i = \frac{1}{r_i - r_f} \int_{r_f}^{r_i} \tilde{E}_i(r) dr .$ $\tilde{E}_i(r) = E_m(r/r) + [r_i - r]/(r_i - r_f)]^{1/2} [E_f - E_m(r/r)]$	0 ÷ 20 nm	Polymer/fiber NP	three-dimensional unit cell model, (Saber-Samandari and Khatibi, 2006)
$E_f=40$ GPa for alumina–epoxy NC; $E_f=30$ GPa for alumina–epoxy NC; $E_f=22$ GPa for the titanium oxide–epoxy NC; Stiffness $E_{BR}=580$ MPa for hydrogenated nitrile butadiene rubber (HNBR)–carbon black NC	Thickness $t=36$ nm for alumina–epoxy NC; Thickness $t=10$ nm for alumina–epoxy NC; Thickness $t=19$ nm for the titanium oxide–epoxy NC; Thickness $t=26$ nm for HNBR/carbon black NC.	oxide NP/epoxy, carbon black NP/elastomer	Analytical prediction: interphase thickness t and elastic modulus E_f were obtained via the best fit of this model obtained via least squares nonlinear regression with respect to the measured data, (Deng and Vliet, 2011)
Formula for E of interphase is as in (Saber-Samandari and Khatibi, 2006). The density and Poisson's ratio of the interphase have been	To model the interphase, the nanoclay is surrounded by a 2 mm thickness and	Epoxy /3 wt.% Cloisite 30B (nanoclay)	Experiment/ FEM with and without interfacial debonding (Heydari-Meybodi <i>et al.</i> 2015)

assumed as the average of the other two phases.	incorporated in the matrix.		
NA	Interphase thickness of Gr/epoxy = 13 nm, for GO/epoxy= 12.5 nm	Epoxy/ Graphene-based NC	Experimental: scanning transmission electron microscopy (STEM) and electron energy-loss spectroscopy (EELS), (Liu <i>et al.</i> 2016)
graphical determination for thickness and E (see fig.4 in the source)	Interphase thickness= 23.32 nm	polyimide/ hexagonal-boron nitride (PI/h-BN) NC	Experimental: Peak Force Quantitative Nano-Mechanical (PF-QNM), Atomic Force Microscopy (AFM) mode, (Lahoud-Dignat <i>et al.</i> 2016)
Following (Saber-Samandari and Khatibi, 2006), the interphase modulus for NP spheres is calculated as: $E_i = \frac{E_m L n (r_i / r_f)}{r_i - r_f} + \frac{2[E_f - E_m (r_i / r_f)]}{n + 2}$	For relative thicknesses (interphase thickness to the particle size ratio) lower than a critical value such as 0.04, the particle size and interphase thickness effects on the elastic modulus of the NC are negligible.	SiO ₂ particles/ Epoxy resin	FEM, (Hosseini <i>et al.</i> 2017)
The interphase region is also modelled as an isotropic material, with elastic modulus setting as: $E_I = m \cdot E_m$ (m=0.25, 0.5, 1.0, 1.5, 2.0) and same Poisson's ratio as that of the matrix	Interphase thickness is simulated to be =1.5; 3.0; 6.0; 9.0; 12.0 nm.	Gr/epoxy, Gr/ PA6	Multi-scale FEM, (Manta, 2018)
NA	The interphase width was estimated to	treated & untreated polyimide/	Experimental: PF-QNM and

	be 30 ± 2 nm and 42 ± 3 nm for untreated and silane-treated nanoparticles, respectively.	silicon nitride (PI/Si ₃ N ₄)	Electrostatic Force Microscopy (EFM), (Houssat <i>et al.</i> 2018)
formulae for E of Interphase – the same as in (Saber-Samandari and Khatibi, 2006)	NA, simulated values. considerable effect of interphase thickness on the crack behavior in NC	Nanoclay/epoxy	3D Multi-scale FEM, (Zahedi <i>et al.</i> 2019)
NA	graphene/polymer interface thickness = 0.03 nm	graphene/epoxy	MD and FE simulations, cohesive interface behaves in the form of elastic-softening exponential regressive law, (Koloor <i>et al.</i> 2019)
NA	Interfacial thickness BaTiO ₃ /epoxy = 22 nm (model), 15–30 nm (exp) Interfacial thickness epoxy/Al ₂ O ₃ = 33 nm (model), 30–50 nm (exp)	BaTiO ₃ /epoxy , epoxy/Al ₂ O ₃	3D FEM + particle size distribution (PSD) analysis/ Experimental EFM, TEM, (Sharma <i>et al.</i> 2020; Sharma and Gupta, 2023)
NA	The thickness of the interphase region is identified as 10.5 Å	Gr/polymer, 5 layers, 2 interphases between 2 polymer layers and 1 graphene layer	Atomistic Local Identification of Stiffness method (ALIAS), (Lu <i>et al.</i> 2021)

NA	the interphase thickness is of the order of 80 nm, while the BN nanoparticle radius is around 20 nm.	low density polyethylene (LDPE)/ boron nitride (BN) spherical nanoparticles	Experimental AFM, PF-NM/electrostatic 3D FEM model, (Villeneuve-Faure <i>et al.</i> 2022)																		
$E_c \approx E_m \left[1 - \frac{t}{T} + \frac{s^2}{12} \frac{\eta_o \eta_a}{(1 + \nu)} \left(\frac{t}{T} \right)^2 \right]$ $\eta_l = \left[1 - \frac{\tanh(ns/2)}{ns/2} \right]$ $n = \sqrt{\frac{2G_m}{E_{eff}}} \frac{t}{T} \text{ and } G_m = \frac{E_m}{2(1 + \nu)}$ G_m, E_m , ν - matrix shear and Young's moduli and Poisson's ratio; T - thickness of the polymer/filler interphase; η_0 varies from 8/15 for randomly oriented to 1 for highly oriented NP; η_l goes from 0 to 1; agglomeration factor η_a varies from 0 to 1; s and t are the aspect ratio and the thickness of the NP	 Interphase thickness T determination <table><thead><tr><th></th><th>GO</th><th>MoS₂</th></tr></thead><tbody><tr><td>T_0</td><td>87.8</td><td>67.6</td></tr><tr><td>A</td><td>340.1</td><td>512.7</td></tr><tr><td>R_0</td><td>-6.29</td><td>-51.6</td></tr><tr><td>R^2</td><td>0.944</td><td>0.983</td></tr><tr><td>$T = T_0 + A \exp(R_0 \phi_f)$</td><td></td><td></td></tr></tbody></table> mass fraction (w_f) and volume fraction (ϕ_f) of the obtained NC		GO	MoS ₂	T_0	87.8	67.6	A	340.1	512.7	R_0	-6.29	-51.6	R^2	0.944	0.983	$T = T_0 + A \exp(R_0 \phi_f)$			PVB/GO, PVB/MoS ₂	Experimental and micromechanical analysis model, (Cremonezzi <i>et al.</i> 2023)
	GO	MoS ₂																			
T_0	87.8	67.6																			
A	340.1	512.7																			
R_0	-6.29	-51.6																			
R^2	0.944	0.983																			
$T = T_0 + A \exp(R_0 \phi_f)$																					
graded interphase is calculated as: $E^{Int} = \frac{1}{1 - \alpha} \int_{\alpha}^1 \left[E^{GNP} - (E^{GNP} - E^m) \left(\frac{r - \alpha}{1 - \alpha} \right)^q \right] dr,$	For interphase thickness of 90 nm, model results show excellent agreement with the experimental results.	Gr NPlates/ Epoxy polymer	3D micromechanical model, graded interphase, (Mehdipour <i>et al.</i> 2024)																		
Defines “stress transfer coefficient” – mean and for each layer for estimate STE:  The strain transfer coefficient is given as $\beta = \frac{\varepsilon_g}{\varepsilon_h} = 1 + (q - 1) \frac{\cosh(kx)}{\cosh(kL_g)}$	NA, line interfaces	5 layers NC (incl.interfaces), gr/PDMS is a sensitive layer, PDMS for the rest layers	Analytical strain transfer model with quadratic distribution of shear stress in each layer, effect of coating accounted, FEM, (Weng <i>et al.</i> 2024)																		

Meanwhile, the average strain transfer coefficient is $\alpha = \frac{2 \int_0^{\frac{L_g}{2}} \varepsilon_g(x) dx}{\varepsilon_0 L_g} = 1 + (q - 1) \frac{2 \sinh\left(k \frac{L_g}{2}\right)}{k L_g \cosh\left(k \frac{L_g}{2}\right)}.$			
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In conclusion, it can be said that the properties and geometric characteristics of the interfacial layer in NCs are a subject of considerable interest both at the experimental and theoretical levels. At present, there is still no method for direct measurement/identification of this layer; there are many theoretical hypotheses about its properties and size. The currently available experimental and theoretical data are summarized and analyzed. There are too many factors that influence the dimensions and properties of the interface/interphase zone. Regardless of the above, the interfacial zone at NCs exists and should be considered in the modeling of design and stress transfer efficiency of both existing and newly created NCs, especially in terms of their ever-increasing number of industrial applications.

2. Parametric (sensitivity) analysis in modeling of NC

The parametric analysis (PA), also known as *sensitivity analysis*, is the study of the influence of different geometric or physical parameters or both on the solution of the problem. Parametric analysis is an important tool for design exploration (*Parametric Analysis vs. Optimization*, 2021). Parametric study is, actually, an elementary form of optimization in which, at each step, one or two of the parameter values are optimized, while the others are kept constant (Stevanović, 2013). This analysis still produces a locally optimal solution.

Nevertheless, in the context of the NC modeling, PA assures an important information for the influence of distinct factors (geometrical, physical, etc.) when modeling and simulating the NC behaviour, independently from the experiments and before manufacturing of devices with NC parts (Vinay *et al.* 2023).

Table 2 summarizes the works found so far, in which an analysis (parametric or for sensitivity) of the factors influencing the main mechanical characteristics of NCs or their behavior has been made. It is noteworthy that a similar analysis was made mainly for graphene-polymer NCs (Lu *et al.* 2021; Manta, 2018; Mehdipour *et al.* 2024; Weng *et al.* 2024; Gong *et al.* 2012; Xu *et al.* 2016; Heidarhaei *et al.* 2017, 2018; Kirilova *et al.* 2018;

Petrova *et al.* 2018; Cui *et al.* 2022; Liu *et al.*, 2022; Apostolov *et al.* 2022, 2024; Vladova *et al.* 2022; Du *et al.* 2022; Peng *et al.* 2024). One work with graphene and a Cu substrate was also found (Kim *et al.* 2021), in which the influence of the substrate thickness and the graphene content on ISS in NCs was considered.

In another group of publications (Zahedi *et al.* 2019; Kim *et al.* 2021; DeviSingh, 2020; Khorasani *et al.*, 2021; Li and Hu, 2023; Zeinedini, 2024; Zhang *et al.* 2024) the influence of various factors (particle volume fraction, length, arrangement/distribution, aspect ratio, NP length, interphase thickness and properties, substrate thickness, aggregation, deboned NP, etc.) on the characteristics of NPs from the older types NCs, such as Si, CaCo₃, Al₂O₃, ZrO₂, Si₃N₄, nano-fibers, nanoclay, carbon nano tubes (CNT) and others, is analyzed.

The influence of the nanoparticle length in the NC, as well as other factors on its properties, especially on the stress transfer in the NC, on interfacial strength, etc., for other than graphene 2D materials has been investigated in far fewer publications. For example, information about the factors influencing NC behaviour with WS₂ is available in (Kirilova *et al.*, 2023; Wang, 2017; Wang *et al.* 2020; Wu *et al.* 2024; Tang *et al.* 2021). For NC with BNNT - in (Gou and Ke, 2019; Yi *et al.* 2019), for NC with hBN - in (Wang *et al.* 2021), for NC with MoS₂ - in (Du *et al.*, 2022; Liu *et al.* 2014; Chae *et al.* 2022; Vladova *et al.* 2024). For NC with Ti₃C₂ Mxene information on factors influencing the stress transfer is available only in (Liu *et al.* 2022a). It can definitely be said that the length of the graphene flake/s has a very significant influence on the ISS and on the stress transfer in the NC, respectively, on the magnitudes of variables/quantities with which the latter is expressed, as can be seen from *Table 2* (Weng *et al.* 2024; Gong *et al.* 2012; Xu *et al.* 2016; Heidarhaei *et al.* 2017, 2018; Kirilova *et al.* 2018; Liu *et al.* 2022; Apostolov *et al.* 2022, 2024; Du *et al.* 2022; Peng *et al.* 2024). It is important to note two main facts here: the researchers are advised to use longer flakes to better strengthen the NC and reduce/retard debonding if it has started; the second fact states that after a certain flake length no dependence between ISS or stress transfer and length is observed. As for the remaining 2D materials, despite the scarcer literature data in *Table 2*, the above trend also applies to them, recommending the use of thicker (several layers) and longer flakes of WS₂, MoS₂, hBN, Ti₃C₂ Mxene (Liu *et al.* 2022; Kirilova *et al.* 2023; Wang, 2017; Wang *et al.* 2020; Vladova *et al.* 2024). However, it should be noted that graphene flakes have weaker interlayer bonds in contrast

to the other 2D nanomaterials, for example hBN (Wang *et al.* 2021), and during the loading stage they begin to slide, which greatly reduces the interlayer stress, and the stress transfer between graphene and other nanomaterials in the nano heterostructures (Du *et al.* 2022; Wu *et al.* 2024). Therefore, in the design of such structures, it is recommended to first simulate and find the optimal combination of materials, as well as the optimal geometry, before fabricating and testing the corresponding device containing the simulated nanostructure (Petrova, 2023; Tang *et al.* 2021).

One of the great challenges for scientists is still the study of the influence of the interfacial zone (more precisely, its thickness and properties) on the mechanical characteristics of NCs. Mainly, the reason is because the direct experimental measurement of the value of the interface shear stress is not yet possible (Wang and Liu, 2023a). The modeling of the NC interfacial zone is the only way, by which the scientists could procure with information about the stress transfer in the NC and, accordingly, about the efficiency of the same. As mentioned, this zone significantly affects the formation and development of the process of debonding/delamination and crack formation in NC (Zahedi *et al.* 2019; Mehdipour *et al.* 2024; Heidarhaei *et al.* 2017, 2018).

At present, scarce (mostly theoretical prediction from shear-lag and its non-linear variants) information is available on the maximum value of ISS or the so-called ISS strength obtained for different NC structures (Du *et al.* 2022; Yi *et al.* 2019; Dong *et al.* 2023). It is known that an approximate theoretical value for ISS can be obtained from shear-lag and its derivative models (Gong, 2012), considering that the interface zone is a material line for the elastic zone and after this zone, in the softening/sliding or cohesion zone, the ISS value must be calculated/modeled in another way – for example, through a cohesion model (Lu *et al.* 2021; Kirilova *et al.* 2018; Petrova *et al.* 2018; Peng *et al.* 2024), or through a balance of forces at the interfaces (Du *et al.* 2022), etc. In (Zhang *et al.* 2024), an approximate formula for calculating the “interfacial debonding strength” for NCs with metallic spherical NPs was recently reported; this quantity depends quadratically on the properties of the matrix E and ν , as well as on the interfacial fracture energy and the radius of the NP. A similar value, “critical debonding stress” was also analytically derived in (Zeinedini, 2024), when modeling the behavior of polymer NPs with spherical NPs - silica nanoparticles/epoxy, CaCO_3 nanoparticles/high density polyethylene, and silica nanoparticles/photopolymer. As can be seen from *Table 2*, for fixed

properties and width of the interface zone, this value decreases as the external load decreases; respectively, at a fixed load, it grows with increasing interface strength and thickness.

The presence of an additional layer (adhesive, glue) to act as an interphase layer between the NM and the matrix is also of great importance in the stress transfer and debonding process (Peng *et al.* 2024; Li and Hu, 2023; Gong, 2012). The observations are that this layer improves the stress transfer, but also determines the behavior of NC under load - rapid delamination or progressive crack propagation; for example, the debonding process is much faster for the Gr/Fo/PDMS interface (Peng *et al.* 2024).

The influence of the properties and geometry of the substrate layer on the ISS and the properties of the entire NC has been studied for three types of NC – with graphene, with MoS₂ and with WS₂ (Weng *et al.* 2024; Heidarhaei *et al.* 2017, 2018; Kirilova *et al.* 2018, 2023; Apostolov *et al.* 2022, 2024; Vladova *et al.* 2022; Wang *et al.* 2020; Tang *et al.* 2021; Liu *et al.* 2014). In Kirilova *et al.* (2018) by a cohesive shear-lag model for graphene/PET, the model interface shear stress is found to be not affected by the host substrate layer thickness. Probably, it is due to the constrained functions and their arguments in the description of the model ISS in both elastic and cohesive model zones. The works Heidarhaei *et al.* (2017, 2018) show, that the matrix elastic modulus can affect the first critical stress when loading Graphene/epoxy NC. According to the 2D stress-function model, applied for the graphene/SU-8/PMMA, graphene/SU-8/PET, graphene/MoS₂/PET and WS₂/SU-8/PMMA NC structures (Apostolov *et al.* 2022, 2024; Kirilova *et al.* 2023) the delamination (or the critical value of ISS) depends on the polymer matrix thickness. About delamination in graphene/SU8/PMMA NC - it has been found out that for thinner PMMA layer the delamination could be observed over 350 MPa external load; for a thicker one it could be seen over 750 MPa (Apostolov *et al.* 2022). In the next work Apostolov *et al.* (2024), more detailed analysis was performed for graphene/SU-8/PET and graphene/MoS₂/PET NC; it was shown, that when the thickness h_2 decreases, the ISS increases. Recently, in the work of Weng *et al.* (2024) a NC with 5 layers, including interfaces, where graphene/PDMS is a sensitive layer and PDMS - for the rest layers, is modeled; the stress transfer coefficient introduced by these authors is found to decrease, when the thickness of the substrate increases, the measured strain in the sensitive layer decreases prominently.

For NC MoS₂/PET in (Vladova *et al.* 2024) it is concluded that for a PET thickness after 50 μm a delamination cannot appear. For the other NC

MoS₂/PDMS investigated earlier (Liu *et al.* 2014) these authors reported that Young’s modulus of the matrix has to be over 1 GPa to ensure 90% stress transfer efficiency (STE) in NC. In (Kirilova *et al.* 2023) for WS₂/SU-8/PMMA it was mentioned, that for a considered thinner (10⁻⁷m) polymer matrix layer the delamination is not observed even for an applied load over 5 GPa, on the contrary to the thicker one (10⁻⁵m) when it appears after applied load of about 1.175 GPa. In (Wang *et al.* 2020) for the same NC structure a shear-lag model recommended for better stress transfer is to use high values of *ns*, i.e. using stiffer substrates (with higher *G_m* values leading to a higher *n*) and long WS₂ flakes with high aspect ratios *s*.

Last, but not least, is the influence of external factors like temperature difference and humidity on the ISS or debonding in NC (Tian *et al.* 2024; Vladova *et al.* 2022, 2024; Apostolov *et al.* 2024; Zhang *et al.* 2024; Tang *et al.* 2021; Chae *et al.* 2022). Swelling of the substrate or high humidity shows influence on the crack-formation in 2D materials; they propagated deep into the substrates. For graphene/polymer and WS₂/polymer NC (Vladova *et al.* 2022, 2024; Apostolov *et al.* 2022, 2024) the temperature has little effect on the delamination, except in the case of an extreme cooling load in combination with a limit value for mechanical loading, at which delamination begins; at these conditions cooling can retard delamination. It should be noted, that in the case of heating and mechanical loading the overall effect is additive. Also, the effect of temperature is more clearly visible for strains in the polymer layer than in graphene.

Table 2: Literature data for studies including PA of factors, influencing NC properties, stress transfer efficiency and debonding in NC

Factors and facts, influencing properties, stress transfer and debonding in NC	Source, NC
- An effective stress transfer and reinforcement are possible at graphene flake length > 30 μm; - If the number of graphene layers and polymer thickness increase, the effective Young modulus of NC decreases; - Additional SU-8 layer improves the stress transfer in NC.	Gong (2012), Graphene/ /SU-8/PMMA
- Increasing the substrate modulus could significantly increase the strain in MoS₂ layer, if a high-quality interface is preserved. A substrate with a modulus >1 GPa may effectively transfer almost 90% of the applied strain to monolayer MoS₂.	Liu <i>et al.</i> 2014, MoS ₂ /PDMS

- The length of the graphene layer significantly affects the stress transfer between the layers of the NC and specifically, τ and the strain in graphene ε; - As the length of the graphene flake/layer increases from 20 to 10000 μm, the interfacial tension τ decreases until complete exfoliation occurs. The interfacial mechanical properties of graphene less than 20 μm long are extremely sensitive to its length, while for graphene longer than 1000 μm they are no longer size dependent; - As the loading in the PET substrate increases, the strain ε in the graphene linearly increases until reaching a sliding mode and a retention plateau, after which exfoliation of the graphene flake/layer follows.	Xu <i>et al.</i> 2016, Graphene/PET
- No reinforcement is expected for flakes $< 4 \mu\text{m}$ in diameter, some reinforcement is expected at $> 4 \mu\text{m}$ and large WS_2 flakes; - About $\sim 40 \mu\text{m}$ are required for full reinforcement to take place. For good reinforcement to occur, the length of fiber should be $\sim 10 L_c$ (L_c is found to be $\sim 4 \mu\text{m}$ for monolayer WS_2); - The interlayer slippage of a few layers WS_2 has been found to be a significant factor that compromises the reinforcing effect.	Wang (2017), $\text{WS}_2/\text{SU8/PMMA}$
- The interfacial shear stress, graphene volume fraction and interfacial fracture energy affect the damage and debonding initiation; their variation does not influence them at near center of the interface; - According to the analytical relations, the matrix elastic modulus can affect the first critical stress; - By increasing the shear strength of the interface, damage initiation retards for the graphene sheets with lengths $> 50 \text{ nm}$ and for smaller lengths, the interfacial shear strength impresses the first critical stress imperceptibly; - After damage initiation at the interface, stress transfer is affected slowly by increasing the applied stress only at the end of graphene; - When the applied stress reaches the second critical stress, debonding progresses at 75% of the length of graphene matrix interface; but the central region of the interface has large resistance against debonding.	Heidarhaei <i>et al.</i> 2017, 2018, Graphene/epoxy
- The rise of the aspect ratio (AR) leads to significant decrease in the resistance; after $\text{AR} > 50$ the effect is negligible; - The graphene shape did not affect the trend of the NC electrical response the rectangular filler exhibited lower percolation threshold than that obtained for the elliptical graphene filler;	Manta (2018), Graphene/epoxy and PA6

- Increasing volume fraction (V_f) of nanoparticles arises two main phenomena in the NC structure with opposing effects on the electrical conductivity – the formation of conductive paths and the formation of agglomerations. For V_f around the percolation threshold, the increase of conductive paths has greater influence on conductance compared to the limited formation of agglomerations; - If the interphase thickness and stiffness increase, the properties of whole NC increased too.	
- If the value of initial displacement u_0 increases, the length of cohesive zone decreases, so the interfacial debonding length d increases; - Increasing the length of the structure, the cohesive length increases too, and respectively, the delamination length decreases; - Influence of the thickness of host layer on ISS is negligible.	Kirilova <i>et al.</i> 2018, Graphene/PET
- Increasing the external load, maximal values of strain in graphene decrease and delamination (debonding) increases.	Petrova <i>et al.</i> 2018, Graphene/PET
- The interphase characteristics such as its thickness and elastic modulus, have significant influences on the critical energy release rate; - There is a considerable effect of the interphase thickness on the crack behavior.	Zahedi <i>et al.</i> 2019, Nanoclay/epoxy
- The occurrence of pull-out event influences the deformation either in a purely plastic or a mixed elastic–plastic manner, which depends on the embedded nanotube length; - Critical embedded length is about 386 nm for the BNNT–PMMA interface, and about 483 nm for the BNNT–epoxy interface.	Gou and Ke (2019), BNNT/PMMA and epoxy
- The average interfacial shear stress reaches about 34.7 MPa; - The obtained maximum IFSS of BNNT-silica interfaces of about 1.25 GPa is much higher than the reported values for BNNT-PMMA and BNNT-epoxy interfaces (i.e., 219 MPa and 323 MPa), indicating a much stronger interfacial binding interactions of BNNTs with silica versus with those two polymers.	Yi <i>et al.</i> 2019, BNNTs from silica /silicon dioxide)
- The stress transfer efficiency is controlled by the parameter ns and the interaction of the WS₂ flake with the substrate PMMA. Better stress transfer is given by high values of ns, i.e. using stiffer substrates (with higher G_m values leading to a higher n) and long flakes with high aspect ratios s; - The critical length for the monolayer WS₂ flakes was found to be 4 μm; - The stress can be transferred effectively to thicker WS₂ flakes in PVA NC.	Wang <i>et al.</i> 2020, WS ₂ /SU-8/PMMA and LPE WS ₂ /PVA

- Longer fibers assured better E and stiffness of the entire NC; - It is found that the nanofibre/matrix debonding can be attributed to the high stress concentrations at the nanofibre ends which can be made more severe with poor interfacial shear stress transfer; - The interface should not be too strong and not too weak to produce an optimized stress transfer. The formation of stress concentrations at the fibre/matrix interface can be regarded as an indication of good matrix to nanofibre stress transfer.	DeviSingh, 2020, nanofiber/matrix
- The strength of the graphene/Cu composites does not increase if the Cu thickness increases. Rather, an increase in Cu thickness in the same tensile direction reduces the strength performance of the graphene/Cu composites; - When the volume fraction of graphene increased, the stress distribution of Cu also increased.	Kim <i>et al.</i> 2021, Graphene/Cu
- The efficiency of internal stress transfer between the different hBN layers was found to be of the order of 99% compared to 60%–80% for graphene, as a result of the stronger bonding between the hBN layers in the BNNSs; - It is found that the ISS between the BNNS and the substrate is of the order of 10 MPa, a factor of around 4 times higher than that for a graphene monolayer; - The critical AR for stress transfer to the substrate is only ~ 350 for BNNSs compared with $>10^4$ for monolayer graphene implying that better stress transfer to the substrate can be achieved with hBN nanosheets.	Wang <i>et al.</i> 2021, BNNS/PMMA
- Elastic modulus of NC rises with changes in geometry. The wrinkling of graphene increases also the stiffness of NC, as well as the increasing of interfacial cohesion by chemical route such as grafting of graphene; - The identification procedure revealed the existence of an interphase on either side of the graphene with a thickness of 1 nm, which is one and a half times stiffer than the polymer bulk matrix.	Lu <i>et al.</i> 2021, Graphene/ polymeric glass, 5 layers, 2 interphases with thickness 1 nm
- As the polymer substrate swells (bi-axial strain), the fracture of the system is initiated with the crack-formation in 2D materials; - Efficient strain transfer from the substrate occurs when MoS_2 reaches a critical size of 4 μm. For graphene it is 1-2 μm.	Chae <i>et al.</i> 2022, Graphene/ PMMA and MoS_2 /PMMA
- The critical length L_c characterizes the transfer efficiency of the interface; the smaller the value of L_c, the higher the load transfer efficiency. The critical length obtained for MoS_2/PET is 28 μm. The critical transfer length for Graphene/MoS_2/PET is 48 μm;	Du <i>et al.</i> 2022, Graphene/ MoS_2 / /PET with 2 interfaces and MoS_2 /PET, 1 interface

- The presence of the upper graphene influences the interface between the lower MoS₂ and PET; the strain in the central stable region of graphene was not equal to that of the lower MoS₂, indicating that the strain of the lower MoS₂ is not completely transmitted to the upper graphene; - The upper graphene entered the sliding stage earlier than the lower MoS₂, which indicated that the interface properties of the Gr/MoS₂ interface and the MoS₂/PET interface were different; - The interface strengths of the MoS₂/PET interface and the Gr/MoS₂ interface obtained are 0.34 MPa and 0.19 MPa, respectively.	
- The number N of MoS₂ layers affect the effective Young's modulus E of NC if $N > 7$; - The strains and ISSs in 1 and 2 layers MoS₂ are comparable, but the transfer lengths rise when N rises; - For MoS₂ the transfer length required for efficient stress transfer will increase with N and large lateral sizes; - The values of ISS, critical length and transfer efficiency for graphene, MoS₂, WS₂, hBN and Ti₃C₂Mxene, are presented in Table 2 in (Dong <i>et al.</i> 2023).	Dong <i>et al.</i> 2023, 1/2/3layer MoS ₂ /substrate
- Ti₃C₂Mxene offers an efficient mechanical reinforcement to a polymer matrix with a flake length of $>10\ \mu\text{m}$ and a thickness of 10s of nanometers; - An effective aspect ratio of the order of >500 (achievable in 1–10 layer MXene flakes) is expected to facilitate good interfacial stress transfer.	Liu <i>et al.</i> 2022a, Ti ₃ C ₂ Mxene/PMMA
- Optimal functionalization and length are important factors in NC design – (synergetic effect!!!); - Oxidation of graphene nanofillers influences the interfacial shear strength.	Cui <i>et al.</i> 2022, GO/PMMA
- Under uniaxial tension, the two layers of BLG show three sequential stages: simultaneous deformation, top layer sliding and the failure of the interface; - The obtained ISS exhibits an inverse proportionality on the size of BLG, and strain is in direct proportionality with size of graphene.	Liu <i>et al.</i> 2022, Bi-layer graphene/ formvar/PDMS
- The magnitude of the applied tension load influences strongly the appearance of delamination in the structure; - For thinner PMMA layer the delamination could be observed over 350 MPa external load; for thicker PMMA it could be seen over 750 MPa. If the structure length decreases, under the above-mentioned conditions, the delamination begins at slightly lower values of the tension load; - The magnitude of the applied load influences also the value of the debond length.	Apostolov <i>et al.</i> 2022, Graphene/SU-8/ PMMA

- Delamination doesn't appear at fixed WS₂ length of 10 μm, if the loading is up to 5 GPa for thinner substrate and up to 1.175 GPa for thicker one, respectively; - With increasing WS₂ length, the delamination occurs at increasingly higher values of the applied external load, for thicker matrix; for thinner one a delamination does not occur; - At fixed applied load, it was found for thicker substrate, that as the length of WS₂ increases, the debonding length increases.	Kirilova <i>et al.</i> 2023, WS ₂ /SU-8/PMMA
- Applying a thermal loading (heating, $\Delta T > 0$) or mixed (thermomechanical) loading, all resultant strains in the structure layers show the same behavior like the mechanical ones, with slight increase in amplitude due to difference in CTE of graphene and PMMA. This is better visible for axial and peel strains.	Vladova <i>et al.</i> 2022, 3-layer graphene/PMMA
- The formvar layer determines the NC behavior - rapid delamination or progressive crack propagation. The former depends on the τ_{max}, L, ε_0, and the latter on L; - The decohesion behavior of the frictional adhesive interface is governed by three dimensionless parameters. Particularly, the dimensionless length of the graphene film essentially determines the decohesion rate; while the other two parameters (ISS strength and λ) affect the critical substrate strain to initiate debonding; - The shear strength τ_{max} and the relative length of full friction slip stage λ of the Gr/Fo/PDMS interface are much larger than those of the Gr/PDMS interface. Also, the dimensionless length of the Gr/Fo/PDMS interface is much larger than that of the Gr/PDMS interface. Therefore, the debonding process is much rapider for the Gr/Fo/PDMS interface.	Peng <i>et al.</i> 2024, Graphene/Formvar/PDMS)
- PA is performed for Poisson's ratio, aspect ratio, interphase thickness and elastic modulus on stresses and ISS. When interphase thickness increases, stresses and ISS decreased, $T=0.4$ mm is critical.	Li and Hu (2023), (three-layer composites)
- The factor with the strongest effect on ISS and delamination in the graphene/polymer NC structures is the magnitude of the applied external mechanical load; - According to the degree of influence, they can be arranged as: thickness of the polymer matrix, thickness of the graphene layer. The thickness of the middle interface layer was found to be negligible; - The temperature has little effect on delamination, except in the case of a large cooling load in combination with a limit value for the mechanical one, at which delamination begins;	Apostolov <i>et al.</i> 2024, graphene/SU-8/PET, graphene/SU-8/PMMA, graphene/MoS ₂ /PET

- The length of the overlap zone has the least influence on the delamination, after 30 μm.	
- It is found that the interface thickness does not affect the ISS value; - The magnitude of the applied mechanical load has a strong influence on the magnitude of the ISS; - The temperature difference (pure thermal loading) also affects the ISS value, but to less extent. It should be noted, that in the case of combined loading (thermo-mechanical) the overall effect is additive; - The impact of the length l on the ISS is seen up to 90 μm; after $l > 90 \mu\text{m}$ - at fixed layers' thicknesses and load, the delamination does not arise. The maximal value of ISS is reached at $l=15 \mu\text{m}$ and then remains unchanged, up to 90 μm; - The thicknesses of MoS₂ and PET mostly affect the type of ISS solution, especially the substrate thickness.	Vladova <i>et al.</i> 2024, MoS ₂ /Int/PET
- The presence of a hygrothermal environment delivers lower levels of stiffness and critical buckling load; - The presence of clusters or CNTs' concentrated regions has a beneficial effect on the mechanical behavior of such models.	Khorasani <i>et al.</i> 2021, PMMA and CNT/FGM/PMMA, Functionally graded materials (FGM) are Al ₂ O ₃ , ZrO ₂ , Si ₃ N ₄ , Al
- The decline in composite modulus at elevated temperature is caused by the combination of the decreases in matrix and fiber modulus and an increase in the number of debonded particles; - Increasing the NP V_f to improve the modulus of composites is a double-edged sword, since although initially harder, MPCs with higher particle volume fractions ultimately become inferior to those with lower V_f as the proportion of debonded particles increases; - Increasing the particle modulus can play a role when debonding does not occur or when the proportion of debonded particles is small, but when the particles are almost completely debonding, this method will fail.	Zhang <i>et al.</i> 2024, (metal particles composite, Si/Al) Size dependent equation for theoretical interfacial debonding strength, for nanospheres (see eq.31 in source)
- For the silica/epoxy NCs, at a certain normalized Young's modulus of the interphase, the normalized debonding stress was decreased by enhancing the loading rate. Under a certain loading rate, the normalized debonding stress enhances as much as the stiffness of interphase material increases; in the presence of stiffer interphase, the critical debonding stress increases; - For both silica/epoxy and CaCO₃/HDPE systems, the normalized debonding stress was reduced by increasing the	Zeinedini, 2024, (Si/epoxy, CaCO ₃ /HDPE, Si/photopolymer)

strain rate at a certain size of the NP. By increasing the size of NP, the normalized debonding stress was reduced significantly; - In the case of CaCO₃/HDPE NC, the normalized debonding stress is enhanced by increasing the normalized interphase radius at any loading rate. At a certain interphase radius, the normalized debonding stress is decreased as the loading rate enhances; - For the nano-silica/photopolymer NC, the Young's modulus of the interphase has a major effect on the normalized debonding stress at any strain rate. For the interphase material with lower Young's modulus, the normalized debonding stress was not influenced by the applied strain rate. Under different strain rates, it is suggested to reinforce the NC with the smaller NP as much as possible.	
- For a specific value of graphene nanoplatelet V_f, the mechanical properties of polymer NC are at the best state. By increasing the V_f beyond the specified graphene content value, the effective properties of graphene are reduced; - The size of graphene nanoplatelets and the thickness and characteristics of the graphene/polymer interphase region have a direct effect on the properties of the NC; - The influence of the GNP interphase thickness on the elastic modulus of the NC diminishes as GNP aggregation increases; - For interphase thickness of 90 nm excellent agreement with the experimental results is demonstrated.	Mehdipour <i>et al.</i> 2024, (Gr Platelets/ Epoxy polymer, graded interphase)
- As the thickness of the substrate increases, the measured strain decreases prominently. The average strain transfer coefficient is also found to decrease as the thickness of the substrate increases; - As the length of the strain gauge decreases, the length of the fully transfer section also decreases, leading to a decrease in the average strain transfer coefficient; - As the thickness of the coating increases, the efficiency of strain transfer indicated a slight linear decrease; - The strain transfer coefficient reaches 0.95 when the coating extends beyond 10 mm at both ends, enabling the flexible sensor to accurately reflect the true structural strain. $\beta = \frac{\varepsilon_g}{\varepsilon_h} = 1 + (q - 1) \frac{\cosh(kx)}{\cosh(kL_g)}$	Weng <i>et al.</i> 2024, (NC with 5 layers, incl. interfaces, Gr/PDMS (sensitive layer) and PDMS for the rest layers)
- Mechanical properties of DLNS deteriorate when compared to those of monolayer WS₂; - Mechanical properties of graphene/WS₂ (layer) composite with both layers deformed are superior than those of WS₂, even though inferior than those of bare graphene. If stress	Wu <i>et al.</i> 2024, (heterostructures: double layer WS₂ nanosheet (DLNS), graphene/WS₂ (layer))

is applied only to the graphene layer, the graphene/WS₂ composite retains most of the strength and toughness of monolayer graphene, decreasing the fracture strength and Young's modulus by only 9.7% and 16.3%, respectively; - In the case of the graphene/WS₂ NT composite the mechanical strength and toughness experience a reduction compared to monolayer graphene, specifically by 15% and 53% for fracture strength and Young's modulus, respectively.	composites and graphene/WS₂ nanotube (NT) composites)
- Temperature plays an essential role in deciding strain sensor performance, as high temperature results in better ductility but strength. Also, a peak of elastic modulus is found at 500 K; - The gauge factor of sensor depends on the electronic properties of WS₂ as well as the mechanical properties (dimensions and Young's modulus) of the substrate; - For flexible WS₂ device - it is better to choose one substrate with low <i>E</i> to achieve a higher gauge factor (GF); - As the strain increased, the current of the sensor gradually increased, which was verified with the DFT results; the conductivity consequently increases.	Tang <i>et al.</i> 2021, WS₂ strain sensor based on PET

In conclusion, it can be said that the performed analyses give us very valuable information about the influence of various factors determining the important characteristics of NCs from the point of view of their industrial applications - mechanical, optical, electrical and other valuable NC properties. A parametric study can and has to be provided in the design of the experiment for the study of NC properties; it helps to reduce the number of experiments and determines the influence of different factors on the quantities we are interested in, as well as the relationships between individual factors. In the presence of a model for NC behaviour, the PA gives us valuable information that cannot yet be obtained experimentally. Based on the reviewed articles in *Table 2*, it should be concluded, that the length, thicknesses of the layers in NC, temperature, material properties of substrate and interphase are general factors, that have influence on the stress transfer and delamination in NC.

3. Results from PA for ISS in the investigated NC structures under project KII-06-H57/3/2021

Here the results from parametric analysis are presented to determine which factors influence the delamination in the nanostructures, considered in the

previous Chapter 1 (section for 2D stress-function model results), as well as these from the abovementioned project works (second stage, after 2022). The criterion for delamination in a 3-layer NC structure is when the model interface shear stress (ISS) exceeds the critical value of the shear stress at tension (or ultimate tensile shear strength) in its middle layer:

$$\sigma_{xy}^{(a)}(x) = h_1 \sigma_1' \geq \sigma_{USS}^{(a)} \tag{1}$$

In this section, the influence of the following parameters on the model ISS - ($\sigma_{xy}^{(a)}$) under criteria Eq. (1) is studied: the influence of the NC structure length (l), the influence of the layers thickness (h_1, h_a, h_2), the influence of external loading (σ_0 and/or ΔT). The principle of performing PA is to vary one of the parameters, fixing the values of the others and checking what is its influence on the ISS. The material properties of the NC structures considered below are shown in *Table 3*.

Table 3: Layers’ material properties of NC structures & studies sources

Case studies, source	Young’s modulus E, GPa			Poisson’s ratio ν , -			USS, MPa
graphene/SU-8/PMMA, Apostolov <i>et al.</i> 2022, 2024	1000	2	3.5	0.13	0.22	0.35	30
graphene/SU-8/PET, Apostolov <i>et al.</i> 2024	1000	2	2.3	0.13	0.22	0.43	30
graphene/MoS ₂ /PET, Apostolov <i>et al.</i> 2024	1000	270	2.3	0.13	0.25	0.43	0.26
WS ₂ /SU-8/PMMA, Kirilova <i>et al.</i> 2023	270	2	3.5	0.22	0.22	0.35	
3-layer graphene/ SU-8/PMMA, Vladova <i>et al.</i> 2022	1000	2	3.5	0.13	0.22	0.35	30
MoS ₂ /Interphase/PET, Vladova <i>et al.</i> 2024	270	3 ÷ 11*	2.3	0.25	0.34**	0.43	0.26

*simulated, not influence on the ISS; **mean value of Poisson’s ratios other 2 layers.

All calculations of the model ISS during the PA are performed in developed Mathcad Prime programs, the graphics were generated by Sigma Plot, v.13.

Results of PA for Graphene/SU-8/PMMA

In the paper [50] the PA is made for the influence of σ_0 and graphene length l on the ISS for two different geometries of layers' thicknesses, corresponding to both model solutions for ISS (for real and complex roots – for details see the *Table 4* and Chapter 1). The graphene length is $l=12\text{ }\mu\text{m}$, unless otherwise noted. The properties of the layers' materials and USS are settled in *Table 3*.

It was found that in the thinner PMMA layers (Case 1) – see *Table 4*, of the considered NC graphene/SU-8/PMMA, the delamination can be observed at values of external load $\sigma_0 \geq 350\text{ MPa}$, while in the thicker layers (Case 2) it occurs for $\sigma_0 \geq 50\text{ MPa}$, at a fixed value of the length l (Fig. 4, (a), (b)). The delamination starts simultaneously from both ends of the structure and graphically the debond length corresponds to the intersection of the model $\sigma_{xy}^{(a)}$ with the critical value (red line).

Table 4: Geometry configuration and details for calculated model solutions for ISS in adhesive layer of nanocomposite structure graphene/SU-8/PMMA

Case	$h_1, \text{ m}$	$h_a, \text{ m}$	$h_2, \text{ m}$	Discriminant for quadratic equation**	Roots of quadratic Equation*
Case 1	0.35×10^{-9}	1×10^{-8}	2×10^{-6}	4.38×10^{24}	1.333×10^{13} ; 1.123×10^{13}
Case 2	0.35×10^{-9}	4×10^{-8}	1×10^{-5}	-3.681×10^{24}	$(4.942 \times 10^{11}) \pm$ $i \cdot (9.593 \times 10^{11})$

*, ** - characteristic equation of ODE in Chapter 1

The value of the calculated debond length (i.e, solution for x for equality in Eq. (2.3.1)) for the maximal applied load (3.5 GPa) is about $1.5\text{ }\mu\text{m}$ for Case 1 and $3.5\text{ }\mu\text{m}$ for Case 2. The maximum of the ISS in both solutions is reached for the values comparable to those obtained in (Anagnostopoulos *et al.* 2015), for the graphene/SU-8/PMMA - about $2\text{ }\mu\text{m}$ (Fig. 4).

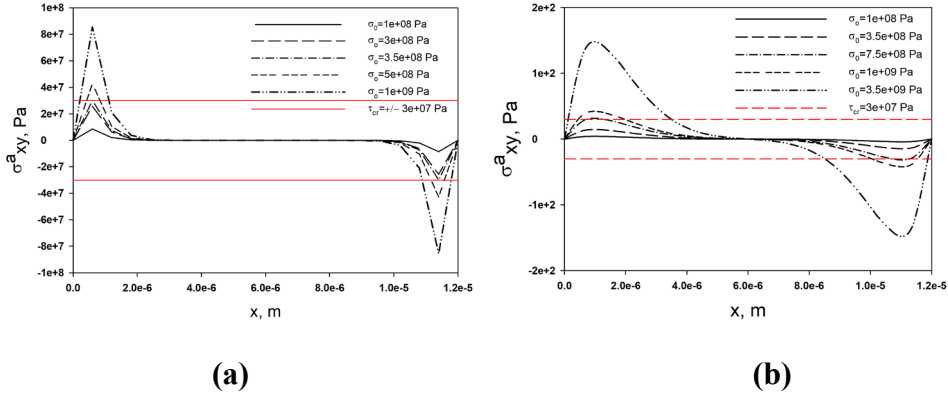


Figure 4: Influence of the magnitude of applied mechanical load σ_0 on the interface shear stress in adhesive layer, for (a) Case 1 solution and (b) – Case 2 solution.

The other part of the parametric analysis in (Apostolov *et al.* 2022) is connected with the influence of the structure length l on the delamination in it. Four different structure lengths (from 6 to 30 μm) were tested to analyze this influence and to determine the critical magnitude of the applied load, after which a delamination will occur. The results are presented in *Table 5*.

Table 5: Critical magnitude of applied load, over which delamination appears for various structure lengths

Case	$l = 6 \mu\text{m}$	$l = 12 \mu\text{m}$	$l = 20 \mu\text{m}$	$l = 30 \mu\text{m}$
Case 1	$\sigma_0 \geq 2.5 \times 10^8 \text{ Pa}$	$\sigma_0 \geq 3.5 \times 10^8 \text{ Pa}$	$\sigma_0 \geq 8.5 \times 10^8 \text{ Pa}$	$\sigma_0 \geq 3.3 \times 10^9 \text{ Pa}$
Case 2	$\sigma_0 \geq 7.5 \times 10^8 \text{ Pa}$	$\sigma_0 \geq 7.5 \times 10^8 \text{ Pa}$	$\sigma_0 \geq 7.2 \times 10^8 \text{ Pa}$	$\sigma_0 \geq 8 \times 10^8 \text{ Pa}$

It can be concluded for Case 1, that delamination depends strongly on the structure length and occurs at higher loads with length increasing. This is confirmed by the experimental observation of (Gong, 2012) for the efficient stress transfer for graphene flakes $> 30 \mu\text{m}$. For Case 2 (thicker structure) practically, there is no essential influence of the length on the critical load after which delamination takes place. The influence of the thickness of SU-8 on ISS is found insufficient and is not presented here.

In (Apostolov *et al.* 2024) the PA for graphene/SU-8/PMMA is enhanced with influence of the temperature difference on the model ISS. The latter is calculated accounting that the coefficients D_i in the ODE for axial stress (and respectively, for ISS too) will change in the conditions of thermo-mechanical loading of NC (see Chapter 1). Also, the coefficients of thermal expansion for graphene ($-8\text{e-}06$ 1/K) and $74\text{e-}06$ 1/K for PMMA will be included in the coefficient D_5 together with the mechanical load.

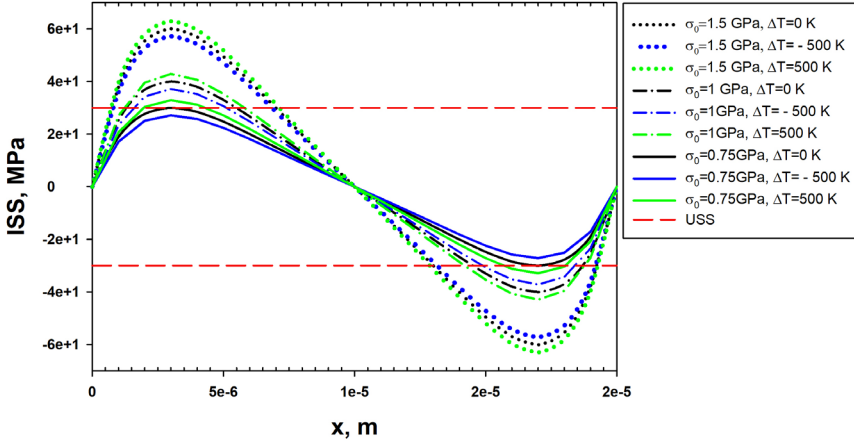


Figure 5: Influence of the magnitude ΔT of applied thermal load on the ISS for graphene/SU-8/PMMA, for complex roots solution.

The illustrative results for the model ISS in the case of complex roots are presented here in Fig. 5. It can be seen that when the mechanical load and the geometry are fixed ($\sigma_0=1.5$ GPa, $h_l=1$ nm, $h_a=0.3\mu\text{m}$, $h_2=30\mu\text{m}$, $l=20\mu\text{m}$) and the delamination already takes place (the model curves of ISS are above the USS), the thermal load influence on the ISS is weak. But for the limit case (the solid black line), the influence of the applied thermal load can be significant, especially during cooling ($\Delta T<0$, the solid blue line below the USS). The heating ($\Delta T>0$), in combination with mechanical load increases the chance of delamination in the considered structure, while cooling provides the opposite effect.

Results of PA for Graphene/SU-8/PET, complex roots

In the recently published paper (Apostolov *et al.* 2024) the influence of the applied mechanical load σ_0 , and geometry parameters h_2 , h_l and length l on

the model ISS for mechanically loaded NC Graphene/SU-8/PET are shown in the next Figs. 6 - 9.

It can be seen, that as the applied load increases at fixed values for the rest of the parameters $l=12\text{ }\mu\text{m}$, $h_l=0.35\text{ nm}$, $h_a=10\text{ nm}$, $h_2=70\mu\text{m}$, the ISS and delamination debond length also increased (Fig. 6). After $\sigma_0 \geq 7.5\text{ GPa}$ the delamination takes place for the almost whole length of the NC structure. The very similar results for ISS at complex roots for the same structure and same σ_0 have been obtained in our previous work (Kirilova *et al.* 2019) for the almost identical geometry $l=12\text{ }\mu\text{m}$, $h_l=0.35\text{ nm}$, $h_a=0.3\text{ }\mu\text{m}$, $h_2=70\mu\text{m}$. This confirmed the fact, that the thickness h_a of SU-8 has no influence on the ISS (see Eq. 1).

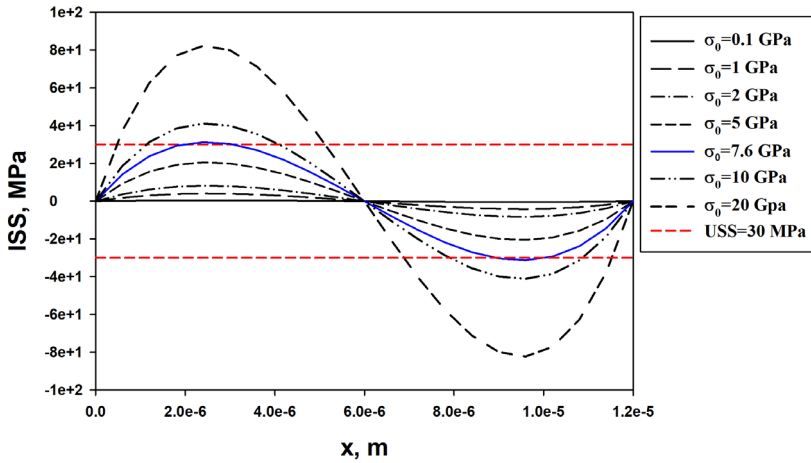


Figure 6: Influence of the magnitude σ_0 of the applied mechanical load on the ISS, for graphene/SU-8/PET, complex roots.

The strong influence of the thickness of the polymer layer h_2 on the ISS can be observed in Fig. 7. When the h_2 (m) decreases, the ISS increases. The thinner the substrate, the less resistant it is to the applied mechanical loads. At $h_2 < 25\text{ }\mu\text{m}$, the behavior of the ISS changes from the elastic one to the sliding case, which is well seen by the change in the slope of the model curve. Practically, the structure is almost completely delaminated and the calculated debond length is $5\text{ }\mu\text{m}$.

Regarding the influence of h_l on the ISS (Fig. 8) it is observed to be very weak. The same could be said for h_a and the corresponding graph is practically the same, as in the previous considered NC.

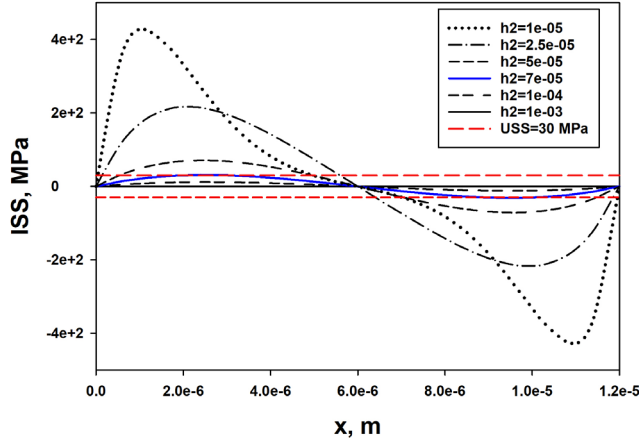


Figure 7: Influence of the thickness h_2 of Layer 2 on the ISS, for graphene/SU-8/PET, complex roots.

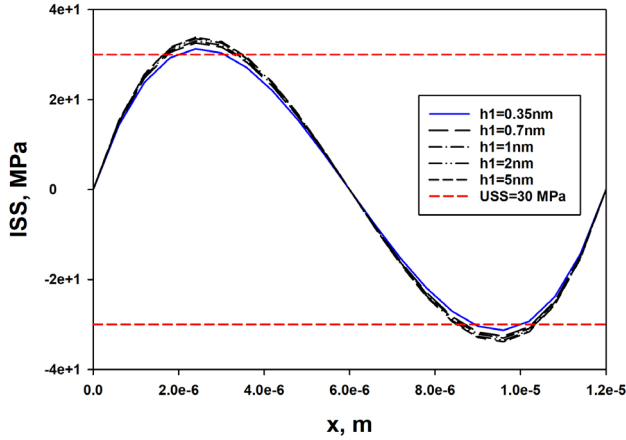


Figure 8: Influence of the thickness h_1 of Layer 1 on the ISS, for graphene/SU-8/PET, complex roots.

The impact of the length l on the ISS is more significant, as is clearly seen in Fig. 9. Up to $l=30\text{ }\mu\text{m}$, the ISS increases with increasing length and reaches its maximum value near the structure ends for this value; the debond length also is maximal, achieving almost complete delamination. After $30\text{ }\mu\text{m}$, with

increasing the length, the ISS amplitude still does not depend on l . Our results agree with those of (Xu *et al.* 2016).

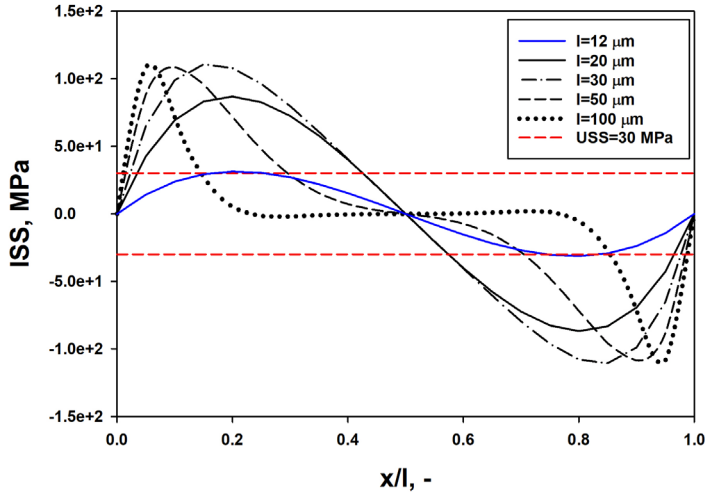


Figure 9: Influence of the layer length l on the ISS, for graphene/SU-8/PET, complex roots.

Results for PA for graphene/MoS₂/PET, complex roots

The influence of the applied mechanical load, h_1 , h_2 and the length l on the ISS is shown in Figs.10 ÷13. The influence of the magnitude of the applied mechanical load on the ISS is similar as for the two cases discussed above – as the load increases, the ISS increases too (Fig. 10). The delamination starts from both structure ends after loads $\sigma_0 > 25$ MPa. The calculated debond length at this load (using eq. 2.3.1) is about 34 μm (for fixed structure length of 72 μm).

Again, the effect of increasing h_2 on the ISS is similar to that in the case graphene/SU-8/PET – as it increases, the ISS decreases (Fig. 11). The influence of h_a on the ISS was calculated and also found to be insignificant, as in previous case structures and there is no sense to be shown here. As the value of h_1 increases, the ISS also increases (Fig. 12), which is not observed in the case of graphene/SU-8/PET. This effect is probably due to the different middle layer properties – MoS₂ is a much stronger material than epoxy adhesive SU-8.

Finally, the influence of the structure length on the ISS is similar to that for the cases discussed above (Fig. 13). After 30 μm , with increasing length, the ISS amplitude still does not depend on l . Our results again are in agreement with the results of (Xu *et al.* 2016).

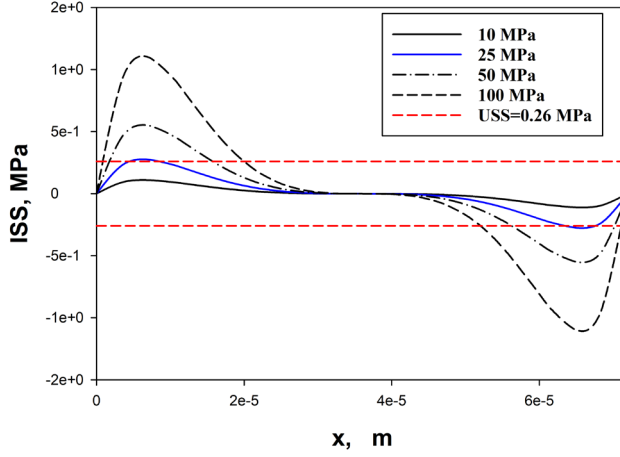


Figure 10: Influence of the magnitude σ_0 of applied mechanical load on the ISS for graphene/MoS₂/PET, complex roots.

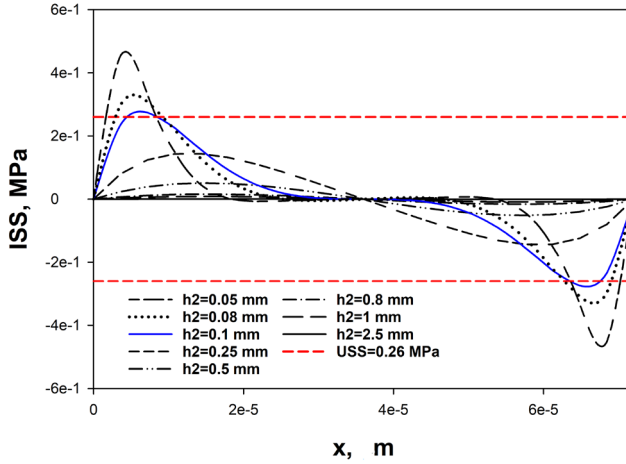


Figure 11: Influence of the thickness h_2 of Layer 2 on the ISS, for graphene/MoS₂/PET, complex roots

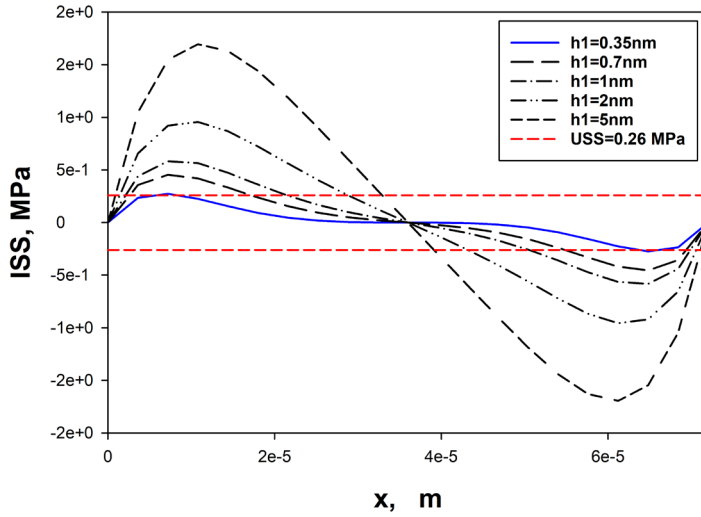


Figure 12: Influence of the thickness h_1 of Layer 1 on the ISS, for graphene/MoS₂/PET, complex roots.

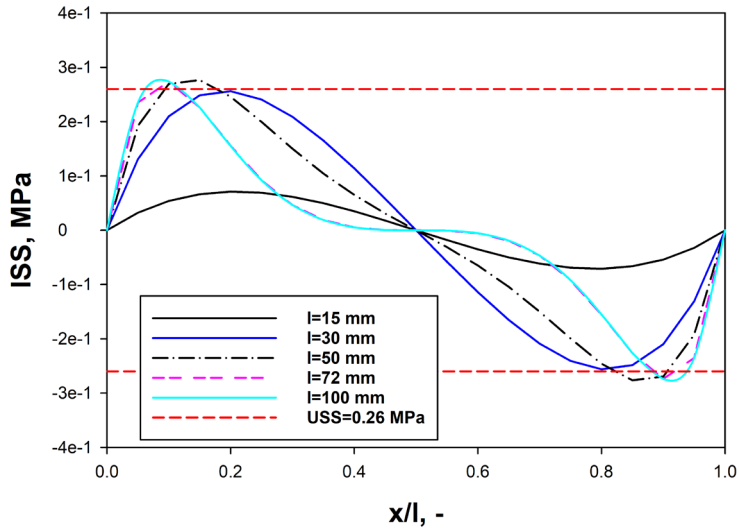


Figure 13: Influence of the layer length l on the ISS, for graphene/MoS₂/PET, complex roots.

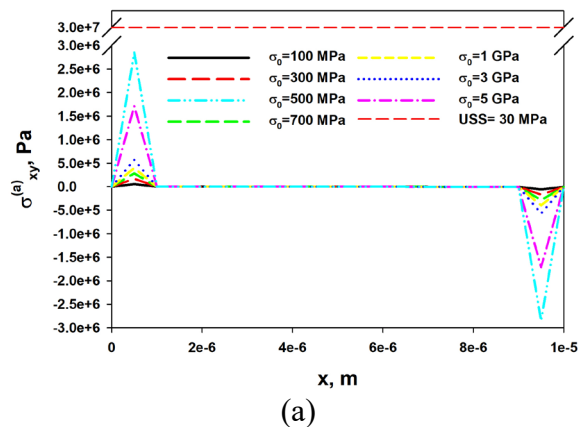
Results from PA for WS₂/SU-8/PMMA, real and complex roots

For the WS₂/SU-8/PMMA NC (Kirilova *et al.* 2023), the parametric analysis follows the same algorithm as before; here using both solutions, the results for external load and length influence on the ISS are depicted in Figs. 14 and 15 and *Table 6*. It was found for fixed WS₂ length 10 μm, that safety intervals (without delamination) in respect to loading could be fixed up to about 5 GPa for the structure with the thinner PMMA layer (Case 1) and up to 1.175 GPa for the structure with the thicker PMMA layer (Case 2). The obtained value for the debond length for this case is 1 μm.

Then a parametric analysis has been performed at a fixed mechanical load, calculating the values for the ISSs varying the length *l* of the considered NC. The results obtained for the critical values for the magnitudes of the applied mechanical load, over which a delamination appears (Case 2), are listed in *Table 6*. For Case 1 a delamination is not observed in the investigated range.

Table 6: Critical values for the magnitudes of applied mechanical load, over which a delamination appears during different length of the nanocomposite structure.

<i>l</i> , (μm)	5	10	15	20	25	30
σ ₀ , (GPa)	σ ₀ ≥1.165	σ ₀ ≥1.175	σ ₀ ≥1.17	σ ₀ ≥1.175	σ ₀ ≥1.27	σ ₀ ≥1.455



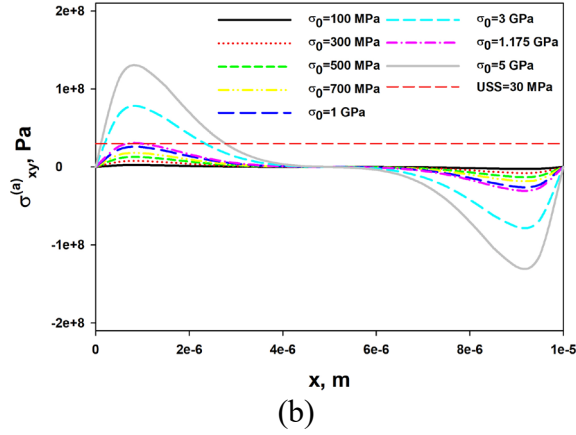


Figure 14: Influence of the magnitude of the external load on the ISS for the monolayer WS₂/SU-8/PMMA NC structure; (a) - real roots, (b) – complex roots.

One can see from *Table 6* that for Case 2 (structure with thicker PMMA layer) with increasing WS₂ length, the delamination is accompanied with a stable increase in the critical applied load, at which it appears.

Results were also obtained for the delamination (debond) length at different structure lengths (Fig. 15). As the length of the structure increases, so does the delamination length. A similar result was also observed by (Wang *et al.* 2020) for the delamination length – 2 μm, for a WS₂/PVA NC structure.

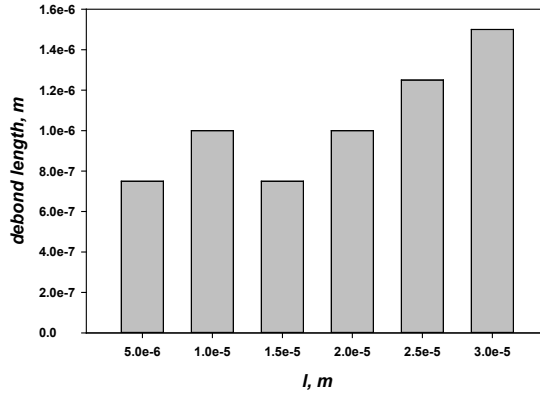


Figure 15: Relationship between the debond length and the length *l* at a fixed load of 3 GPa, monolayer WS₂/SU-8/PMMA, for complex roots.

Results from PA for 3 - layered graphene/SU-8/PMMA

The main emphasis in (Vladova *et al.* 2022) is the comparison between the model solutions for the deformations (strains) in the layers of the considered 3-layered graphene/SU-8/PMMA NC, under different types of external loads (pure thermal, mechanical and thermo-mechanical). This comparison has shown mainly the effect of temperature not only on the ISS value, as well as for all strains in the considered NC. The details for taking into account the temperature load in the 2D stress-function model are given also in Chapter 1.

In the case of a purely thermal effect, the axial deformations in graphene layer are nearly three times smaller than in the case of a purely mechanical effect. In the thermomechanical loading, a superposition effect is observed in the amplitudes of the two loads, or in other words, the behavior is the same as in the mechanical load, but stronger, with the addition of the temperature effect. This effect is better visible for the axial and the normal strains. Also, the effect of temperature is more clearly visible for the deformations in the polymer layer than in graphene.

A similar observation is also found in the model results of Banarouei, (2021) obtained with FEM. This source is the first (to the best of our knowledge) to report results related to the distribution of stresses and longitudinal strains in graphene at different external temperatures. Since the simulation tool used is FEM, no direct quantitative comparison is possible, only a qualitative assessment.

Results for PA for MoS₂/Interphase/PET, complex and real roots

The parametric analysis of the factors, influencing interface delamination, was performed and investigated for numerical examples of combined loaded MoS₂/Interface/PET nanocomposite (Vladova *et al.* 2024). The factors taken into account are: influence of mechanical load on the ISS, layers' thicknesses, layers' length and influence of temperature load. All calculations and corresponding parametric analyses were done in Mathcad environment. PA is performed for both types of solutions (real and complex roots) for the ISS.

The mechanical load σ_0 influence on the ISS at complex roots is depicted in Fig. 16. The figure shows that up to 25 MPa external mechanical load at a fixed geometry of the considered MoS₂/interface/PET nanocomposite structure, delamination is observed.

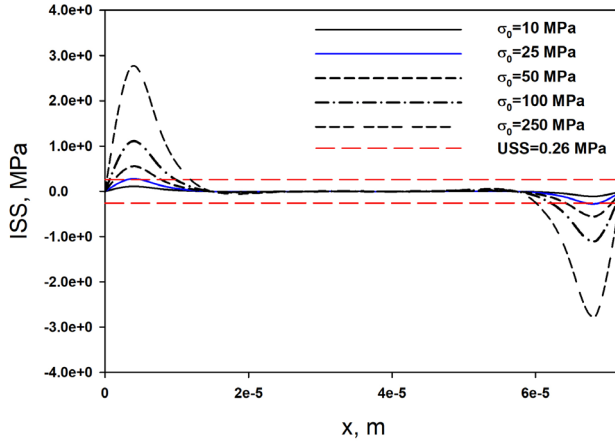


Figure 16: Influence of the magnitude σ_0 of mechanical load on the ISS, for considered MoS₂/interface/PET, for complex roots.

Regarding the influence of h_1 , it is depicted in Fig. 17. Keeping the monolayer thickness h_1 for MoS₂ and choosing the appropriate load, the delamination cannot appear. If $h_1 > 0.65$ nm, the delamination arises.

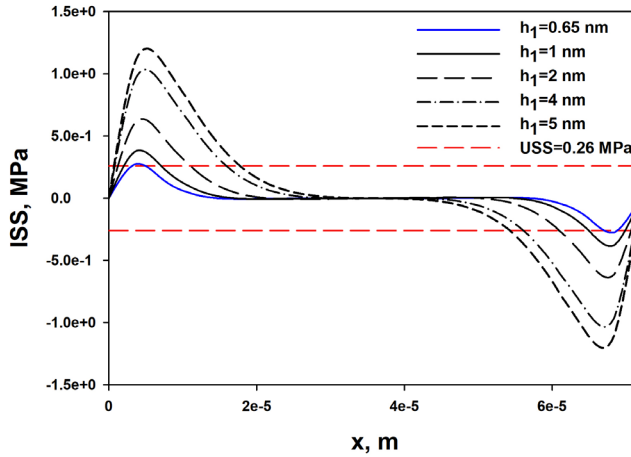


Figure 17: Influence of the thickness h_1 on the ISS for MoS₂/Interface/PET, for complex roots.

Fig. 18 portrays the influence of h_2 . If the PET thickness $h_2 > 50$ μ m, the delamination is not appearing. The influence of h_a is negligible, the ISS does not depend on h_a and it is not presented here.

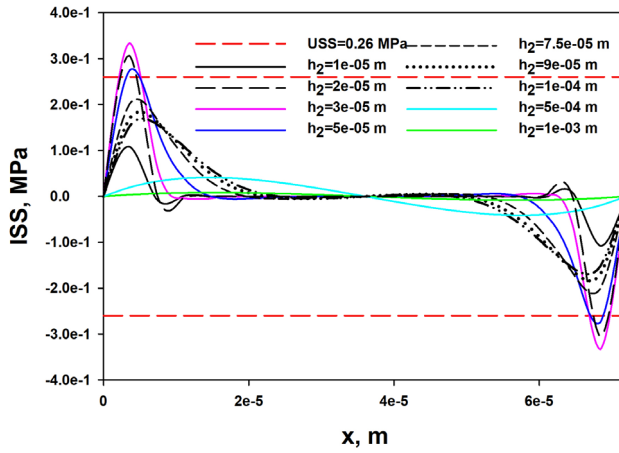


Figure 18: Influence of the thickness h_2 on the ISS for MoS₂/Interface/PET, for complex roots.

The impact of the length l on the ISS is seen up to 90 μm ; after $l > 90 \mu\text{m}$ - at fixed layers' thicknesses and load, the delamination does not arise. The maximal value of the ISS is reached at about $l=15 \mu\text{m}$ as is clearly seen in Fig. 19.

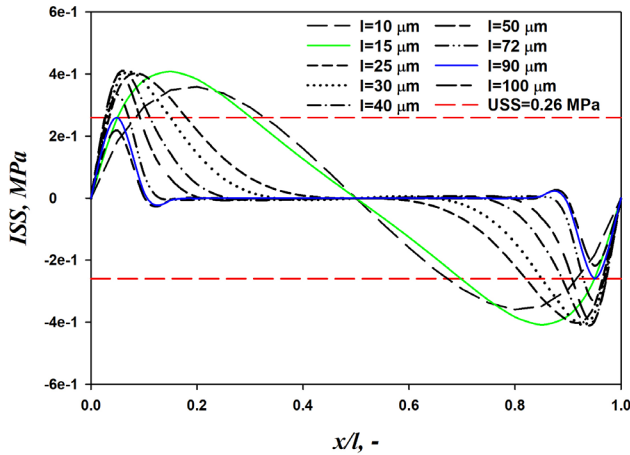


Figure 19: Influence of length on the ISS for MoS₂/Interface/PET, for complex roots.

The effect of thermal loading on ISS is depicted in Fig. 20. If a sufficient cooling temperature difference ($\Delta T = -100\text{K}$ or more) is applied to the

mechanical loading where we have already established delamination, as a result the debonding is no longer observed in the considered structure.

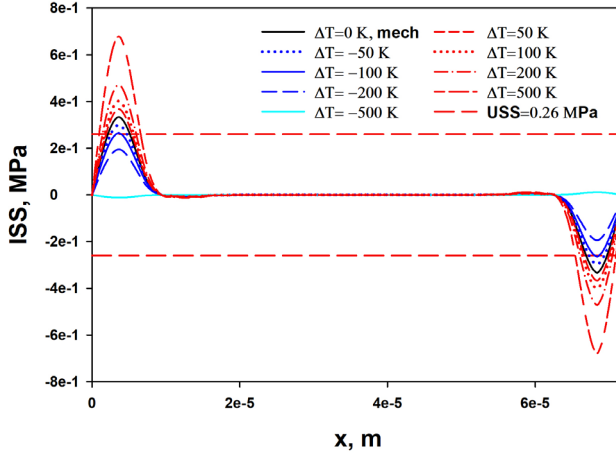


Figure 20: Influence of temperature load on the ISS for MoS₂/Interface/PET, for complex roots.

This is probably due to the differences in TEC of MoS₂ and PET and resulting additional compressive strains occurring after an applied thermal load; all this ultimately reduces the ISS value below the critical one. In contrast, the opposite situation is observed (the positive temperature difference increased already the observed delamination) in the case of heating, applied to the mechanically loaded nanostructure.

The parametric analysis of the factors, affecting interface delamination was performed at real roots too, for MoS₂/Interface/PET nanocomposite under combined loading. The influence of the mechanical load σ_0 on the ISS at real roots is shown in Fig. 21. At a fixed geometry of the considered MoS₂/interface/PET nanocomposite structure, delamination is not observed for applied loads even above 3 GPa (elastic limit).

The influence of h_I on the ISS is depicted in Fig. 22. The figure shows, that keeping MoS₂ thickness $h_I < 2.66$ nm, at fixed other parameters, the delamination is not appearing; over this value it appeared. The influence of h_a on ISS is negligible and is not represented here.

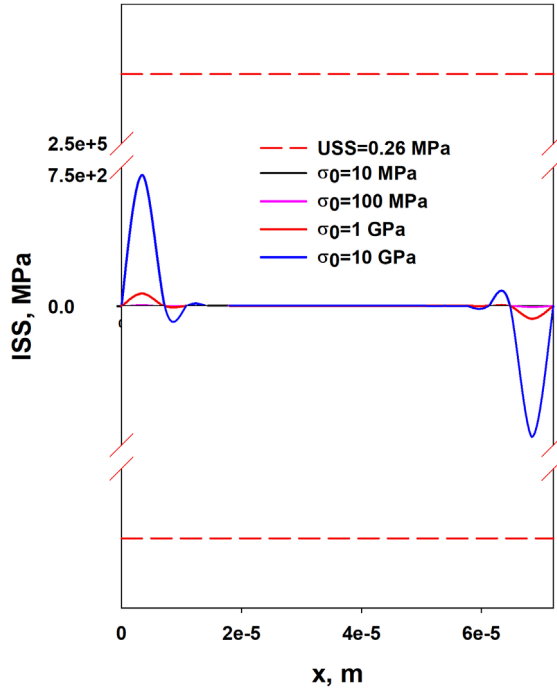


Figure 21: Influence of the magnitude σ_0 of the mechanical load on the ISS for considered MoS₂/Interface/PET, at real roots.

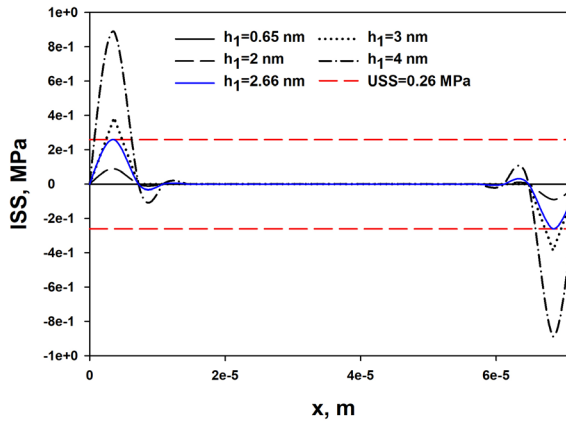


Figure 22: Influence of the thickness h_1 on the ISS for MoS₂/Interface/PET, at real roots.

Fig. 23 portrays the influence of h_2 on the ISS for real roots. Keeping the PET thickness h_2 in the range of $0.81\mu\text{m} \div 1.2\mu\text{m}$, the delamination is not appearing. It should be noted, that the existence of positive roots and, the existence of model solutions for the axial stress and the ISS, respectively, are inextricably bound up with a very thin interval for the values of h_2 .

Fig. 24 presents the influence of the length l on the ISS: after $l > 38.25\mu\text{m}$ at fixed other layers' thicknesses and load of 1 GPa, the delamination does not spring up.

The effect of thermal loading is determined: for longer lengths, at $72\mu\text{m}$ and more, the influence of ΔT on ISS is negligible, as seen in Fig. 25 (a). If an extreme cooling temperature difference ($\Delta T = -500\text{K}$) is added to the mechanical loading where we have already established delamination, at fixed length $38.25\mu\text{m}$, as a result debonding is no longer observed in the considered structure (Fig. 25, (b)).

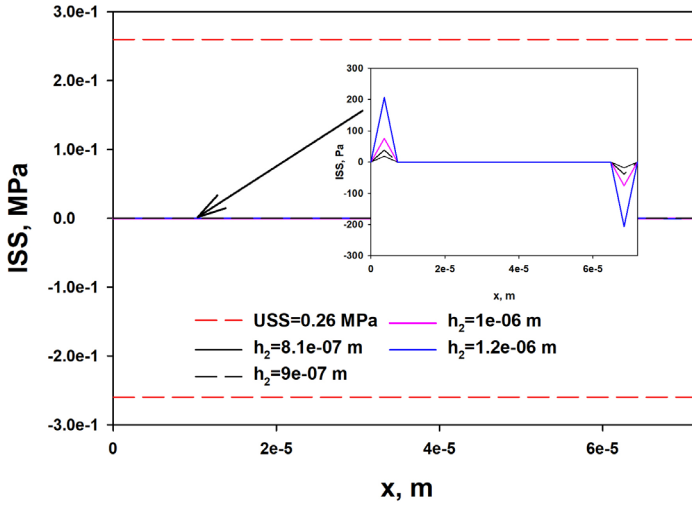


Figure 23: Influence of the thickness h_2 on the ISS for MoS₂/Interface/PET, for real roots.

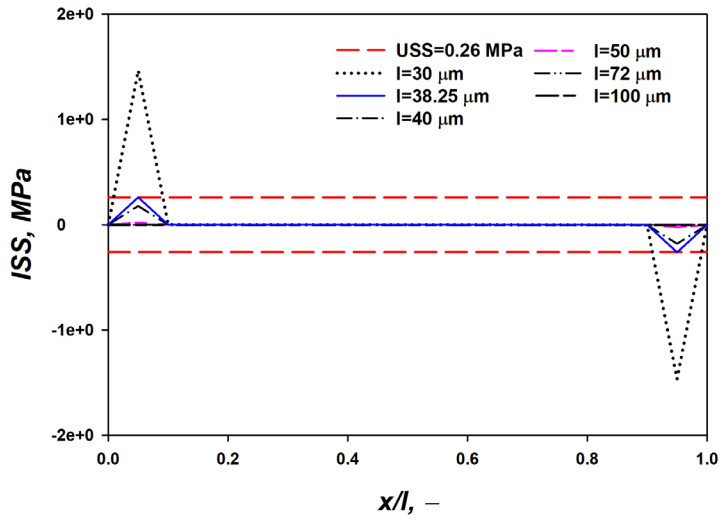
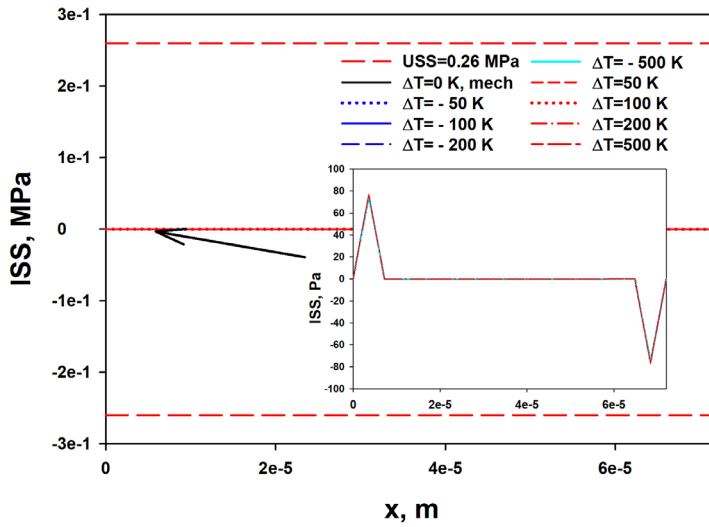
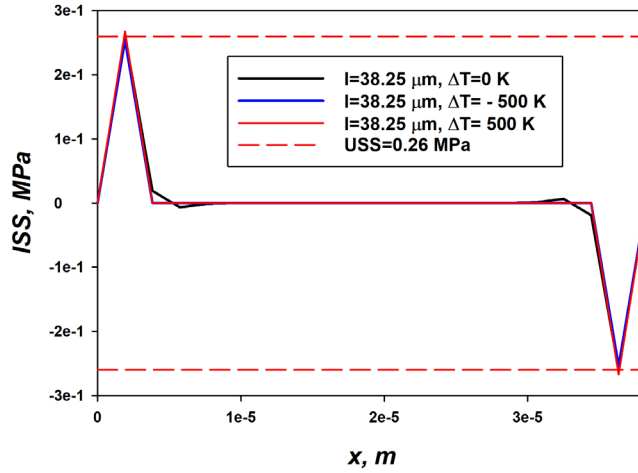


Figure 24: Influence of length l on the ISS, for MoS₂/Interface/PET, for real roots.



(a)



(b)

Figure 25: Influence of temperature load on the ISS, for MoS₂/Interface/PET for real roots: (a) at fixed length 72 μm; (b) at fixed length 38.25 μm.

4. Conclusions

It can be said that the properties and geometric characteristics of the interfacial layer in NCs are a subject of considerable interest both at the experimental and theoretical levels. At present, there is still no method for direct measurement/identification of this layer; there are many theoretical hypotheses about its properties and size. The currently available experimental and theoretical data on this subject are summarized and analyzed. There are too many factors that influence the dimensions and properties of the interface/interphase zone. Regardless of the above, the interfacial zone at NCs exists and should be considered in the modeling of design and stress transfer efficiency of both existing and newly created NCs, especially in terms of their ever-increasing number of industrial applications.

PA gives us very valuable information about the influence of various factors determining the important characteristics of NCs from the point of view of their industrial applications - mechanical, optical, electrical and other valuable NC properties. A parametric study can and has to be provided in the design of the experiment for the study of NC properties; it helps to reduce the number of experiments and determines the influence of different factors on

the quantities we are interested in, as well as the relationships between individual factors. In the presence of a model for NC behaviour, the PA gives us valuable information that cannot yet be obtained experimentally. It should be noted, that the length, thicknesses of the layers in NC, temperature, material properties of substrate and interphase are among the main factors, that influence the stress transfer and delamination in NC.

The obtained results from PA in 6 NC, performed during the project KII-06-H57/3/15.11.21 help to draw the following conclusions: PA could identify the factors that influence the delamination of the interface, as well as their significance (weight) on the value of the interfacial shear stress. The most significant factor stands out as the magnitude of the external mechanical load, followed by the thicknesses of the nanolayer and the substrate. The length of the NC, as well as temperature differences, have less influence on this interfacial stress, but can be significant in combination with specific values of the external load. The results obtained from PA facilitate the definition and solution of the multiparametric optimization problems presented in the Chapter 6 on optimization of NC structures.

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Notations list

Notation	Meaning
σ	Stress, Pa
τ	Interfacial shear stress (ISS), Pa
ε	Strain (deformation) in nanomaterial, -
l	Length of the structure/flake, m
x, y, z	Cartesian coordinate system, m
E	Young's modulus, Pa
G	Interface/adhesive shear modulus, Pa
ν	Poisson ratio, -
t	Thicknesses of the layers in NC, m
h_i	Thickness of the layers in NC, m
$s=L/a$	Thread size ratio (aspect ratio), length to diameter, -
L_c	Critical length, m
V_f	Volume fraction of NM in NC, %
n	Parameter in shear-lag model, -
$T, \Delta T$	Temperature and temperature difference, K

Chapter 3. Numerical modelling of functionally graded piezoelectric cracked nanocomposites subjected to dynamic loads by boundary element method

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Annotation

This chapter deals with modelling of time-harmonic SH scattering in infinite, semi-infinite and finite functionally graded cracked piezoelectric nanocomposite 2D solids. The computational tool is a non-hypersingular traction boundary integral equation method (TBIEM) based on an analytically derived fundamental solution or half-plane Green's function for functional graded piezoelectric material (PEM) combined with the boundary conditions derived in surface elasticity theory. The proposed numerical schemes are verified in respect to their accuracy and convergence. The simulation results illustrate the sensitivity of the fracture state of the cracked nanocomposites to the type and properties of the material gradient, to the surface elasticity properties, to the nanocracks existence and their dynamic interaction, to the coupled properties of the PEM and to the type of the dynamic load.

The obtained results are with theoretical application in solid, computational and fracture mechanics and with important regard to practical matters concerning the technology of new multifunctional structural materials and modern design of advanced electromechanical systems.

1. Introduction

The piezoelectric heterogeneous materials containing nanoscale objects possess unique mechanical and electrical properties different from those at the macro-scale. The mechanical behavior of materials at the nanoscale has begun attracting a great deal of recent attention from researchers in solid mechanics. The new field nanomechanics of materials may be concerned with extending concepts and methods of traditional solid mechanics to describe the mechanical response of nanostructures. Along this direction we should

mention the pioneering work of Gurtin and Murdoch (1975), who developed a general theoretical framework to represent both surface and interface stresses and their influence on the overall stress-strain state of the nanocomposites. In their model, the interfaces between the nanoheterogeneity and the surrounding matrix are regarded as thin membranes that possess their own mechanical properties and surface tension. It is assumed additionally that residual stresses develop around the surface and the interface, even in the absence of external loading. The effect of this residual stress is size-dependent and its influence becomes very significant for nanosized objects for which the ratio of surface to volume is high. The reason for surface elasticity existence is that molecules near the surfaces and interfaces have different equilibrium positions and energy levels from those of the bulk material. For structures with sizes larger than 100 nm, the surface-to-volume ratio is negligible and the effective material properties are governed by the classical bulk elastic strain energy through the fourth order elastic stiffness tensor. For smaller sizes, the strain energy can be dramatically altered by surface effects and hence both the local and macroscopic properties of the material are different enough to serve as the basis for nanotechnology. Compared with the elastic surface/interface model of Gurtin-Murdoch, the surface energy density in the piezoelectric nanostructures could also depend on the surface electric displacement in addition to mechanical surface stress. The coupling of stress and electric displacement results in a complex distribution of elastic stress and electric displacement. The electrical and mechanical properties in the vicinity of surfaces as well as the interplay between electricity and elasticity therein are more complicated at nanolevel. In the engineering practice, the sensors of piezoelectric nanocomposites are often subjected to all kinds of static and dynamic loads. The strength and reliability of these sensors will greatly influence their function in the serving life. In a wide range of fields as engineering, physics, material science, biomechanics, non-destructive testing, geophysics, etc., a catastrophic fracture, failure and damage remain a major challenge. The fracture is generally initiated locally from a crack tip. In continuum mechanics a crack is defined as a cut in a body which has its ends inside the body volume. This end of the crack is referred to as a crack-tip. Crack's lines are defined as two opposite boundaries formed by the cutting line and are generally treated at macro-scale as traction-free, see Gross and Seelig (2011). The fracture process leads to a global failure of materials through crack propagation across the entire structure. Fracture mechanics established on the basis of continuum mechanics provides a theoretical framework to describe the critical conditions at which a crack becomes mechanically unstable and begins to propagate. Understanding the nanoscale fracture behaviour is crucial for tailoring the mechanical properties of

nanomaterials. It is known that classical continuum theory fails in predicting the material behaviour at nanoscale where the surface elasticity effects play an important role.

New classes of advanced functionally graded piezoelectric materials (FGPM) are investigated intensively in our days due to their applications in smart intelligent systems. The FGPM is brittle, and the applied electromechanical loads in manufacturing and service conditions can cause different types of defects provoking damage and fracture. FGPMs are challenging regarding modeling and numerical simulation of their inhomogeneous structure. The mathematical background of models describing the behavior of these materials involves the solution of partial differential equations with spatially varying coefficients. The application of the BIEM to dynamic problems in inhomogeneous piezoelectric solids meets serious difficulties because the method requires the fundamental solution for the governing wave equation of the corresponding FGPM. In general, partial differential equations with variable coefficients do not possess fundamental solutions that can easily be implemented in the existing BIEM software. This prevents the reduction of a boundary value problem (BVP) to a system of boundary integral equations (BIEs) which can be treated by standard numerical quadrature techniques. The authors' results and a detailed review of the solutions existing in the literature for dynamic behavior of 2D functionally graded piezoelectric infinite and finite solids with macro-cracks subjected to time-harmonic plane waves can be found in Dineva *et al.* (2014). The computational tool is a nonhypersingular traction BIEM based on: (i) fundamental solutions derived by Radon transform for a homogeneous or a restricted class of inhomogeneous materials in the whole plane; (ii) Green's function derived by Fourier transform for homogeneous or a restricted class of inhomogeneous materials half-plane.

To the authors' knowledge, there is a lack of published results for nanocracks in functionally graded piezoelectric solids.

What follows is a review concerning 2D mechanical models of dynamic behavior of single and multiple nanocracks in infinite, semi-infinite and finite homogeneous or functionally graded elastic or piezoelectric solids in the frame of *Gurtin-Murdoch* theory.

- *Results for infinite homogeneous or graded, elastic or piezoelectric, nanocracked solids under static loads*

The boundary integral equation method (BIEM) is developed in Xu and Dong (2016) and Dong and Lo (2013) to study the nanocrack behavior in an infinite homogeneous elastic isotropic plane subjected to remote anti-plane shear.

Few results are known for homogeneous piezoelectric material with a nanocrack under far-field anti-plane mechanical and in-plane electrical loads, see Xiao *et al.* (2016) and Fang *et al.* (2012) where conformal mapping technique and complex variable approach is applied as computational tool.

- *Results for semi-infinite and finite, homogeneous or graded, elastic or piezoelectric, nanocracked solids under static loads*

To the authors' best knowledge there are no results for anti-plane strain case.

- *Results for infinite homogeneous or graded, elastic or piezoelectric, nanocracked solids under dynamic loads*

There is a lack of results in this field with an exception of the authors' results for the PEM anti-plane case of graded PEM planes, see Rangelov and Dineva (2022).

- *Results for semi-infinite homogeneous or graded, elastic or piezoelectric, nanocracked solids under dynamic loads*

There is a lack of results in this field with an exception of the authors' result, see Rangelov and Dineva (2023a).

- *Results for finite homogeneous or graded, elastic or piezoelectric, nanocracked solids under dynamic loads*

Results for finite exponentially inhomogeneous piezoelectric solid with nanocracks are available in Marinov *et al.* (2018) and Dineva *et al.* (2019).

Based on the above state-of-the-art, a number of conclusions can be done:

- (a) There is a certain lack of work for the solution of anti-plane dynamic problems for homogeneous and graded piezoelectric solids with nanocracks;
- (b) Despite well-known advantages of the BIEM, the application of this method as an effective numerical technique in fracture mechanics of nanocomposites is still limited;
- (c) At macroscopic scale the crack's front profile is considered to be infinitely sharp and the corresponding elastic and elasto-plastic near field zones are well established in the classical fracture mechanics. However, in reality the crack-tips are not ideally sharp but blunt with a curvature radius in the order of microns or nanometers. Experiments and simulations by atomic models (Hoagland *et al.* (1991)) show that the stresses obtained via the atomic models are in a good agreement

with the predictions of linear fracture mechanics except in a very small vicinity of the crack tip, where the effect of surface elastic energy should be accounted for. Or, the surface elasticity effect is localized at the crack-tip.

- (d) There are a limited number of papers considering surface elasticity effects on the stresses near the crack-tip and the most of them are for static loads.
- (e) To the authors' knowledge there is a lack of results in dynamic fracture mechanics of functional graded nanocracked elastic and piezoelectric nanocomposites.

The aim of this chapter is to develop, verify and insert in parametric studies new mechanical models which give solutions for the dynamic stress field near crack-tips of blunt nanocracks subjected to incident time-harmonic plane SH- wave propagating in anisotropic piezoelectric infinite, semi-infinite and finite solids by BIEM taking into account the surface elasticity effect by Gurtin-Murdoch model.

2. Problem formulation by governing partial differential equation

The main goal in this section is to formulate 2D elastodynamic problems in frequency domain for infinite, semi-infinite and finite functionally graded transversely isotropic piezoelectric solids of nanocomposites with multiple cracks at nano-scale under anti-plane load.

- *Problem 1:* Dynamic behaviour of an infinite graded piezoelectric solid (Fig.1a) containing a number of nanocracks $\Gamma_{cr} = \bigcup_{n=1}^K \Gamma_{cr}^n$ of arbitrary size and configuration under time-harmonic incident SH plane waves, see Rangelov *et al.* (2020b). In addition, electrical load can be taken into account.
- *Problem 2:* Dynamic behaviour of a finite anisotropic piezoelectric solid (Fig. 1b) with external boundary Γ_{ext} containing a set of K nanocracks $\Gamma_{cr} = \bigcup_{n=1}^K \Gamma_{cr}^n$ of arbitrary size and configuration under uniform time-harmonic mechanical and/or electrical loads, see Dineva and Rangelov (2016), Luo and Wang (2009).
- *Problem 3:* Dynamic behaviour of a graded (Fig. 1c) piezoelectric half-plane with boundary Γ_{ff} and containing a number of nanocracks $\Gamma_{cr} = \bigcup_{n=1}^K \Gamma_{cr}^n$ under incident time-harmonic SH plane waves and/or electrical load, see Rangelov and Dineva (2021).

The nanocrack S is modelled as a blunt one with a root in the shape of a semi-ellipse, with semi-axes denoted as d, d_0 , respectively, see Fig. 1d. The perimeter of the crack is $|S| = 4(c - d_0) + 4d_0E(g)$, with $d_0 = 0.0375c$, and the size parameter c falls in the range $[10^{-10}, 10^{-7}m]$. Furthermore, $E(g) = \int_0^{\pi/2} \sqrt{1 - g^2 \sin^2 \varphi} d\varphi$ is the complete elliptic integral of second kind, see Gradshteyn and Ryzhik (1965), and $g = \sqrt{1 - (d/d_0)^2}$ is a dimensionless length parameter. If $d_0 = d$, then the blunt nano-crack has a semi-circular crack root of radius d_0 , while if $d_0 = 0$, we have Griffith line crack of length $2c$. The blunt nanocrack's contour S can be expressed as $S = S^+ \cup S^- \cup S^l \cup S^r$, comprising a flat part (indices $+/-$) and left and right crack roots of semi-elliptical shapes (indices l/r).

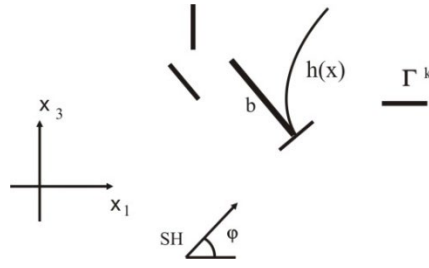
Assume that piezoelectric material shows hexagonal symmetry with respect to the axis Ox_3 and the poling axis is collinear with this axis. The plane $x_3 = 0$ is isotropic plane, while plane $x_2 = 0$ is transversely isotropic. The uncoupling of 3D deformation state into two 2D states, i.e. anti-plane and in-plane deformation states, is only possible if the material is monoclinic. Fortunately, the PEM falls into the crystallographic class 6mm and thus belong to this group of materials.

For the considered anti-plane strain state the poling axis is collinear with the axis Ox_3 . The material properties are as follows: elastic stiffness variable $c_{44}(x)$, piezoelectric variable $e_{15}(x)$, dielectric variable $\varepsilon_{11}(x)$ and density $\rho(x)$. The inhomogeneity function for exponentially graded material is $h(x) = e^{2\langle b, x \rangle}$, where $\langle, \rangle$ is a scalar product and the inhomogeneous vector $b = |b|(\cos\alpha, \sin\alpha)$, where α and $|b|$ are direction and magnitude of the material gradient.

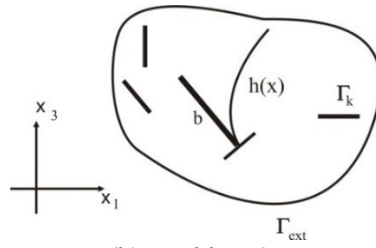
In the considered deformation case the only non-zero field quantities depend on the coordinates (x_1, x_2) are: (a) mechanical field variables: displacement component u_3 ; stress tensor components σ_{13}, σ_{23} ; strain components s_{13}, s_{23} ; (b) electrical field variables: electric field components E_1, E_2 , electrical displacements D_1, D_2 and electrical potential ϕ . The following generalized notations for the displacements and stresses are used: $u_J = \begin{cases} u_3, J = 3, 4 \\ \phi \end{cases}$;

$$\sigma_{ij} = \begin{cases} \sigma_{ij}, J = 3 \\ D_i, J = 4 \end{cases};$$

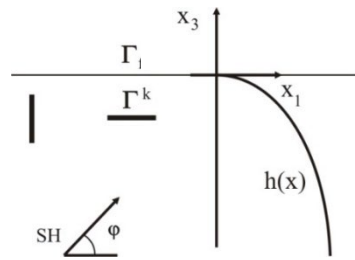
The boundary-value problem (BVP) under consideration is defined by the governing partial differential equations and the corresponding boundary conditions given below.



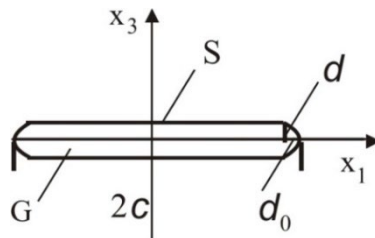
(a) Problem 1



(b) Problem 2



(c) Problem 3



(d) Problem 4

Figure 1: Geometry of nanocracked problems: (a) infinite PEM plane; (b) finite PEM solid; (c) PEM half-plane; (d) blunt nano-crack geometry.

Governing partial differential equations

The constitutive equation is:

$$\sigma_{ij} = C_{ijkl}(x)u_{k,l} = C_{ijkl}(x)s_{kl} \quad (1)$$

where $i, l = 1, 2$ and $C_{i33l}(x) = \begin{cases} c_{44} & i = l \\ 0 & i \neq l \end{cases}$; $C_{i34l}(x) = \begin{cases} e_{15} & i = l \\ 0 & i \neq l \end{cases}$; $C_{i44l}(x) = \begin{cases} -\varepsilon_{11} & i = l \\ 0 & i \neq l \end{cases}$.

The elastic strain-displacement and the electrical field-potential kinematic relations are given by:

$$s_{i3} = \frac{1}{2}(u_{3,i}), E_i = -\phi_{,i} \quad (2)$$

The mechanical and electrical balance equation for time-harmonic processes in absence of body forces and electric charges can be written in the following compact form

$$\sigma_{ij,i} + \rho_{JK}(x)\omega^2 u_K = 0, \quad \rho_{JK}(x) = \begin{cases} \rho, & J = K = 3 \\ 0, & J = 4 \text{ or } K = 4 \end{cases} \quad (3)$$

The governing equations (1)-(3) are given by the equation of motion for the mechanical displacement (3) and by the equation of electrostatic in (2). The electric field that develops in piezoelectrics can be assumed to be quasi-static because the velocity of the elastic wave is much smaller than the velocity of the electromagnetic wave. Therefore, the magnetic field due to the elastic waves is negligible. This fact implies that the time derivative of the magnetic field B is close to zero, i.e. $\partial B/\partial t \approx 0$. Thus one of Maxwell's equations of electrodynamics becomes $\text{rot} E = \partial B/\partial t \approx 0$, hence $E = -\text{grad} \phi$. Consequently, a piezoelectric continuum is based on the governing equations of elastodynamics in the case of small deformations and quasi-electrostatic fields, see Dineva *et al.* (2014).

Boundary conditions in the case of anti-plane wave motion

• Problem I

The non-classical boundary condition in the frame of Gurtin and Murdoch model for the traction defined by $t_3 = \sigma_{13}n_1 + \sigma_{23}n_2$, where n_1, n_2 are the

components of the outward normal vector along the interface S between a blunt nano-crack and a piezoelectric matrix M , is (Dineva *et al.* (2019)):

$$t_3^M(x, \omega) = -\mu^S \frac{\partial^2 u_3(x, \omega)}{\partial l^2}, x \in S \quad (4)$$

where μ^S is the shear modulus of the infinitely thin surface layer S between the nanocrack and matrix.

In sum, the *Problem 1* is given by the equation of motion (3), the boundary condition (4) on each nanocrack's boundary I^k , plus Sommerfeld's radiation condition for the scattered wave field at infinity. If $\mu^S = 0$ the boundary condition (4) degenerates to the classical traction free boundary condition and we consider the macro-crack. If $\mu^S \neq 0$ we have a nanocrack. In both cases for the electrical part of the boundary condition we have that $t_4^M = D_n^M = 0$, i.e. the nanocrack is electrically impermeable.

- *Problem 2*

The *Problem 2* is given by the equation of motion (3), the boundary condition (4) on each nanocrack's boundary I^k and the prescribed generalized displacement or traction along the external boundary Γ_{ext} of the finite PEM solid.

- *Problem 3*

The *Problem 3* is given by the equation of motion (3), the boundary condition (4) on each nanocrack's boundary I^k , the zero tractions along the half-plane boundary Γ_{ff} plus Sommerfeld's radiation condition for the scattered wave field at infinity.

Note that the generalized stiffness tensor depends on the radius vector of the observer point, i.e. $C_{ijkl}(x) = C_{ijkl}^0 h(x)$, where C_{ijkl}^0 are the reference stiffness coefficients of the homogeneous material. The exponential type of material gradient is assumed at numerical realization of all three problems with $\alpha \in [0, \frac{\pi}{2}]$ for Problems 1 and 2 and $\alpha = \frac{\pi}{2}$ for *Problem 3*.

The aim is to determine numerically the mechanical and electrical field variables at any point of the infinite, semi-infinite and finite graded piezoelectric solid containing a set of nanocracks and to evaluate the dynamic generalized stress concentration fields near the perimeter of any nanocrack subjected to time-harmonic load.

3. Problems reformulation by boundary integral equations

The above formulated BVPs are now reformulated by equivalent integro-differential equations along the existing boundaries. In the case of cracks the displacement BIEs degenerate and due to this the authors developed for the case of graded cracked continuum the method of non-hypersingular traction BIE based on the two-state conservation integral of elastodynamics, see Dineva *et al.* (2014). Note that the system of derived boundary integro-differential equations takes into account the non-classical boundary condition in the Gurtin-Murdoch model along the nanocrack surface.

Problem 1 for a system of blunt nanocracks in an infinite graded piezoelectric plane with common boundary $\Gamma = \Gamma_{cr} = \bigcup_{n=1}^K \Gamma_{cr}^n$ (Fig. 1a), *Problem 3* with common boundary $\Gamma = \Gamma_{cr} \cup \Gamma_{ff}$ (Fig. 1c) for blunt nanocracks in a graded PEM half-plane subjected to plane wave and *Problem 2* for a finite piezoelectric solid with common boundary $\Gamma = \Gamma_{cr} \cup \Gamma_{ext}$ (Fig. 1b) subjected to time-harmonic electro-mechanical load along its external boundary are reformulated via the following non-hypersingular traction BIE (12):

$$\begin{aligned} \gamma_{RJ}(t_R^{in or ff}(\mathbf{x}, \omega) - t_R^M(\mathbf{x}, \omega)) = \\ C_{ijkl}(\mathbf{x})n_i(\mathbf{x}) \int_{\Gamma} \{[\sigma_{\eta PK}^*(\mathbf{x}, \boldsymbol{\xi}, \omega)u_{P,\eta}^{sc}(\boldsymbol{\xi}, \omega) - \rho_{QP}\omega^2 u_{QK}^*(\mathbf{x}, \boldsymbol{\xi}, \omega)u_P^{sc}] \delta_{\lambda l} \\ - \sigma_{\lambda PK}^*(\mathbf{x}, \boldsymbol{\xi}, \omega)u_{P,l}^{sc}(\boldsymbol{\xi}, \omega)\} n_{\lambda}(\boldsymbol{\xi}) d\boldsymbol{\xi}, \quad \mathbf{x} \in \Gamma. \end{aligned} \quad (5)$$

Where: γ_{RJ} is the jump term depending on the local geometry at source point $\mathbf{x} \in \Gamma$; u_{QK}^* is the fundamental solution (in case of *Problems 1* and 2) and Green's function, i.e. fundamental solution that in addition satisfies traction free boundary conditions on Γ_{ff} (in case of *Problem 3*) of Eq. (3) with Dirac delta at the right hand side; $\sigma_{ijk}^* = C_{ijkl}(\mathbf{x})U_{QK,l}^*$ is its corresponding stress; n_q is the unit outward normal; $u_j^{sc} = u_j - u_j^{in}$ and $t_j^{sc} = t_j - t_j^{in}$ for *Problem 1* and $u_j^{sc} = u_j - u_j^{ff}$ and $t_j^{sc} = t_j - t_j^{ff}$ for *Problem 3*, $\delta_{\lambda l}$ is the Kronecker symbol. The fundamental solutions and Green's function and solutions for incident wave field and anti-plane free-field wave motion in a graded plane and graded half-plane, correspondingly, are given in Dineva *et al.* (2014), Rangelov *et al.* (2020a,b).

After the standard discretization and collocation procedure applied to Eq. (5) and satisfaction of the boundary condition discussed above, the

resulting solution takes into consideration the effects of surface elasticity via the Gurtin –Murdoch model. Once the solution of BIE (5) is known for a fixed frequency ω , the displacement and traction produced by the scattered wave field and by this the total wave field in the piezoelectric plane/half-plane or finite solid under consideration can be determined via the known representation formulae, see Dineva *et al.* (2014).

The normalized SCF and Electrical Field Concentration Factor (EFCF) close to the blunt crack-tip at the point $(\pm x_1, 0)$ is evaluated using the formulae (6) for anti-plane wave motion.

The normalized stress concentration factor (SCF) F_{III}^* and electrical field concentration factor (EFCF) F_E^* close to the blunt nano-crack-tip at the point $(\pm x_1, 0)$ are evaluated by the formulae:

$$F_{III}^*((\pm x_1, 0), \omega) = \frac{\sigma_{23}((\pm x_1, 0), \omega)}{\sigma \sqrt{\pi c}} \sqrt{2\pi(x_1 \mp c)}, |x_1| > c; \quad (6)$$

$$F_E^*((\pm x_1, 0), \omega) = e_{15}^0 \frac{E_3((\pm x_1, 0), \omega)}{\sigma \sqrt{\pi c}} \sqrt{2\pi(x_1 \mp c)}, |x_1| > c.$$

where:

$$E_3 = \frac{\sigma_{24}((\pm x_1, 0), \omega) c_{44}^0 - \sigma_{23}((\pm x_1, 0), \omega) e_{15}^0}{c_{44}^0 e_{11}^0 + (e_{15}^0)^2}; \quad \sigma \text{ is the magnitude of the mechanical load.}$$

The final aim of the defined three mechanical problems is to obtain numerically the dynamic stress-strain field at any point in the corresponding infinite, semi-infinite and finite graded piezoelectric solids and to evaluate the local dynamic stress concentration fields near the nanocracks.

4. Numerical scheme and its verification

In the numerical scheme the displacements and tractions are approximated with parabolic shape functions which satisfy Hölder continuity at least at the collocation points and show an asymptotic $O(\sqrt{r})$ behavior for the displacements near the crack tips. Quarter-point boundary elements are implemented in a quadratic boundary element discretization. The disadvantage of the standard quadratic approximation regarding the smoothness at all irregular points is overcome by the shifted point method, see Dineva *et al.* (2014). After discretization the obtained integrals are at least Cauchy principal value (CPV) integrals. The regular integrals are computed

employing the Gaussian quadrature scheme for one-dimensional integrals and Monte Carlo integration scheme for two-dimensional integrals. All integrals with singular kernels are solved analytically in the small neighborhood of the field point, using the approximation of the fundamental solution for a small argument. After discretization of the non-hypersingular traction BIEs and satisfying the boundary conditions on the existing boundaries, an algebraic system of equations in respect to the unknowns is obtained and solved.

The usage of Gurtin-Murdoch surface elasticity model requires the knowledge of a group of new surface material constants which is difficult to be obtained, especially for materials with coupled properties such as are the PEM. This therefore causes remarkable difficulty in the study of relevant problems of piezoelectric nanostructures. Our work is based on the assumption that the infinitely thin interface layer is elastic isotropic with own surface elastic properties. The surface elastic constants of some single-crystalline materials have been determined by atomic simulations (Miller and Shenoy (2000)) or elaborate experiments (Jing *et al.* (2006)). In Miller and Shenoy (2000) via atomic simulations of FCC Al and diamond Si it is shown that the absolute value of the surface layer thickness h_s is in the order of several angstroms or nanometers. In Zhang *et al.* (2012) it is discussed that the surface modules f^S are merely the scaled versions of their bulk counterparts f^M , that is $f^S \leftrightarrow h_s f^M$, with h_s being the surface layer thickness. In Fang *et al.* (2012) the surface constants which are related to their bulk counterparts through an introduced characteristic length are used. The results available in the literature show that the surface elastic characteristics depend on the material type and on the surface crystal orientation. For real nanomaterials, the value of $\alpha^S = \lambda^S + 2\mu^S$ is in the neighborhood of ± 10 N/m, and negative values are also possible, see Miller and Shenoy (2000). Since our main goal is to gain an intuitive physical picture of the surface effects by applying an efficient numerical BIEM scheme, the surface constants are taken from the literature and for the anti-plane wave motion the following value $\alpha^S = \mu^S = \pm 6.091$ N/m are used, see Sharma *et al.* (2003) and Duan *et al.* (2005).

A dimensionless surface parameter defined as $s = \frac{\mu^S}{2c_{44}^0 d d_s}$ is introduced. A multiplier d_s is used in order to increase a fixed value of the curvature radius d of the semi-circle crack-root of the blunt crack. A dimensionless parameter s is introduced to better gauge interface effects at the nanoscale. More specifically, a macroscopic blunt crack with large radius d leads to values $s \ll 1$, and surface effects can be neglected. In opposite, when this radius shrinks to the nanoscale, then s becomes noticeable and the surface effect should be taken into account.

A non-dimensional frequency defined as $\Omega = c\omega\sqrt{\rho^0 a_0^{-1}}$, $a_0 = \left(c_{44}^0 + \frac{(e_{15}^0)^2}{\varepsilon_{11}^0}\right)$ is used in numerical simulations. The mechanical properties of the used material PZT-4 are given in *Table 1*.

Table 1: Material properties

Material	Elastic stiffness ($10^{10}[N/m^2]$) c_{44}^0	Piezoelectric coefficient (C/m^2) e_{15}^0	Dielectric constants ($10^{-10}[C/Vm]$) ε_{11}^0	Density ($10^3[kg/m^3]$) ρ^0
PZT-4	2.56	13.44	60	7.5

To our best knowledge, no results are currently available for SH-wave scattering by nanocracks in an exponentially graded PEM plane.

Due to this reason the verification of the proposed numerical scheme for the case of anti-plane wave motion is done by solution of the test example for a line macro-crack in a homogeneous PEM plane under an incident normal SH-wave. This test example has been solved by Wang and Meguid (2000) using singular integral equation method. For the aim of comparison the authors use their proposed numerical scheme for:

(a) A single nanocrack with surface parameter $s = 0$ in a graded PEM at prescribing zero values to all coefficients relevant to the inhomogeneity;

(b) Two collinear nanocracks with distance $e = mc$, between them with $m = 0.25c; 0.5c; c; 10c$

The numerical scheme is realized by the verified code basing on *Mathematica 6.0*, see MAT (2007). The following dimensionless parameters are introduced:

(a) dimensionless surface parameter $s = \frac{\mu^S}{2c_{44}^0 d d_S}$, $\mu^S = \pm 6.091$ N/m, c_{44}^0 is the reference stiffness coefficient for homogeneous material. The notation d_S is used in order to decrease or increase the fixed value of the curvature radius d of the semi-elliptic nanocrack root.

(b) dimensionless frequency Ω , defined above;

Fig. 2 presents a comparison between the frequency dependent BEM authors' solution and the solution by Wang and Meguid (2000) for the normalized stress intensity factor defined as $K_{III}^* = \frac{K_{III}}{t_3^{in}\sqrt{\pi c}}$. The PZT-4 material is used in this test example with properties given in Tab. 1. Note that

$\lim_{x_1 \rightarrow \pm c} F_{III}^* = K_{III}^*$ and $\lim_{x_1 \rightarrow \pm c} F_E^* = K_E^*$, see Rangelov and Dineva (2022). Both solutions are very close with percentage difference no more than 5%. The obtained results demonstrate the well-known fact that at a large distance between both collinear cracks the solution of BVP for two cracks recovers the solution of the BVP for a single crack.

The mesh of the blunt nano-crack consists of 10 quadratic boundary elements, 8 along the flat parts and 2 along semi-circles with a fixed radius $d = 0.0375c$. More details for study of the accuracy and convergence of the developed numerical schemes based on the non-hypersingular traction boundary integral equation can be found in Dineva *et al.* (2014), Rangelov and Dineva (2017), (2022), Dineva *et al.* (2019), Rangelov *et al.* (2020a, b).

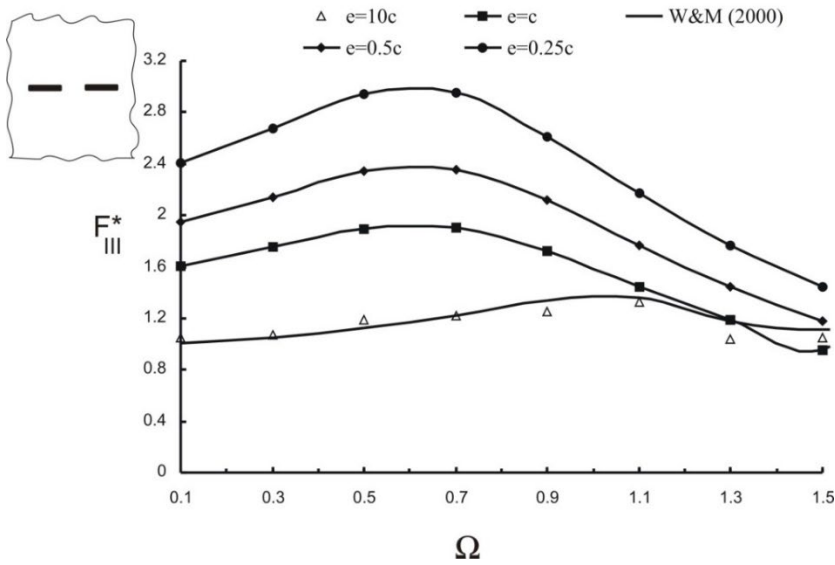


Figure 2: Normalized SCF F_{III}^* at the right crack-tip of the reference nanocrack which is at distance $e = 10c; c; 0.5c; 0.25c$ from the neighbouring collinear nanocrack versus normalized frequency Ω of normal SH-wave in homogeneous PZT-4 plane. Dimensionless surface parameter is zero, i.e. $s=0$.

5. Parametric study

A set of numerical results for a wave loaded blunt nano-crack or a set of nanocracks in a piezoelectric solid is presented highlighting the dependence of

the dynamic stress concentration field on the key model parameters such as: (a) the wave type and wave characteristics; (b) the bulk coupled electroelastic reference material properties; (c) the surface material properties and the corresponding surface effect; (d) the type and properties of the material gradient; (e) the crack-size, the wave-crack, the crack-crack and the crack-solid's boundary interactions.

Illustrative numerical example for Problem 1

Two nanocracks in a graded piezoelectric infinite plane under time-harmonic shear SH wave

Consider a transversally isotropic piezoelectric plane $x_3 = 0$ exponentially graded along the arbitrary direction α in a Cartesian coordinate system $Ox_1x_2x_3$. The plane contains two blunt nano-cracks and the following couples are considered, see Fig. 3a, where S is the reference nanocrack given in Fig.3b: a) two collinear nano-cracks, see the couple S and S_1 in Fig. 3a; b) two parallel nanocracks, see the couple S and S_2 in Fig. 3a; c) two shifted nanocracks, see the couple S and S_3 in Fig. 3a. The model of the reference nanocrack S and the corresponding notations for its length $2c, c \in (10^{-10}m, 10^{-7}m)$ and semi-axes d, d_0 where $d \leq d_0$ of the crack's root presenting as a semi-elliptical shape are given in Fig. 3b.

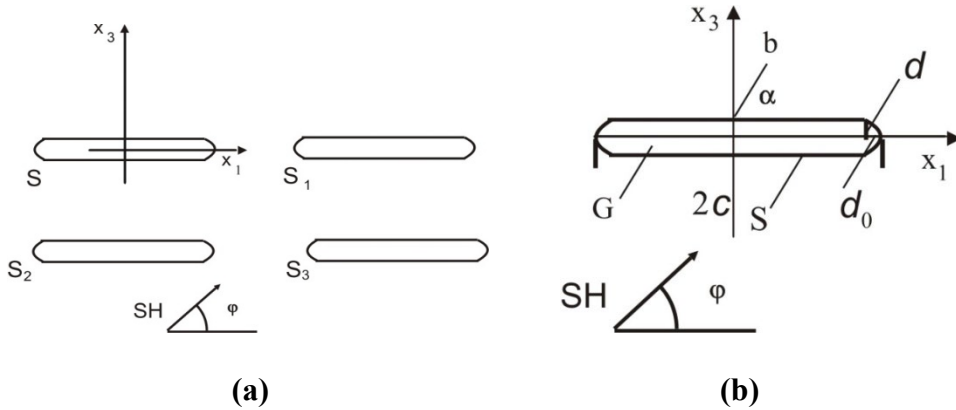


Figure 3: A graded PEM plane under normally incident time-harmonic SH-wave containing: a) collinear nanocracks with boundaries S and S_1 , parallel nanocracks with boundaries S and S_2 , shifted nanocracks with boundaries S and S_3 ; b) reference model of a single blunt nano-crack S .

The nanocracked graded PEM plane is subjected to incident time-harmonic shear SH-wave with frequency ω under incident angle φ with respect to the axis Ox_1 . The poling axis of the piezoelectric material is collinear with the Ox_3 axis and the antiplane deformation state is considered in the plane perpendicular to the poling axis. The non-zero field quantities in the plane $x_3=0$ are mechanical displacement $u_3(x, \omega)$, electrical displacement components $D_i(x, \omega)$, mechanical stress components $\sigma_{i3}(x, \omega)$, strain components $s_{i3}(x, \omega)$, electric field components $E(x, \omega)$ and electric potential $\phi(x, \omega)$, where the position vector is $x = (x_1, x_2)$ and $i = 1, 2$. The material parameters vary in the following way $C_{ijkl}(x) = C_{ijkl}^0 h(x)$, where C_{ijkl}^0 are the reference material properties for homogeneous material, $h(x) = e^{2\langle b, x \rangle}$, $\langle \dots, \dots \rangle$ is scalar product, $b = (b_1, b_2)$, $b_1 = |b| \cos \alpha$, $b_2 = |b| \sin \alpha$, α is the direction of the material gradient and $|b| = \sqrt{b_1^2 + b_2^2}$ is its magnitude. The model of electrically impermeable nanocrack is considered.

All the details describing this problem such as: (a) analytical solution for the incident SH-wave propagating in an exponentially graded PEM plane; (b) the BIEM based on analytically derived fundamental solution for graded PEM; (c) non-classical boundary conditions in the frame of Gurtin-Murdoch theory along anti-plane nanocracks are given in Rangelov and Dineva (2022).

The reference material used in all the simulations is PZT-4 and the dimensionless inhomogeneity magnitude is defined as $\gamma = 2c|b|$.

Let us define the cut-off frequency as $\omega_0 = |b| \sqrt{\frac{a_0}{\rho^0}}$, $a_0 = \left(c_{44}^0 + \frac{(e_{15}^0)^2}{\varepsilon_{11}^0} \right)$. There exist the following three types of solutions with respect to the frequency of the applied load:

- (a) at $\omega = \omega_0$ we have the static case;
- (b) at $\omega < \omega_0$ we have the simple vibration case;
- (c) at $\omega > \omega_0$ we have the wave propagation case.

The mesh employed for each nanocrack S_j , $j = 1, 2, 3$ with $c_0 = 0.0375a$, $a = 2.5 \times 10^{-9}m$, consists of 10 quadratic BEs, 8 BEs along the flat part of the crack's boundary S and 2 BEs along the semi-elliptic left and right parts of S denoted as S^l and S^r correspondingly. Quarter-point BEs for correctly modelling the crack-tip zones where asymptotic generalized displacement behavior is as $O(\sqrt{r})$ at $r \rightarrow 0$ are used.

After discretization of the non-hypersingular traction BIE (12) and satisfying the boundary conditions on the nanocracks, an algebraic system of equations with respect to the generalized displacements along the cracks boundaries is obtained and solved. Note that the obtained integrals are at least

Cauchy principal value integrals. The size of the discretization mesh should satisfy the well-known accuracy condition $\lambda_{SH} > 10l_{BE}$, where λ_{SH} is the wavelength and l_{BE} is the boundary element size.

Once the solution of BIE is known for a fixed frequency ω , the displacement and stress produced by the scattered wave field and by this the total wave field in every point of the piezoelectric plane can be determined via the well-known representation formulae, see Dineva et al. (2014).

What follows is to present a parametric study revealing the dependence of the mechanical and electrical stress concentration zones on the direction and magnitude of the material gradient, on the surface elasticity effect, on the frequency and direction of the incident wave, on the electro-elastic coupling and on the nanocracks dynamic interaction.

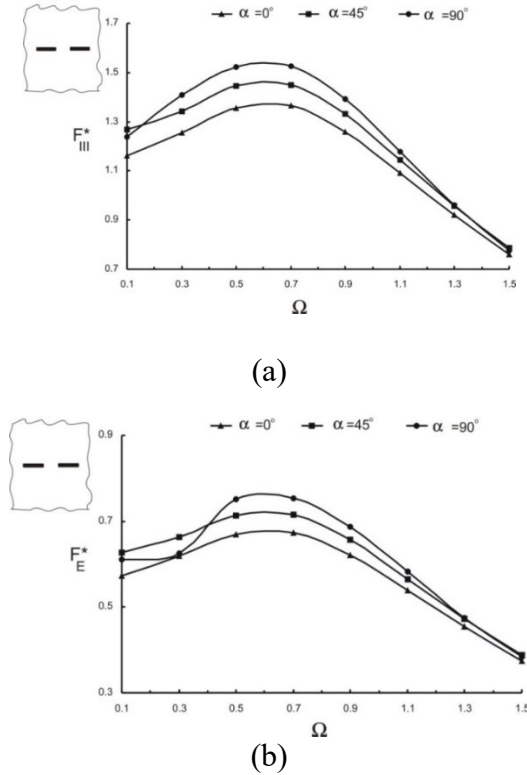


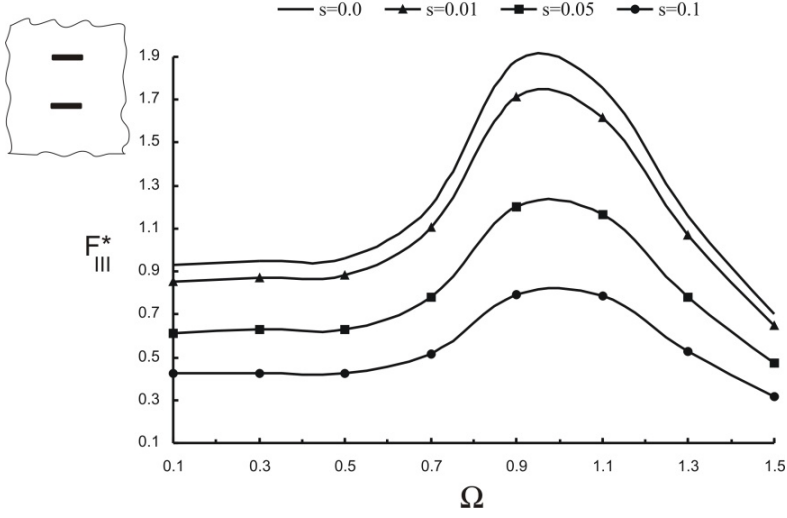
Figure 4: Normalized SCF (a) and EFCF (b) at the right crack-tip of the reference crack versus normalized frequency of a normally incident SH-wave propagating in the graded plane with two collinear nano-cracks S and S_1 at distance $e = 0.25c$ with dimensionless surface parameter $s = 0.02$ for $\gamma = 0.2$ and $\alpha = 0^\circ; 45^\circ, 90^\circ$: a) F_{III}^* ; b) F_E^* .

Fig. 4a and 4b illustrate the sensitivity of the normalized mechanical SCF and EFCF, correspondingly, to the normalized frequency Ω of the incident SH-wave and to the material gradient direction α in the case of two collinear nanocracks S and S_1 with the distance between them $e = \text{dist}(S, S_1) = 0.25c$ and for fixed dimensionless surface parameter $s = 0.02$ at normalized inhomogeneity magnitude $\gamma = 0.2$. These figures show that with increasing angle of the material gradient direction, both SCF and EFCF increase too. Fig. 5a and 5b show the dependence of both SCF and EFCF, correspondingly, on the frequency of the incident shear wave and on the dimensionless surface parameter s in the case of two parallel nanocracks S and S_2 with the distance between them $e = 2c$ and for fixed values of $\gamma = 0.2$ and $\alpha = 0$. Fig. 5a and 5b reveal that with increasing surface elasticity parameter the generalized (mechanical and electrical) stress concentrations decrease significantly. Fig. 6a and 6b are analogous to the scenario in Figs. 5a and 5b but for the case of shifted nanocracks S and S_3 . A comparison between Fig. 4 and 5 shows that the geometrical configuration of nanocracks is in addition an important key factor responsible for the mechanical and electrical fields developing around nanocracks.

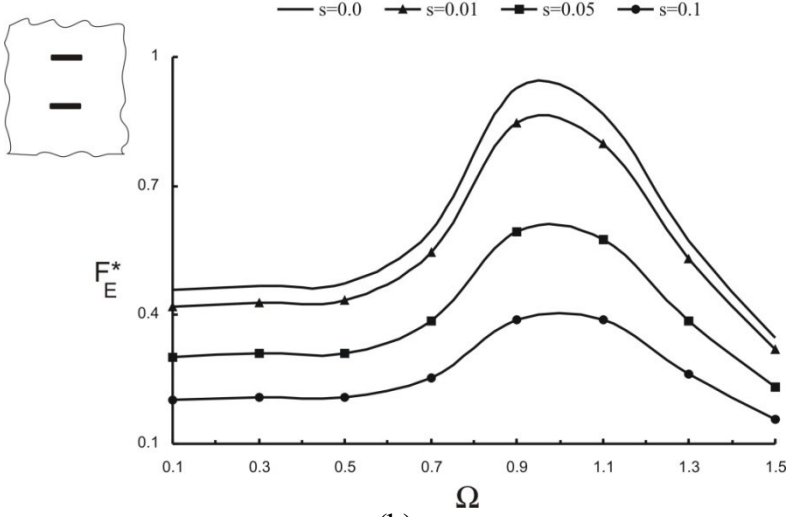
As a conclusion, we can write that an exponentially graded piezoelectric plane containing two nanocracks in arbitrary mutual disposition and subjected to incident time-harmonic SH-wave is studied in this illustrative example.

To the authors best knowledge there is no available results in the literature for the problem under consideration. The proposed numerical scheme is well suited for stress concentration problems by the high BIEM accuracy, since numerical quadrature techniques are directly applied to the BIEs, which represent an exact solution to the problem at hand. Additionally, the fracture mechanics parameters can be accurately recovered from the computed nodal data along the nanocracks in a straightforward manner. BEM formulations have proven to be powerful tools for treating exterior BVPs, as the fundamental solutions obey the Sommerfeld's condition. Therefore, infinite boundaries are automatically incorporated, in contrast to other numerical methods where special transmitting and/or non-reflecting viscous boundaries must be used.

The simulations conducted here illustrate that the non-uniform dynamic stress and electrical field distribution is strongly dependent on several key factors discussed in the presented parametric study. The proposed methodology can be applied in computational nanomechanics, fracture nanomechanics and non-destructive testing of nanomaterials.



(a)



(b)

Figure 5: Normalized SCF (a) and EFCF (b) at the right crack-tip of the reference crack S in Fig. 3a vs normalized frequency of a normally incident SH-wave propagating in the graded plane with two parallel nanocracks S and S_2 at distance $e = 2c$ with dimensionless surface parameter $s = 0, 0.01, 0.05, 0.1$ for normalized inhomogeneity magnitude $\gamma = 0.2$ and nonhomogeneous direction $\alpha = 0^\circ$: a) F_{III}^* ; b) F_E^* .

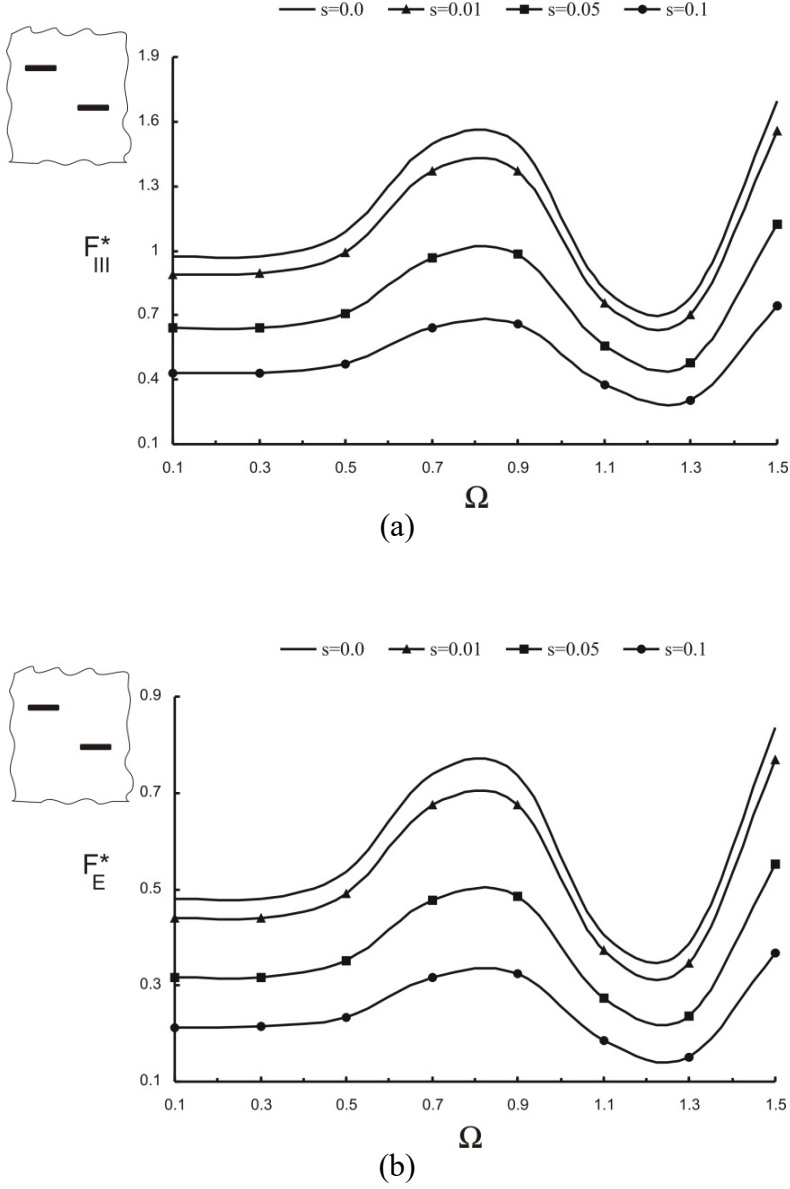


Figure 6: Normalized SCF (a) and EFCF (b) at the right crack-tip of the reference crack S in Fig. 3a versus normalized frequency of a normally incident SH-wave propagating in the graded plane with two shifted nano-cracks S and S_3 at distance $e = 5c$ with dimensionless surface parameter values $s = 0, 0.01, 0.05, 0.1$ for inhomogeneity magnitude $\gamma = 0.2$ and nonhomogeneous direction $\alpha = 0^0$: a) F_{III}^* ; b) F_E^* .

Illustrative numerical example for Problem 2

A rectangular graded piezoelectric finite solid with a nanocrack under time-harmonic electromechanical load

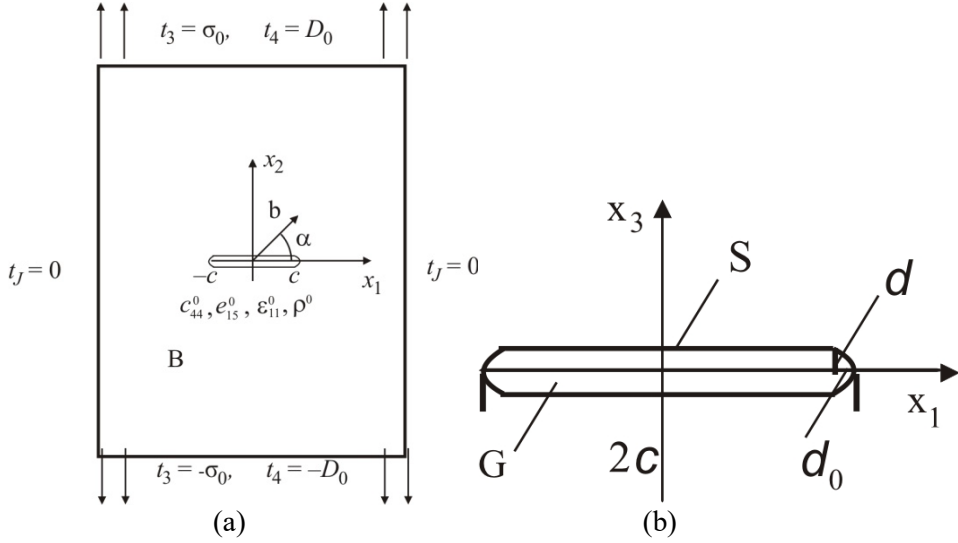


Figure 7: A rectangular graded piezoelectric finite solid (a) with a nanocrack (b) under time-harmonic load.

Consider a finite transversally isotropic piezoelectric rectangular solid B exponentially inhomogeneous along direction α with boundary ∂B in a Cartesian coordinate system $Ox_1x_2x_3$. The solid contains an internal nanocrack (Fig. 7a). The model of the nano-crack is presented by a blunt crack G with boundary S and a crack root with a semicircular shape of radius d , and the perimeter of the crack is $|S| = 2[2(c-d) + \pi d]$, with $d \ll c$, see Fig. 7b. Assume that the piezoelectric material shows hexagonal symmetry with respect to the axis Ox_3 and the poling axis is collinear with the Ox_3 axis. Consider an anti-plane strain state with time-harmonic uniaxial along Ox_2 uniform mechanical traction $t_3 = \pm \sigma_0 e^{i\omega t}$ and electrical displacement $t_4 = \pm D_0 e^{i\omega t}$, where σ_0 and D_0 are the corresponding amplitudes of the applied time-harmonic loads. The boundary conditions along the boundary ∂B are given in Fig. 7a, and along the nanocrack the non-classical condition in the Gurtin-Murdoch model is applied. The inhomogeneity function here is denoted again by $h(x) = e^{2\langle b, x \rangle}$, where the inhomogeneity vector is denoted by b , the direction of material magnitude is α and dimensionless inhomogeneity magnitude is $\gamma =$

$2c|b|$. The reference material is PZT-4. In the numerical analysis, we use the following values for the surface parameter $s = -0.048, 0, 0.024, 0.12$.

The numerical study aims to illustrate the dependence of the mechanical and electrical stress concentration fields on the type and properties of the applied dynamic electromechanical load, on the direction and magnitude of the material gradient, on the coupled electro-elastic fields, on the surface elasticity effects, wave-crack-external solid's boundary and on the wave-crack-material gradient interactions.

All results are for the following cases of loadings: (a) pure mechanical uniaxial load uniform in vertical direction load with amplitude $\sigma_0 = 400 \times 10^6 \text{ N/m}^2$, see Figs. 8-10, 14; (b) uniform time-harmonic electromechanical uniaxial load uniform along the vertical direction with amplitudes $\sigma_0 = 400 \times 10^6 \text{ N/m}^2$ and $D_0 = 0.1 \frac{\epsilon_{11}^0}{e_{15}^0} \sigma_0$, see Figs. 11-14.

Fig. 8 shows the normalized mechanical SCF F_{III}^* and the electrical field concentration factor F_E^* at the left tip of the blunt nanocrack in a homogeneous center-cracked plate for different values of the surface parameter s versus normalized frequency Ω of the mechanical load with amplitude $\sigma_0 = 400 \times 10^6 \text{ N/m}^2$. This figure illustrates the surface elasticity effects when the piezoelectric plate is homogeneous. It is seen that the influence of the surface effect increases with increase of the surface parameter s . For the frequency interval $\Omega > \Omega_0$ and for $s > 0$, the stress concentration factors decrease when the surface parameter s increases. This figure confirms the suggestion that the surface elasticity has a strong effect on the non-uniform stress distribution in a finite nanocracked homogeneous piezoelectric solid. The combined influence of two different phenomena such as the material inhomogeneity and surface elasticity on the stress concentration fields in a finite nanocracked piezoelectric solid can be seen in Fig. 9 and Fig.10 for the case of pure mechanical load and in Fig. 11 and Fig. 12 for the case of electromechanical load. In Figs. 9, 10, 11 and Fig. 12, the material gradient is with magnitude $\beta = 0.2$ and direction $\alpha = 0$. Figs. 9 and 11 show the results for the left crack tip, while Figs. 10 and 12 for the right crack tip. Figs. 9, 10, 11 and 12 illustrate that due to the existence of material gradient, the stress concentration effects are different at the left and at the right crack tip even at one and the same applied loading. It is also evident that the type of the load has also its influence on the mechanical and electrical SCFs, comparing Figs. 9 and 10 with Figs. 11 and 12.

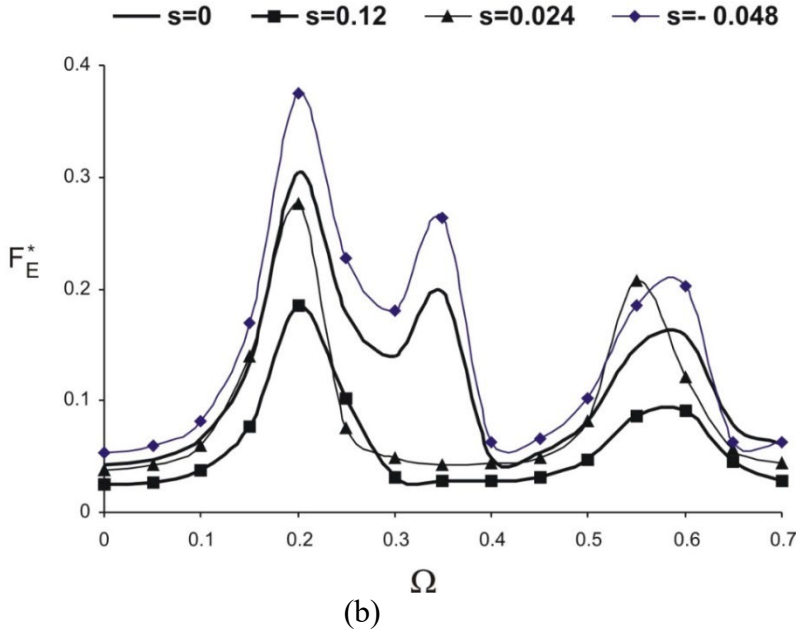
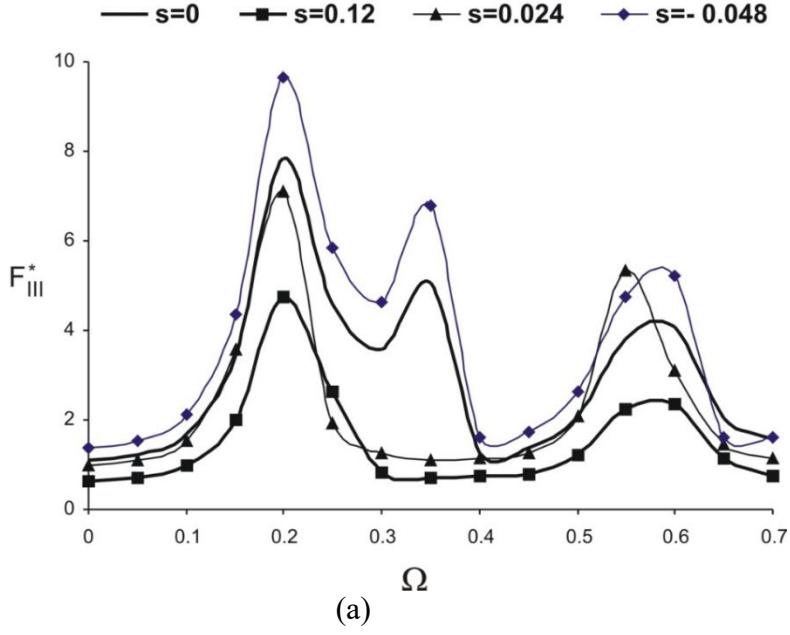
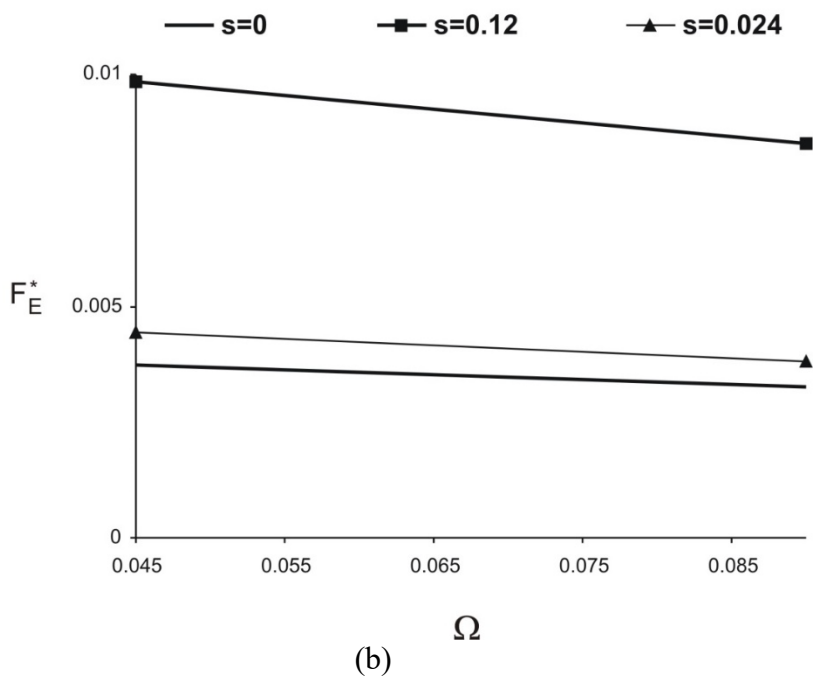
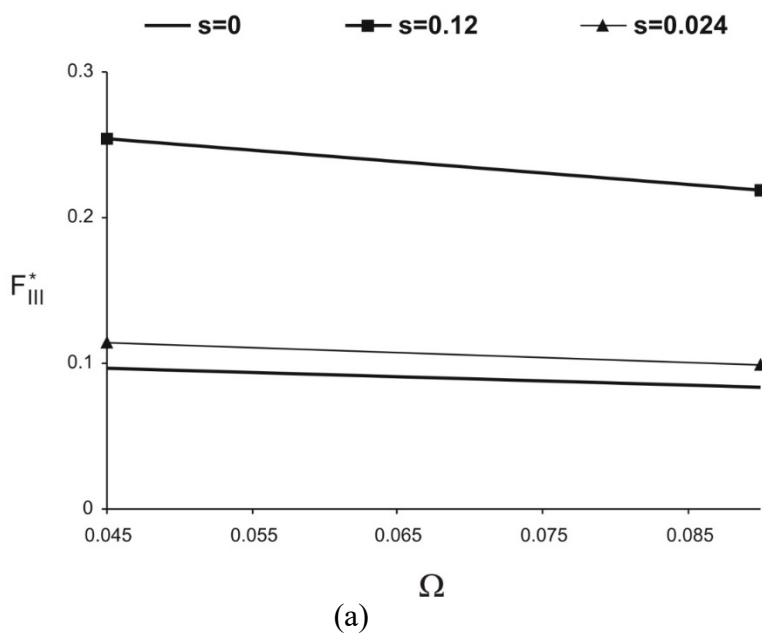
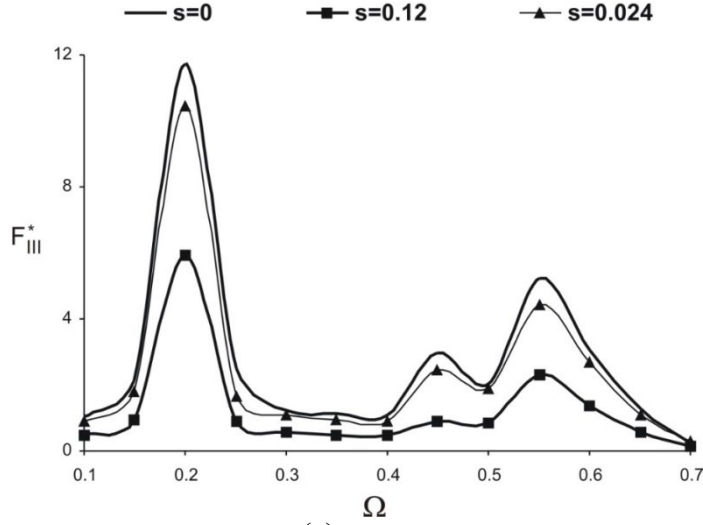
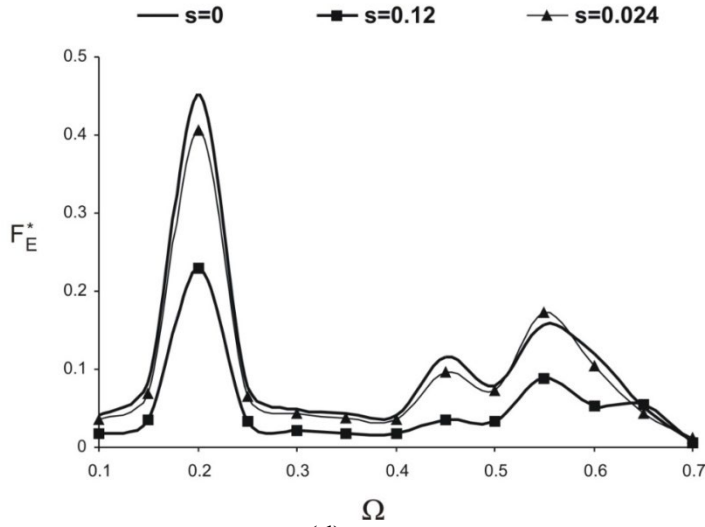


Figure 8: Normalized SCFs F_{III}^* (a) and F_E^* (b) at the left tip of a blunt nanocrack in a homogeneous center-cracked plate for different values of the surface parameter s vs normalized frequency Ω of mechanical load with amplitude $\sigma_0 = 400 \times 10^6 \text{ N/m}^2$.





(c)

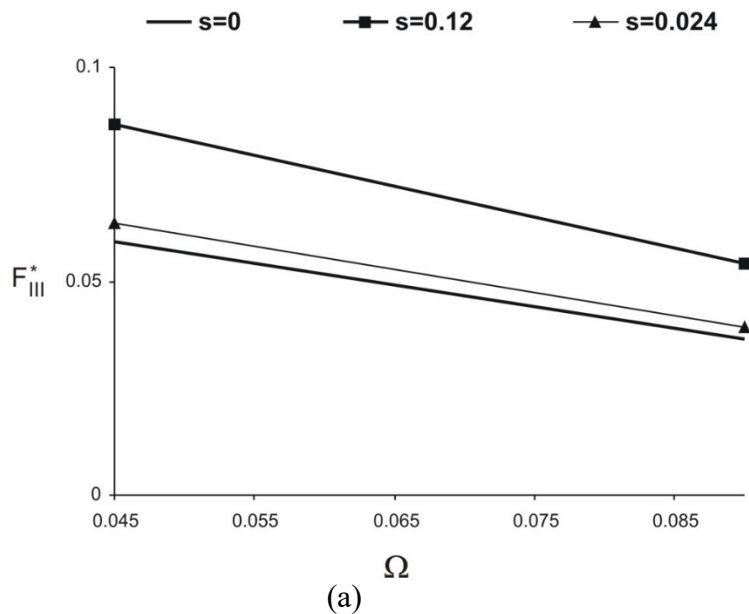


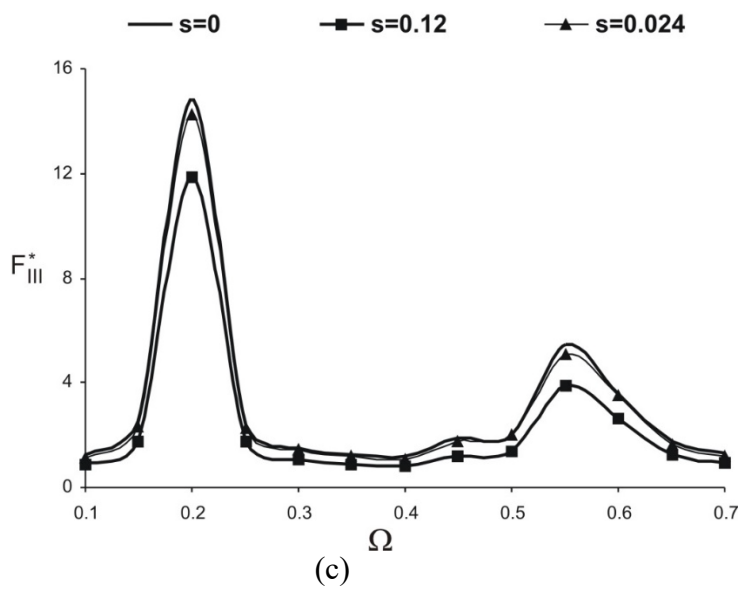
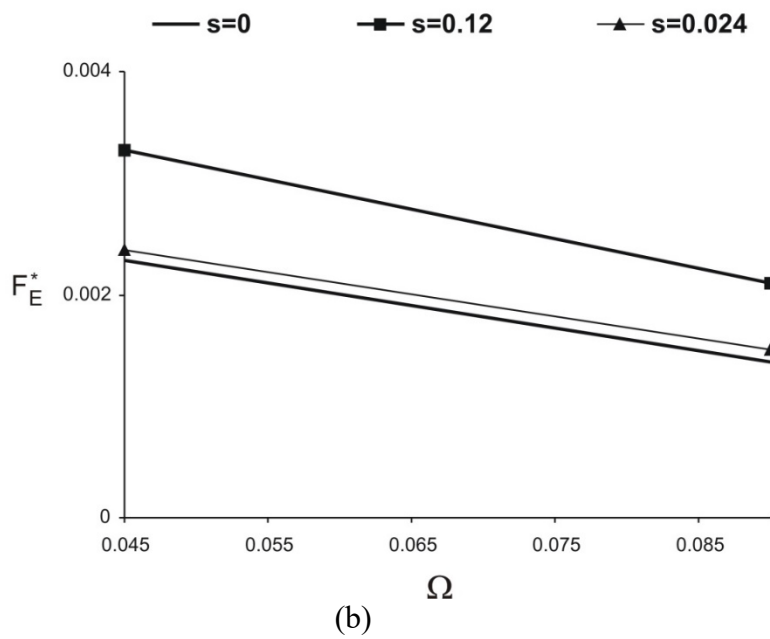
(d)

Figure 9: Normalized SCFs F_{III}^* and F_E^* at the left tip of the blunt nanocrack for different values of surface parameter s vs normalized frequency for inhomogeneous ($\gamma = 0.2$ and $\alpha = 0$) center-cracked plate under mechanical load $\sigma_0 = 400 \times 10^6 \text{ N/m}^2$: (a), (b) F_{III}^* and F_E^* for $\omega < \omega_0$; (c), (d) F_{III}^* and F_E^* for $\omega > \omega_0$.

Additionally, to the above factors, we should add the strong influence of the surface elasticity effect appearing due to the size of the crack, i.e., due to

the existence of nanocracks in the solid under consideration. Fig. 13 presents the normalized SCFs F_{III}^* and F_E^* at the right tip of the blunt nano-crack for different values of the surface parameter s versus the normalized frequency Ω for an inhomogeneous ($\gamma = 0.2$ and $\alpha = \pi/2$) center-cracked plate under electromechanical load for frequencies $\Omega < \Omega_0$ and for $\Omega > \Omega_0$. The sensitivity of the SCFs to the direction of the material gradient is visible when comparing Fig. 12 and Fig.13. Note that in the case of $\alpha = \pi/2$, i.e., when the material gradient is perpendicular to the crack, the SCFs at the left and at the right crack tips are equal, in opposite of the case when the material inhomogeneity is with direction along the crack. Fig. 14 shows the normalized SCFs at the right tip of the blunt nano-crack for two different values of the surface parameter $s = -0.048, 0, 0.12$ versus magnitude $\gamma = 0, 0.05, 0.1, 0.15, 0.2$ of the material gradient in the center-cracked piezoelectric plate under mechanical load at fixed values of the normalized frequency $\Omega = 0.2$ and inhomogeneity direction $\alpha = \pi/2$. This figure illustrates the combined role of the key factors such as the surface elasticity due to the cracks with sizes at nanoscale, continuous inhomogeneity and electromechanical effects due to the graded and coupled nature of the piezoelectric material.





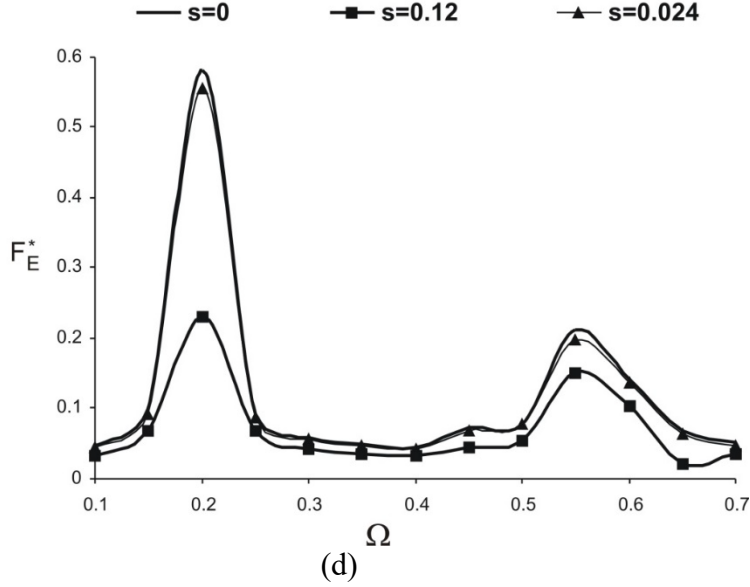


Figure 10: Normalized SCFs F_{III}^* and F_E^* at the right tip of the blunt nanocrack for different values of the surface parameter s vs the normalized frequency Ω for an inhomogeneous ($\gamma = 0.2$ and $\alpha = 0$) center-cracked plate under mechanical load $\sigma_0 = 400 \times 10^6 \text{ N/m}^2$: (a), (b) F_{III}^* and F_E^* for $\omega < \omega_0$; (c), (d) F_{III}^* and F_E^* for $\omega > \omega_0$.

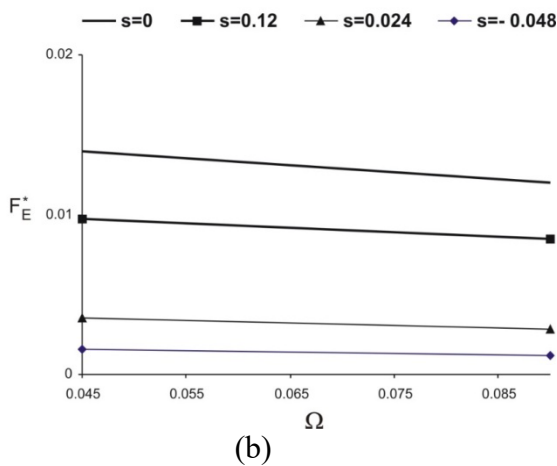
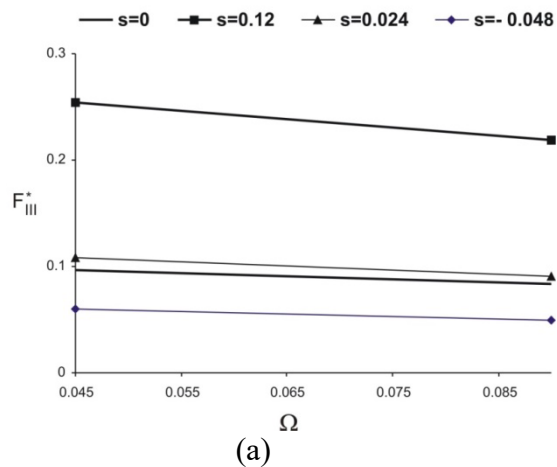
The following conclusions can be drawn from the above-shown parametric study:

- (i) In most of the obtained results, the SCFs for the inhomogeneity case are lower than for the homogeneous one but this effect is frequency dependent and SCFs are continuous at the critical normalized frequency Ω_0 ;
- (ii) For the inhomogeneity direction $\alpha = \pi/2$, the SCF is equal at points close to both left and right crack tips;
- (iii) For the inhomogeneity direction $\alpha = 0$, the magnitude of the SCF at the left crack tip and at the right crack tip is different;
- (iv) For the frequencies above the critical ones, the decrease of the dimensionless surface parameter $s > 0$ provokes increase of the SCF near the crack tip in the whole considered frequency interval, while for frequencies below the critical ones the situation is reverse.

The simulations reveal that the dynamic non-uniform stress and the electric field distribution in a finite inhomogeneous piezoelectric nano-

cracked solid is a complex result of the mutual interaction of different key factors such as: the type and the characteristics of the applied load; the type of material gradient and its magnitude and direction; the crack interaction with the external boundary of the bounded solid; the wave–crack interaction; the size of the blunt crack root curvature and surface elasticity effects.

The proposed methodology can be applied further for the solution of dynamic nanocrack problems in finite functionally graded nano-composites with multiple cracks, holes and inclusions. The proposed approach has the potential to be used as a base for the evaluation of the fracture state of different nanostructural elements with different type of defects at nanoscale.



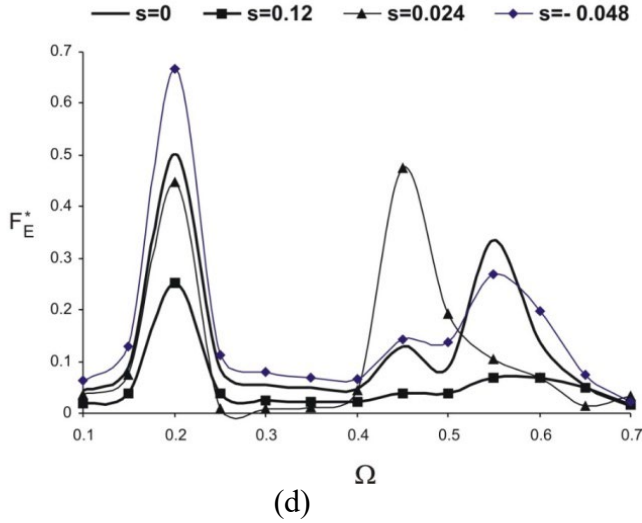
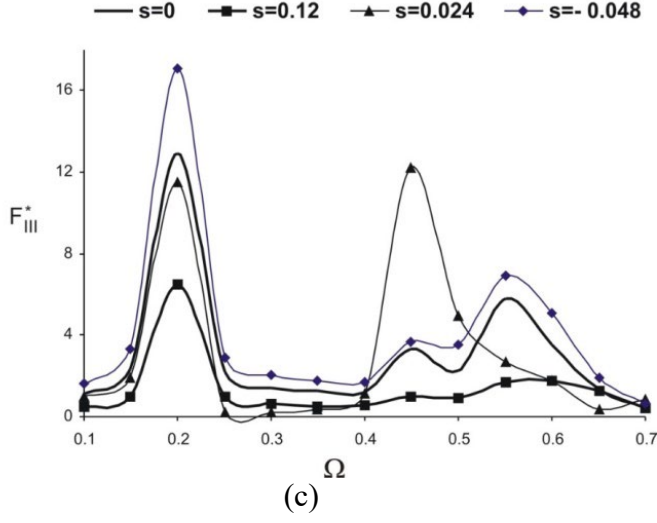
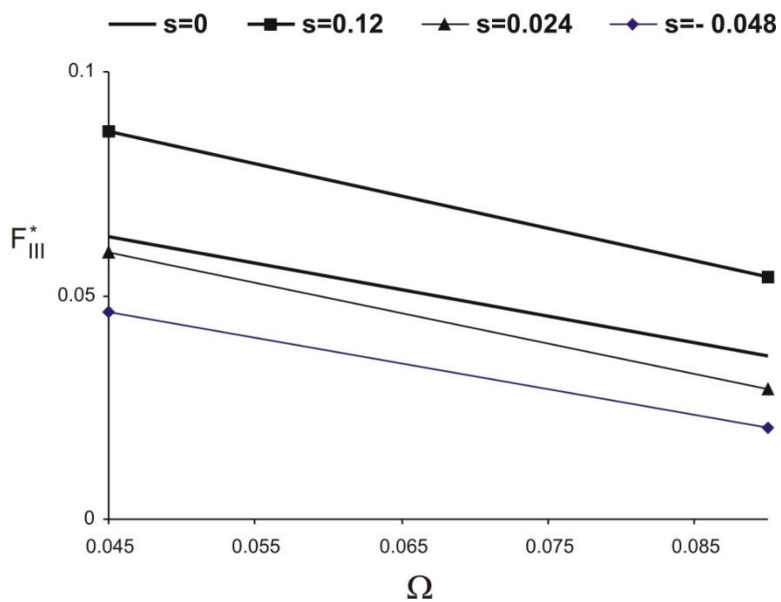
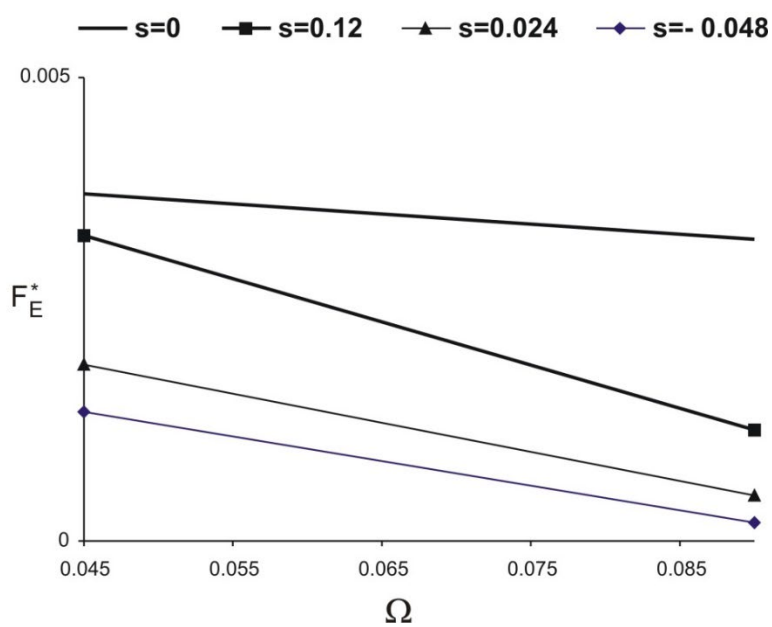


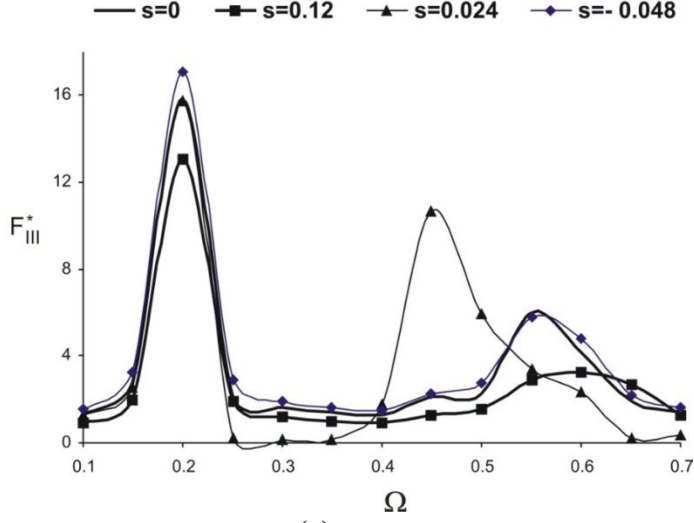
Figure 11: Normalized SCFs F_{III}^* and F_E^* at the left tip of the blunt nanocrack for different values of the surface parameter s vs the normalized frequency for an inhomogeneous ($\gamma = 0.2$ and $\alpha = 0$) center-cracked plate under mechanical load $\sigma_0 = 400 \times 10^6 \text{ N/m}^2$ and electrical load $D_0 = 0.1 \frac{\epsilon_{11}^0}{e_{15}^0} \sigma_0$: (a), (b) F_{III}^* and F_E^* for $\omega < \omega_0$; (c), (d) F_{III}^* and F_E^* for $\omega > \omega_0$.



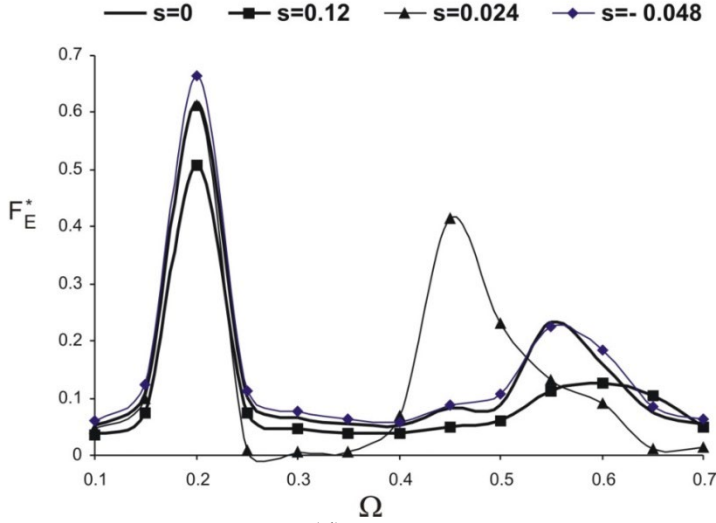
(a)



(b)

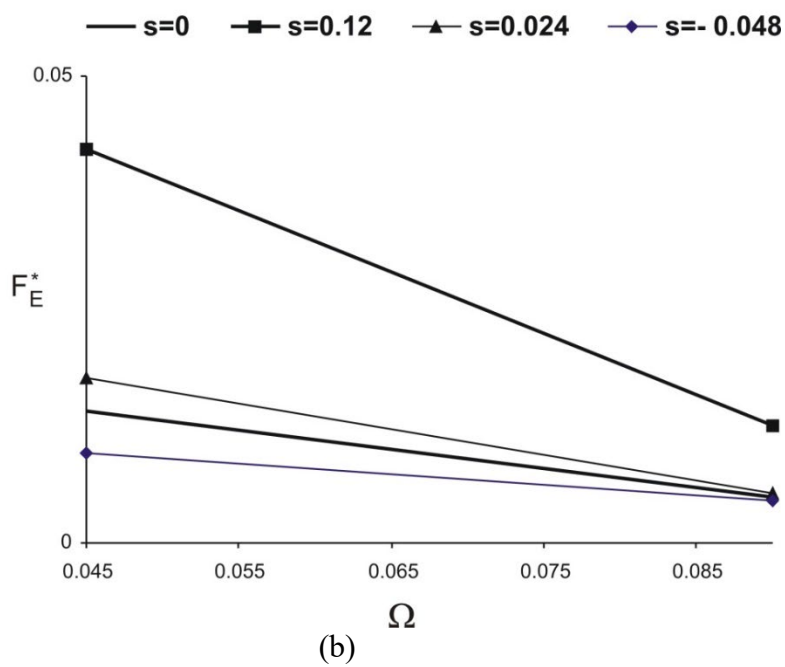
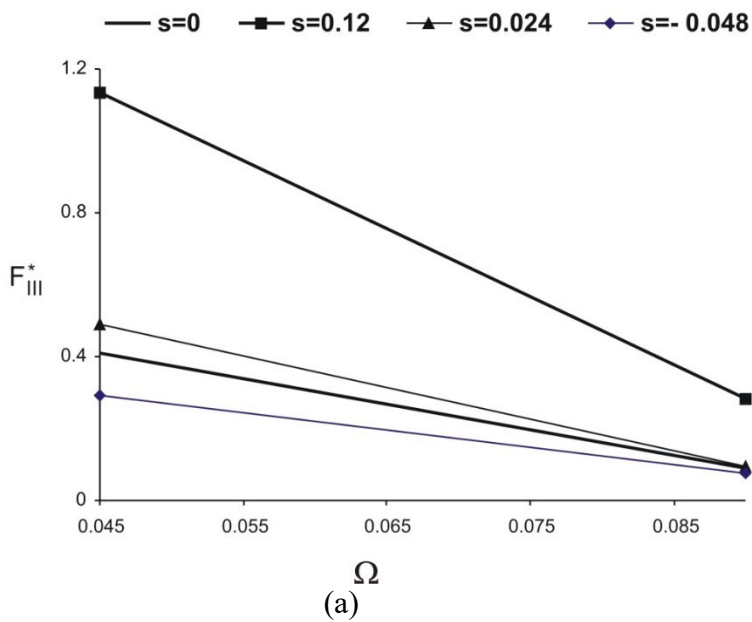


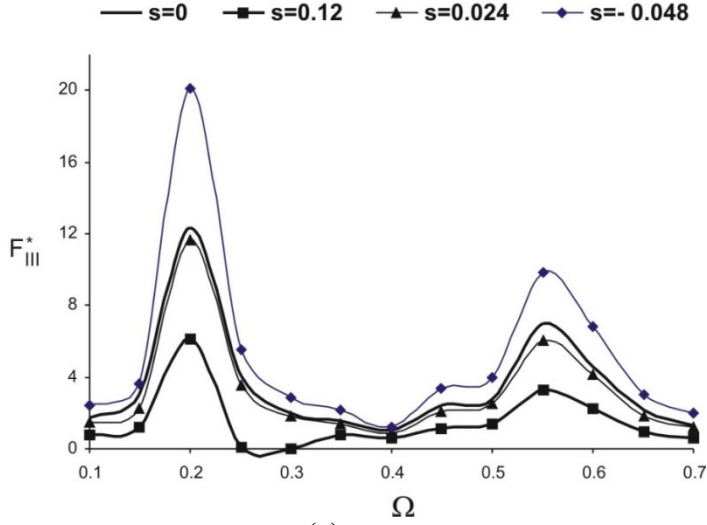
(c)



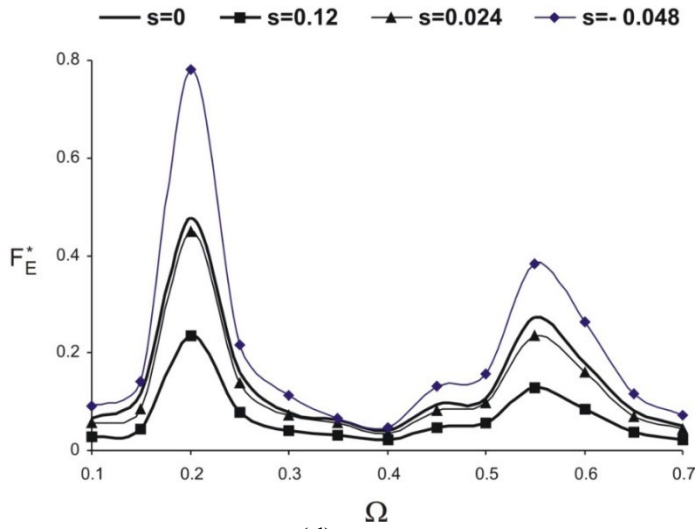
(d)

Figure 12: Normalized SCFs F_{III}^* and F_E^* at the right tip of the blunt nanocrack for different values of the surface parameter s vs the normalized frequency for an inhomogeneous ($\gamma = 0.2$ and $\alpha = 0$) center-cracked plate under mechanical load $\sigma_0 = 400 \times 10^6 \text{ N/m}^2$ and electrical load $D_0 = 0.1 \frac{\epsilon_{11}^0}{e_{15}^0} \sigma_0$: (a), (b) F_{III}^* and F_E^* for $\omega < \omega_0$; (c), (d) F_{III}^* and F_E^* for $\omega > \omega_0$.



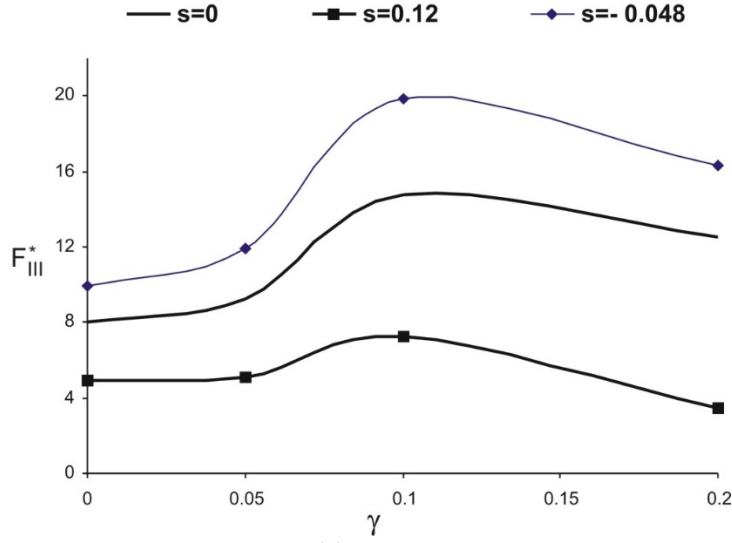


(c)

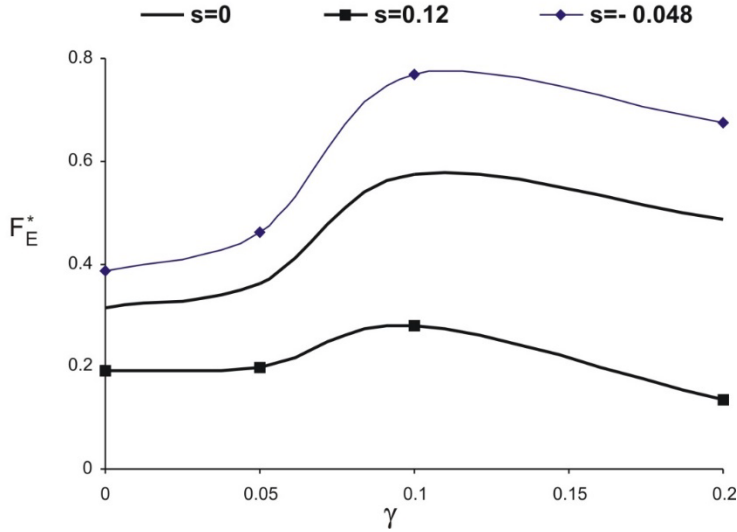


(d)

Figure 13: Normalized SCFs F_{III}^* and F_E^* at the right tip of the blunt nanocrack for different values of the surface parameter s vs the normalized frequency for an inhomogeneous ($\gamma = 0.2$ and $\alpha = \pi/2$) center-cracked plate under mechanical load $\sigma_0 = 400 \times 10^6 \text{ N/m}^2$ and electrical load $D_0 = 0.1 \frac{\epsilon_{11}^0}{e_{15}^0} \sigma_0$: (a), (b) F_{III}^* and F_E^* for $\omega < \omega_0$; (c), (d) F_{III}^* and F_E^* for $\omega > \omega_0$.



(a)



(b)

Figure 14: Normalized SCFs F_{III}^* (a) and F_E^* (b) at the right tip of the blunt nanocrack for different values of the surface parameter s vs different values of the magnitude γ of material gradient in a center-cracked plate under mechanical load $\sigma_0 = 400 \times 10^6 \text{ N/m}^2$ at fixed value of normalized frequency $\Omega=0.2$.

Illustrative numerical example for Problem 3

Time-harmonic nano-cracks interaction in functionally graded piezoelectric half-plane, see Fig. 15.

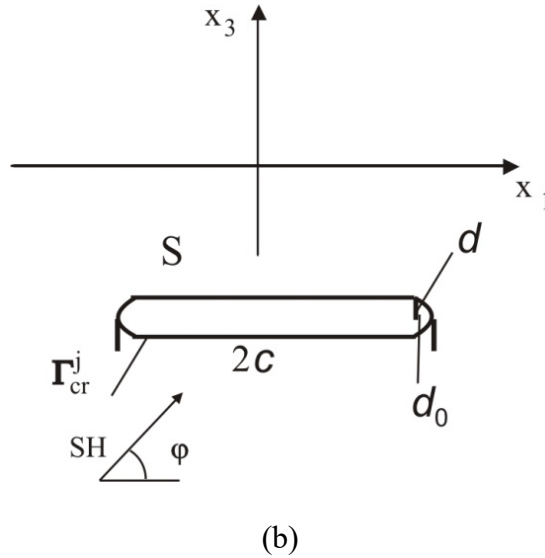
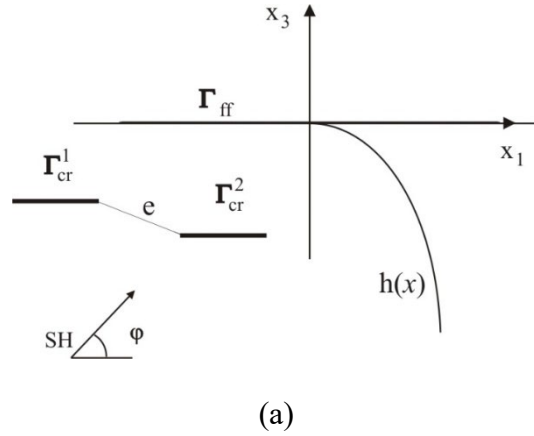


Figure 15: Two nanocracks in a functionally graded half-plane under an incident SH wave in (a); Reference model of a single blunt nano-crack in (b).

In a Cartesian coordinate system $Ox_1x_2x_3$ a graded piezoelectric half-plane $R_-^2 = \{x = (x_1, x_2), x_2 < 0\}$ is considered poled in x_3 - direction and

subjected to a time-harmonic incident SH-wave with frequency ω , see Fig. 15. The only non-vanishing displacements are the anti-plane mechanical displacement $u_3(x, \omega)$ and the in-plane electrical displacements $D_i(x, \omega)$, $i = 1, 2$. The exponential inhomogeneity function $h(x) = e^{2bx_2}$ is characterized by the coefficient b and $c_{44}^0, e_{15}^0, \epsilon_{11}^0, \rho^0$ are the reference material constants.

The boundary condition along the free surface is: $t_j = \sigma_{ij}(x, \omega)n_i(x) = 0$, where $n_i(x)$ is the outward normal vector. Following the Gurtin-Murdoch model, the boundary condition for the mechanical stresses along the crack's line Γ is: $t_3(x, \omega) = -\mu^S \frac{\partial^2 u_3}{\partial l^2}$, where μ^S is the shear modulus of the infinitely thin surface layer S between the crack and matrix. Both nano-cracks are electrically impermeable, i.e., $D_n(x, \omega) = 0$ for $x \in S$.

The total wave field in the graded PEM half-plane is a sum of the free-field wave motion displacements u_K^{ff} and tractions t_K^{ff} and the ones u_K^{sc}, t_K^{sc} scattered by the cracks. The free-field wave displacement and traction in the graded half-plane is the wave motion in the cracks' free half-plane. It is the sum of the incident waves and the reflected ones by the traction-free half-plane boundary. An analytically derived solution for the free-field wave motion is presented in Rangelov and Dineva (2023b).

The aim is to obtain solutions for the frequency-dependent displacements, strains and stresses in the graded PEM half-plane. In addition, the stress concentration fields near the nanocracks are evaluated. The computational tool used for the solution of this boundary-value problem (BVP) is an efficient non-hypersingular traction BIEM based on Green's function analytically derived in Rangelov and Dineva (2023b) for an exponentially graded piezoelectric half-plane. The applied BIEM based on the fundamental solution for a graded PEM full plane is described and verified in Dineva *et al.* (2014). The innovative element here is the solution of the dynamic fracture problem for multiple nanocracks in a graded PEM half-plane with BIEM based on the Green's function.

The numerical scheme is based on discretization and collocation technique. The mesh employed for each nano-crack with half-length $c = 2.5 \times 10^{-9} m$ and curvature radius $d = 0.375 c$ consists of 10 quadratic boundary elements (BEs), 8 BEs along the flat part of the crack's boundary Γ denoted by $\Gamma^+ \cup \Gamma^-$ and 2 BEs along the semi-elliptic left and right parts of Γ denoted as Γ^l and Γ^r correspondingly. Quarter-point BEs for correctly modelling the crack-tip zones where the asymptotic generalized displacement behavior as $O(\sqrt{r})$ at $r \rightarrow 0$ are used.

After discretization of the system of non-hypersingular traction BIEs (12) an algebraic system of equations with respect to the generalized

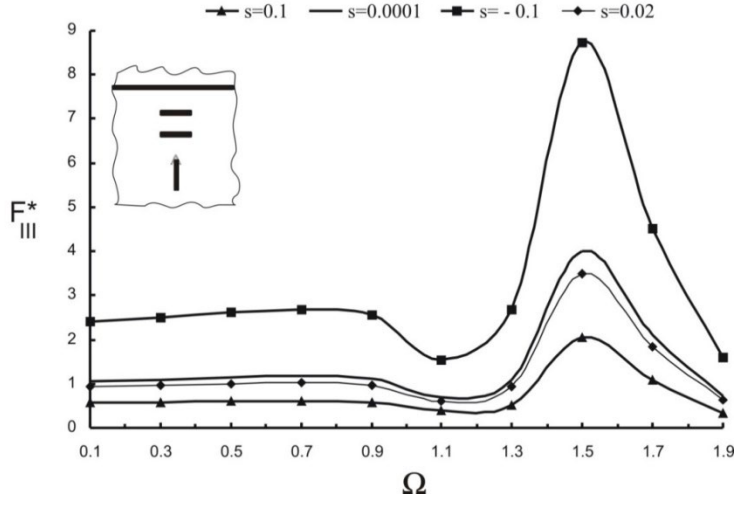
displacements along the cracks' surfaces is obtained and solved. The displacements and strain-stress state at any point of the graded half-plane can be determined by the usage of the well-known integral representation formulae, see Dineva *et al.* (2014). The numerical scheme is realized by the verified code basing on Mathematica software. The reference material is PZT-4.

What follows is a parametric study shown by Figs. 16-19. All the figures illustrate the sensitivity of both the mechanical and electrical concentration fields near the nano-cracks on the following factors:

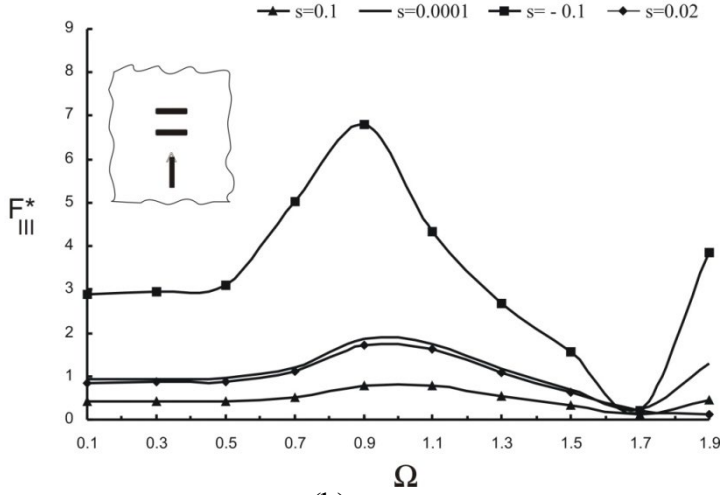
- (a) The frequency of the incident wave and the value of the resonance frequency;
- (b) The geometry of the nanocracks configuration – collinear (Fig.19), parallel (Fig.16, Fig.17) or shifted cracks (Fig.17, Fig.19);
- (c) The influence of the half-plane boundary when Figs. 16a, 17a and Figs. 16b, 17b are compared;
- (d) The surface elasticity phenomenon: the dynamic response decreases with increase of the positive surface elasticity parameter and increases with the negative surface elasticity parameter. This happens because of the destruction and reorganization of the atom symmetry along the interfaces at nano-level.

The size of the crack has strong influence on the scattered and diffraction wave field and also on the local zones of the stress and electrical field concentrations. With decreasing crack size, surface elasticity phenomena arise and *vice versa* -cracks with size at macro-level do not show surface elasticity properties. The normalized displacement amplitude $|u_3|$ along the free surface of the PEM graded half-plane is presented in Fig. 19 for the following fixed data: inhomogeneity magnitude is $\beta = 0.2$, surface elasticity parameter is $s = 0.02$, separate distance between both nano-cracks is $e = 0.5a$, embedded depth is $d = a$, the normalized frequencies of the incident normal SH wave are $\Omega=1.1; 1.3; 1.7$.

Two different crack configuration geometries were studied, namely: (a) two collinear nano-cracks; (b) two shifted nano-cracks.

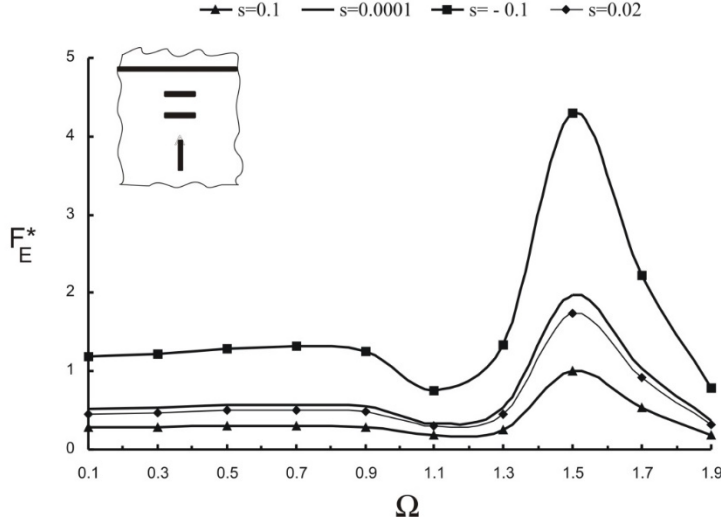


(a)

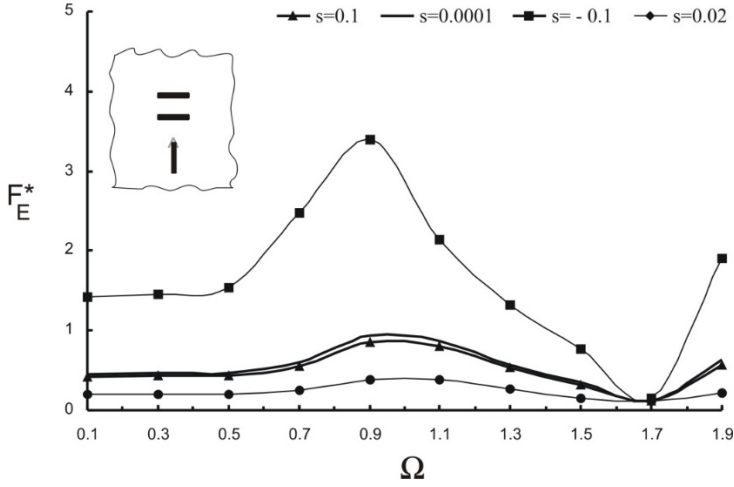


(b)

Figure 16: Normalized SCF F_{III}^* versus Ω at upper nano-crack with embedded depth $d = a$ and distance $e = 0.5a$ from the lower nano-crack due to an incident normal SH wave propagating in: (a) graded PEM half-plane with inhomogeneity magnitude $\gamma = 0.2$; (b) graded PEM full plane with inhomogeneity magnitude $\gamma = 0.2$.

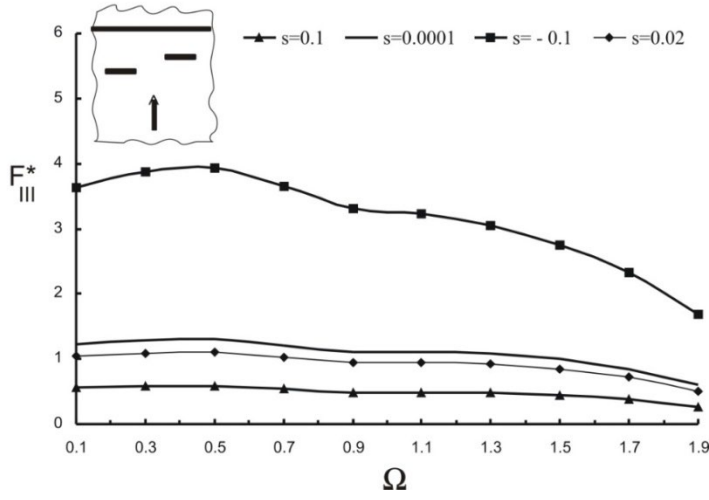


(a)

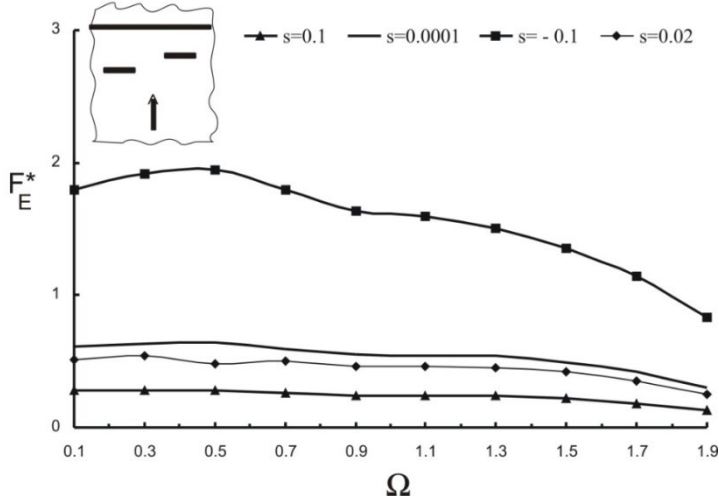


(b)

Figure 17: Normalized EFCF F_E^* vs Ω at upper nano-crack with embedded depth $d = a$ and distance $e = 0.5a$ from the lower nano-crack due to an incident normal SH wave propagating in: (a) graded PEM half-plane with inhomogeneity magnitude $\gamma = 0.2$; (b) graded PEM full plane with inhomogeneity magnitude $\gamma = 0.2$.

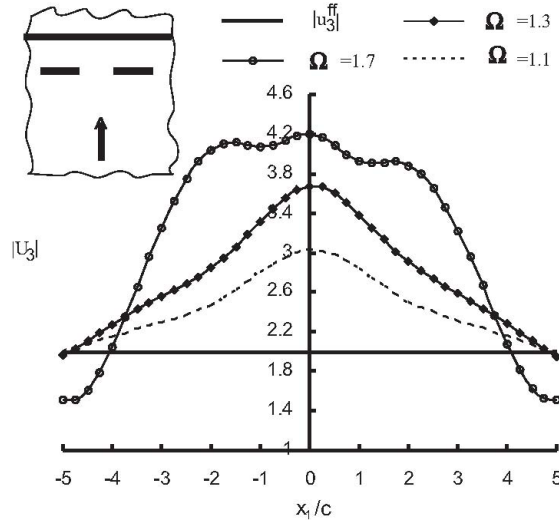


(a)

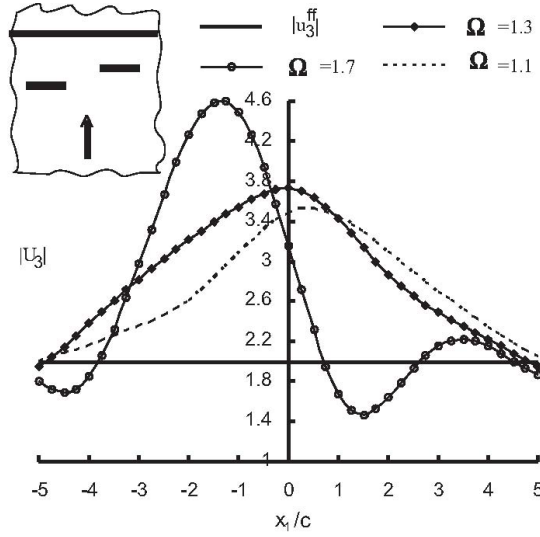


(b)

Figure 18: Normalized mechanical F_{III}^* (a) and electrical F_E^* (b) intensity factors *versus* Ω at the left nano-crack with embedded depth $d = c$ and distance $e = 0.5c$ from the second collinear nano-crack due to an incident normal SH wave propagating in a graded PEM half-plane with inhomogeneity magnitude $\gamma = 0.2$.



(a)



(b)

Figure 19: Normalized displacement amplitude $|u_3|$ along the free surface of the PEM graded half-plane with the following fixed data: inhomogeneity magnitude $\gamma = 0.2$, surface parameter $s = 0.02$, distance between both nano-cracks $e = 0.5c$, embedded depth $d = c$, frequencies of the incident normal SH wave $\Omega = 1.1; 1.3; 1.7$ for two different cracks configuration geometries: (a) two collinear nano-cracks; (b) two shifted nano-cracks.

Figures 19a-19b clearly demonstrate that the scattered wave displacement along the traction-free surface of a graded PEM half-plane is strongly sensitive to the dynamic nano-cracks interaction and mutual nano-cracks configuration.

The obtained results have the potential to be used as a base for the solution of the inverse problems for identification of nano-cracks existence and their position in the functionally graded piezoelectric half-plane. All presented figures show surface elasticity effects. They appear due to the following solids state at nano-level. The number of atoms at the surface increases in respect to that in the bulk as the structural size reduces to the nanoscale. Since the surface atoms are more unstable (broken atomic bonds) than the bulk ones, they may induce the unique properties of nanomaterials.

At the nano scale, the atomic structures in the vicinity of the piezoelectric surface are far from steady. Because of the broken symmetry, they automatically change to be a self-equilibrated state different from those in the underlying piezoelectric bulk. The creation of an additional surface leads to excess of free energy E in the solid, i.e., the surface free energy, which is the origin of the surface effects.

The simulations conducted here illustrate that the non-uniform dynamic stress and electrical field distribution depends on the following key model factors:

- (a) The incident wave characteristics;
- (b) The geometry of the crack configuration and the graded half-plane boundary;
- (c) The type, magnitude and properties of the material gradient;
- (d) The reference material properties;
- (e) The coupled material properties of piezoelectric composite materials;
- (f) The surface elasticity phenomenon and the nano-crack size;
- (i) The ratio of the wave length and the crack length.

The strong influence of the size-effect of nanocracks to the dynamic fracture behavior of cracked piezoelectric material can significantly affect the overall effective dynamic fracture behavior of cracked piezoelectric nanocomposites. The obtained results demonstrate clearly that the piezoelectric cracked solids containing nanoscale cracks possess a unique fracture behavior different from those at macroscale.

The proposed, developed and verified numerical tool has a direct application in nanomechanics and in non-destruction testing of nanomaterials.

6. Conclusion

2D elastodynamic analysis of impermeable nanocracks in graded anisotropic piezoelectric infinite, semi-infinite and finite solids is presented by non-hypersingular traction BIEM in the frequency domain in conjunction with the surface elasticity model of Gurtin and Murdoch. In this model a surface/interface is regarded as an elastic but negligibly thin membrane with the properties that is adhered to the underlying bulk material without slipping and with elastic constants different from the bulk. The equilibrium and constitutive equations in the bulk are the same as those in the classical piezoelectric theory, but the presence of surface stresses gives rise to non-classical boundary conditions taking into consideration the residual surface tension and surface deformation. The use of conventional mechanical models based on continuum mechanics with the appropriate modifications to account for surface effects produces software that is efficient, both in terms of time and memory requirements. This is in contrast to the advanced mechanical models that consider the atomic level, which in turn yields software with very high computational requirements

The novelty of the developed mechanical models and accompanied numerical methodology lies in the effective combination of four stages: *(a)* mechanical modeling based on linear piezoelectricity for graded bulk nanocracked solids combined with the linear fracture mechanics principles; *(b)* introduction of non-classical boundary conditions stemming from localized constitutive equations for the material interfaces; *(c)* efficient numerical implementation of the non-hypersingular traction boundary integral equations based on the closed form frequency dependent free-field wave motion solutions, fundamental solutions and half-plane Green's functions obtained by Bessel or Radon transform, and *(d)* creation and verification of software with low computational cost as numerical modeling is restricted to the surface of the problem in question.

A parametric study for wave scattering and local dynamic stress concentration field near nano-cracks in piezoelectric nanocomposites is presented. The numerical results illustrate that the resulting wave field and non-uniform stress distribution depend on the combined influence of the incident wave type and its properties, the ratio of the wave length and the crack's size, the type of the reference piezoelectric material, the type of material gradient and its characteristics, the size of the blunt crack's root

curvature, the coupled electromechanical field, the nanocracks interaction and the influence of the existing boundaries of the solids under consideration. The decreasing of the radius curvature of the blunt crack to the nano-scale provokes a strong reduction of the intensity of the stress concentration field near the crack-tip in the whole considered frequency interval. The influence of the size effect on the mechanical properties of the nanocomposites is of fundamental interest for the new advanced nano-technologies.

The development of nanomechanical models in a systematic way is still underway, the reason being that such a goal requires multidisciplinary knowledge and skills, which blend continuum mechanics, computational mechanics, material science, mathematical physics, chemistry and physics. In this sense, the results obtained here (a knowledge package of mechanical model, efficient computational methodology, verified authors' software, parametric simulations) are useful and timely for nanomechanics.

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Notations list

Notation	Meaning
$c_{44}(x)[N/m^2]$	elastic stiffness variable
$e_{15}(x)[C/m^2]$	piezoelectric variable
$\varepsilon_{11}(x)[C/Vm]$	dielectric variable
$\rho(x)[kg/m^3]$	density variable
$c_{44}^0[N/m^2]$	reference elastic stiffness coefficient
$e_{15}^0[C/m^2]$	reference piezoelectric coefficient
$\varepsilon_{11}^0[C/Vm]$	reference dielectric constant
$\rho^0[kg/m^3]$	reference density
$h(x)$	inhomogeneity function
b	inhomogeneous vector
α and $ b $	direction and magnitude of the material gradient
u_3 [m]	displacement component
σ_{13}, σ_{23} [N/m ²]	stress tensor components
s_{13}, s_{23}	strain tensor components
E_1, E_2 [V/m]	electric field components

D_1, D_2 [C/m ²]	electrical displacements components
ϕ [V]	electrical potential
$u_J, J=3,4$	generalized displacement
u_J^{sc} u_J^{in}	generalized scattered displacement generalized incident displacement
u_J^{ff}	generalized free-field motion displacement
$\sigma_{ij}, i = 1,2, J=3,4$	generalized stress tensor
$C_{ijkl}(x)$	generalized stiffness tensor variables
C_{ijkl}^0	reference generalized stiffness tensor
$\rho_{JK}(x)$	generalized density
ω [1/sec]	frequency
t_3 [N/m ²]	mechanical traction
$t_J, J=3,4$	generalized traction components
t_J^{sc} t_J^{in} t_J^{ff}	generalized scattered traction generalized incident traction generalized free-field motion traction
n_1, n_2	outward normal vector components
μ^S [N/m]	shear modulus of the infinitely thin surface layer S between the nanocrack and matrix
$\delta_{\lambda\lambda}$	Kronecker symbol
u_{QK}^*	fundamental solution (in Problems 1 and 2) and Green's function (in Problem 3)
σ_{iJK}^*	stress tensor corresponding to u_{QK}^*
γ_{RJ}	the jump term at the source point in BIE
F_{III}^*	normalized stress concentration factor
F_E^*	normalized electrical field concentration factor
σ [N/m ²]	magnitude of the mechanical load
s	dimensionless surface parameter
Ω	dimensionless frequency
γ	normalized inhomogeneity magnitude
c [m]	crack's size parameter
d, d_0 [m]	semi-axes of blunt nanocrack-root in the shape of a semi-ellipse

$\Gamma; \Gamma_{ff}; \Gamma_{cr}$	general notation for boundary; half-plane boundary; nanocrack boundary
φ [degree]	incident wave angle

Chapter 4. Numerical modelling of elastic nanocomposites with nanoholes and nanoinclusions subjected to dynamic loads by boundary element method

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Annotation

This chapter presents a systematic BEM study on the dynamic response of infinite, semi-infinite, and finite isotropic/anisotropic nanocomposite solids with nanocavities, nanoinclusions, or nanorelief under time-harmonic or rapidly applied transient stress pulses along the existing boundaries. In nanostructured composites, the nanoscale is a key factor offering significant advantages, and the surface/interface can have a substantial impact on the mechanical properties of solids. Surface stress relates the variation in excess free energy to the strain at the surface. For this reason, the surfaces and interface boundaries of solids exhibit different mechanical properties compared to their bulk counterparts. *The mechanical models developed here are based on the classical elastodynamic theory for the elastic isotropic/anisotropic bulk solid and the non-classical boundary conditions along its boundary derived in surface elasticity theory by Gurtin and Murdoch (1975). The computational tool is an efficient direct displacement boundary element method (BEM) based on the frequency-dependent elastodynamic fundamental solution for elastic isotropic or generally anisotropic material. The numerical scheme verification is discussed.*

The simulations illustrate the dependence of the wave field in nanocomposites on the material anisotropy, on the surface elasticity properties, on the nanorelief peculiarities, on the nanocavities/nanoinclusions existence and their dynamic interaction, and on the type of the dynamic load.

The obtained results demonstrate the potential of the mechanical models developed using boundary integral equations within the framework of surface elasticity theory to produce highly accurate results, while employing a significantly reduced discretization mesh compared to domain-based methods.

The developed knowledge package on the dynamic behavior of nanocomposites has applications in high technology fields such as bioengineering, biomedicine, optics, electronics, photonics, pharmaceuticals, new structural materials and design of advanced electromechanical systems.

1. Introduction

Static and dynamic analyses of elastic media containing cavities, inclusions, cracks, relief peculiarities or layers are important problems with many applications in material science, non-destructive evaluation, computational geophysics and fracture mechanics. Elastic wave propagation through heterogeneous materials causes reflection, refraction, diffraction, and scattering phenomena which are further complicated by the presence of discontinuities such as cracks, cavities, and inclusions as they are scatterers and stress concentrators. In addition, due to these heterogeneities size-dependent phenomena appear in the scattered wave and dynamic stress concentration fields in the contemporary nano-mechanical systems. Miniaturization of electronic industry and nanofabrication requires an in-depth understanding of surface effects on the mechanical properties of the bulk. Surface elasticity is negligible for macroscopic bulk materials which, to some extent, explain why surface elasticity did not draw significant interest until recent years. The reliability of interconnects in integrated circuits is crucial, and their failures often arise from various mechanisms such as thermal stress and mechanical fatigue. In some cases, the nucleation and growth of even a single nanocavity can cause interconnects failure. Due to their specific behavior, nanostructures play an important role in modern hi-tech smart systems. At the same time their brittleness and low toughness make them very sensitive against defects like nanoholes, nanoinclusions, nanocracks or others. One reason for that is the observation that a precursor of final failure often is the formation of interacting nanodefects which subsequently coalesce to a macro-one.

With the rapid development of nano-mechanical systems, size-dependent phenomena emerge in both the scattered wave fields and the localized dynamic stress concentration fields of nano-structures with heterogeneities. The manifestation of surface energy at the nanoscale is due to the relaxation of bonds between surface atoms, leading to the formation of surface residual stress. As a result, the mechanical properties of nano-structured materials exhibit a strong size dependency, which has been explained within the framework of continuum mechanics by incorporating the effects of surface stresses. The physical origin of surface/interface energy and surface/interface

stresses in solids has been discussed by many researchers (e.g., Gibbs (1906) among others). The basic conceptual models in nanomechanics are as follows: (a) discrete models such as ab initio models ($\approx 10^{-9}$ m) governed by Schrödinger equation (Kudin *et al.* (2001)), atomistic/molecular models ($\approx 10^{-7}$ m) described by Newtonian mechanics (Belytschko *et al.* (2002)), mesoscopic ones ($\approx 10^{-7}$ m) (Müller-Plathe (2002)); (b) continuum mechanics based models comprising pure solid mechanics models ($\approx 10^{-2}$ m) (Guz and Rushchitsky (2003)) and models extending the range of classical continuum mechanics by bridging its basic theoretical principles with the most fundamental effects observed at the nanolevel, such as higher order non-local elasticity models Sladek *et al.* (2018) and surface elasticity models, see Parvanova and Dineva (2015), Rangelov *et al.* (2020), Dineva *et al.* (2019, 2021); (c) multiscale models, see Xiao & Belytschko (2004).

This work focuses on the Gurtin and Murdoch (1975) model, which belongs to the group of surface elasticity models based on continuum mechanics. They developed a mathematical framework for studying the mechanical behavior of nanosolids, incorporating surface stress within the continuum mechanics formalism. The Gurtin-Murdoch theory was partly motivated by empirical observations that indicated the presence of compressive surface stress in certain types of crystals. The surface elasticity phenomena arise from different sources, among them: (a) interatomic bond-breaking when new surfaces are created; (b) surface relaxation or reconstruction, see Wan *et al.* (1999), Ojaghnezhad and Shodja (2012) and (c) interatomic bond stretching and reorientation under applied macroscopic strains. The relevance of the *Gurtin-Murdoch* theory hinges on accurate experimental measurement of the surface elasticity tensor modulus. Experimental progress along this direction is still limited, except for a few important efforts by Goudeau *et al.* (2001), Hurley *et al.* (2001), Cuenot *et al.* (2004), Gavan *et al.* (2009), Paulitschke *et al.* (2013). In this theory, a solid surface is considered as a zero-thickness layer which is attached to the bulk, and a second-order tensor representing the “surface stress” is introduced. The surface stress tensor is associated with the bulk stress tensor and the external load by means of a force balance equation established on the solid surface. Under the assumption of small deformation, a linear constitutive relationship between surface stress and surface strain is established via a fourth-order tensor consisting of the “surface elastic moduli” and the resulting equation system is thus completed.

Below is a review of the modeling of the dynamic behavior of single and multiple nanocavities and nanoinclusions within the framework of the Gurtin-Murdoch theory.

(A) Models in respect to the type of the stress-strain state in nanocomposites:

(A1) Static and dynamic anti-plane problems

The anti-plane strain problem for an elliptic nanoinclusion, nanocavity and nanocrack in an infinite elastic matrix under uniform static loading was considered by Luo and Wang (2009), who used a semi-analytical method based on conformal mapping with complex number formalism. The influence of interfacial effects on the dynamic stress field that develops around nanocavities and nanoinclusions swept by time-harmonic, horizontally polarized shear (SH) waves can be found in a limited number of papers. Since fatigue-induced failure often occurs in regions with high stress concentrations, understanding how dynamic stresses redistribute around nanoheterogeneities is crucial for design purposes. In particular, SH wave diffraction by nanoinclusions was studied analytically by Fang *et al.* (2010a, 2010b, 2013) and Yang *et al.* (2012). More specifically, the elliptical nanoinclusion in an infinite plane under SH waves was studied using a combination of conformal mapping and the wave function expansion method by Fang *et al.* (2010a). Also, the wave function expansion method combined with the method of images was used by Fang *et al.* (2013) for tracing dynamic stress concentration effects around two nanowires in the infinite plane, and similarly by Yang *et al.* (2012) for solving the cylindrical nano-inclusion problem embedded in a semi-infinite solid.

(A2) Static in-plane problems

Plane strain elastostatic solutions for holes and inclusions at the nano-scale are presented in Dong (2012), Fu and Wang (2010), Morozov and Semenov (2013), Sharma and Wheeler (2007), Xu and Dong (2016). In-plane problems for a single nanoinclusion or a nanocavity of circular or elliptic shape in an infinite plate subjected to far-field static loads were solved by Tian and Rajapakse (2006, 2007a, 2007b), Wang and Wang (2006) and Mogilevskaya *et al.* (2008) using analytical or semi-analytical methods. Next, Dong and Pan (2011), Jammes *et al.* (2009) and Dong (2012) developed BEM formulations capable of handling surface effects at the nanoscale, while similar developments using the finite element method (FEM) were accomplished by Gao *et al.* (2006) and Wang *et al.* (2010a, 2010b). More specifically, multiple circular cavities and/or inclusions at the nanoscale are considered in Mogilevskaya *et al.* (2008), Dong and Pan (2011), Dong (2012) and Gao *et al.* (2006), while the case of a halfplane containing nanoinhomogeneities can be found in Jammes *et al.* (2009). Finally, Fu and Wang (2010) evaluated the elastic stress fields around nanosized

heterogeneities and grooves indented across solid surfaces. These last researchers also examined the static in-plane problem for an infinite plane under remote loading containing a circular and an elliptic nanocavity, an elliptic nanoinclusion and finally square plus triangular nanoinclusions.

(A3) Dynamic in-plane problems

This category of problems involves wave diffraction of time-harmonic pressure (P) and vertically polarized shear (SV) waves by nanocavities and nanoinclusions. These were studied analytically by Wang (2009) who considered two circular cavities, by Zhang *et al.* (2011) for an array of cylindrical cavities, by Wang *et al.* (2006) for a single circular cavity and finally by Ru *et al.* (2009) for a single cylindrical nanocavity and a single nanoinclusion. Furthermore, Fang *et al.* (2010b) analytically evaluated the influence of both surface and interface effects on the dynamic stress field around a single circular cavity, a single circular inclusion and two interacting circular inclusions in an infinite matrix under P-waves.

(B) Models in respect to the type of the nanocomposite solid:

(B1) Elastostatic results for infinite solids with holes and inclusions at the nano-scale

Nano-holes with elliptical, circular and arbitrary shapes, respectively, are studied in Wang and Wang (2006), Wang *et al.* (2010b) and Wang *et al.* (2014), while nano-inclusions are considered in Mogilevskaya *et al.* (2008), Dong and Pan (2011), Tian and Rajapakse (2007a). The original Gurtin and Murdoch model was used for the first time in Mogilevskaya *et al.* (2008) to solve the problem of multiple, arbitrarily located, circular nano-inclusions and nano-pores in an infinite bulk material. In most publications, simplified versions of the complete Gurtin and Murdoch equations are used, where either the entire or part of the surface displacement gradient term is neglected. In Dong and Pan (2011), results for an infinite plane with both a nano-cavity and a nano-inclusion are given, where in the latter case a square and an equilateral triangle are considered. Anti-plane strain static results can be found in Wang and Schiavone (2013), where a nanosized elliptical hole for the anisotropic solid is studied and in Luo and Wang (2009), where a nanosized elliptical inclusion in a plane under shear loading is considered.

(B2) Elastostatic results for semi-infinite solids with holes and inclusions at the nano-scale

A model for a half-plane with a circular nano-hole, a circular nano-inclusion, two circular nano-inclusions, a system of nano-holes and nano-inclusions, a

group comprising a circular nanohole and two elliptic inclusions are all presented in Dong and Lo (2013). Surface tension-induced stress concentration around a nanosized hole of arbitrary shape inside an elastic isotropic half-plane is given in Dai *et al.* (2014), while in Dai *et al.* (2016a) the same problem is solved for an anisotropic half-plane. Anti-plane strain cases are solved in Dai *et al.* (2016b), where a half-plane containing a nearby nanosized hole incorporating surface effects not only at the edge of the hole but also at the edge of the half-plane is studied. Finally, a screw dislocation interacting with a nanoscale cylindrical inclusion in an elastic half-plane is considered in Li *et al.* (2013).

(B3) Elastostatic results for finite solids with holes and inclusions at the nano-scale- to the authors' knowledge there are no results for this BVP.

(B4) Elastodynamic results for infinite solids with holes and inclusions at the nano-scale

Plane strain problems for wave scattering, diffraction and stress concentration are solved in Qiang *et al.* (2013), Wang (2009) for cylindrical nano-holes and in Parvanova *et al.* (2015), (2016a), (2016b), Wang *et al.* (2006), Ru *et al.* (2009), Zhang *et al.* (2011), Ou and Lee (2012), Sodagar and Guran(2012) for multiple circular/elliptic nano-cavities and nano-inclusions. Anti-plane strain models can be found in Fang *et al.* (2010a, 2010b, 2013).

(B5) Elastodynamic results for semi-infinite solids with holes and inclusions at the nano-scale

Again, to the authors' best knowledge there are no results for the case of plane strain. Anti-plane strain results are available in Yang *et al.* (2012), where propagation of SH time-harmonic waves in an elastic half-plane containing an elastic cylindrical nano-inclusion is investigated. In Parvanova and Dineva (2024) in-plane wave motion in an elastic anisotropic half-plane with nanotopography and embedded nanocavities is studied by direct displacement BEM based on the fundamental solution for anisotropic elastodynamics derived by the Radon transform in frequency domain. The nanorelief is presented by a single step of semicircle/semielliptic hill-canyon nanotopography.

(B6) Elastodynamic results for finite solids with holes and inclusions at the nano-scale

Solutions for in-plane wave motion are available in Parvanova *et al.* (2016a), (2016b), where the elastodynamic problem for a finite, isotropic and anisotropic elastic solid at the nano-scale containing multiple inclusions or

cavities of arbitrary configuration, shape and size is considered. Parvanova *et al.* (2016b) gives results for a finite elastic/viscoelastic anisotropic solid with nanosized multiple cavities of arbitrary shape, number and configuration. There are no available results for the case of anti-plane wave motion in elastic solids.

The most common computational methodologies for solving mechanical problems in the frame of the surface elasticity model are: (a) *analytical or semi-analytical, such as the complex variable technique* (see Tian and Rajapakse (2007a, 2007b); Wang and Wang (2006); (b) *the complex variable boundary element method* Mogilevskaya *et al.* (2008), Jammes *et al.* (2009)); (c) *the wave function expansion method* (see Wang (2009); Zhang *et al.* (2011); Wang *et al.* (2006); Ru *et al.* (2009)); (d) *the wave function expansion method and the image method* (Yang *et al.* (2012)); (e) *the conformal mapping* (Dai *et al.* (2016b)), (e) *the method of potential displacements* (Avazmohammadi *et al.* (2009)); (f) *the finite element method* (Fu *et al.* (2011), Tian and Rajapakse (2007a), Wang *et al.* (2008), Wang and Li (2013), Gao *et al.* (2006); Wang *et al.* (2010a, 2010b); Fu and Wang (2010)); (i) *the boundary element method* (Parvanova *et al.* (2015, 2016a, 2016b, 2017, 2021), Dineva and Rangelov (2016), Dineva *et al.* (2019), Dong and Pan (2011), Dong and Lo (2013), Rangelov and Dineva (2017), Dineva *et al.* (2021)), (j) *the boundary elements with fractional derivatives* (Rangelov *et al.* (2018, 2021, 2023)).

The advantages of the BEM are widely discussed in the literature, particularly for solids with high surface-to-volume ratios, as the problems are described through integral equations along existing boundaries, see Manolis and Dineva (2015). The BEM is an attractive candidate for modelling wave propagation in infinite/semi-infinite media because of certain advantages, namely: (a) *the formulation via boundary integral equations is equivalent to the original boundary-value problem (BVP) described by partial differential equations*. This fact, coupled with the use of the analytically derived fundamental solution guarantees a high level of accuracy; (b) *the fundamental solution obeys the Sommerfeld radiation condition and thus infinitely extended boundaries are automatically accounted for without resorting to special types of viscous boundaries*; (c) *since only surfaces need to be modelled, there is a reduction of the problem dimensionality, with a corresponding reduction in the size of the algebraic system as compared with domain-type numerical methods*; (d) *a selective solution at internal points in the domain of interest is possible once the BVP has been solved by the use of the well-known integral representation formulae, which obviates the large scale volume discretization*; (e) *flexibility in modelling of arbitrary geometry*; (f) *high accuracy in the computation of stress concentration factor (SCF) near*

heterogeneity, since the solution at internal points is expressed in terms of boundary values without recourse to domain discretization; (g) the possibility to obtain directly, with no other intermediate source of error, the displacements and tractions.

The conclusions that can be drawn from the above discussion are as follows:

(a) To date, there are only a limited number of theoretical and numerical studies on surface effects observed at the nanoscale. Additionally, understanding the scattering of elastic waves by microstructures in solids is of significant engineering importance, due to the numerous potential technical applications;

(b) Numerical results generated by the BEM for elastic wave diffraction and scattering problems in nanostructure are largely lacking. Furthermore, the majority of the existing BEM solutions are for static load conditions, excluding the authors' results Parvanova *et al.* (2015), (2016a,b), (2017), (2021), Rangelov and Dineva (2017, 2021);

(c) There is a paucity of numerical results for boundary value problems involving a free surface or finite boundaries of the solid matrix surrounding the nanostructure;

(d) While results for the mechanical behavior of single defects can be found in few publications, there is a lack of results concerning the behavior of multiple ones;

(e) There is still a lack of results concerning the surface effects in the transient behavior of elastic anisotropic solids. To the authors' knowledge there are no available results for bounded or unbounded anisotropic solids with nano-cavities or nano-inclusions subjected to transient loads, except for the authors' own finding in Parvanova *et al.* (2021);

(f) The limited number of results for dynamic behaviour of nanomaterials or structural elements made of them containing different types of nanoheterogeneties are only for pure elastic isotropic cases. The influence of the material anisotropy is taken into account only in few authors' papers, see Parvanova *et al.* (2016b, 2017, 2021);

(i) There are no results for elastodynamic models describing the dynamic stress-strain state and stress concentration zones in materials and solids with surface roughness and with nanorelief peculiarities even for the case of a pure elastic isotropic solid. The majority of the available results have been concentrated on the nanostructures having perfect surfaces without any topological defects, although it is almost impossible to avoid them during production. The only known solution in the field can be seen in Wu and Ou (2022) where the scattering of incident plane shear waves (SH-waves) by a

nano-sized arc-shaped hole along the half-plane boundary is analyzed through the wave function expansion method.

The present chapter aims to propose a systematic BEM study on the dynamic response of infinite, semi-infinite and finite isotropic/anisotropic solids with nanocavities/nano-inclusions under time-harmonic or transient stress pulses rapidly applied along the existing boundaries.

The importance, the innovation character and applicability of the defined above aims in hi-tech industry based on nanomechanics are as follows:

- (1) The obtained results could be valuable for studying the mechanical behavior of perforated nanomembranes, whose development through advanced nanofabrication techniques has progressed rapidly in recent years. Their applications, extending beyond separation processes, now span various high-tech fields. Today, numerous nanoscale fabrication techniques are being developed to create artificial nanoporous membranes. Perforated nanomembranes have been produced by numerous groups and many are derived from inorganic silicon-based materials (Schuster *et al.* (2018)), noble metals (Monaico *et al.* (2020)) or polymers (Ulbricht (2006));
- (2) To the best of the authors' knowledge, elastodynamic solutions for elastic anisotropic nanocomposites containing anisotropic nano-inclusions are not available in the literature. The model developed here will reveal additional effects compared to the case of nanocavities, as demonstrated in the presented parametric study. The computational tool developed is a direct BEM based on the frequency-dependent fundamental solution derived via the Radon transform for general anisotropic continua. This analytically derived fundamental solution, based on the Radon transform, allows for the consideration of all types of anisotropy, whereas many existing models in the literature, even at the macroscale, are limited to specific classes of anisotropic materials. We believe the results generated here will be valuable to the computational mechanics' community and can serve as benchmark examples for researchers developing new numerical tools;
- (3) The results concerning the nanotopography refer to specific surface features which are generated by nanograins, nanopores, nanotubes, nanoparticles, nanoridges or novalleys at the nanoscopic scale. Modern technologies such as plasma functionalization, abrasive blasting, etching, electron beam lithography and particle deposition are available for the production of nanotopography. The evaluation,

identification and control of the nanotopography change is readily applied to cell engineering (McNamara *et al.* (2010)), to crystallography (He *et al.* (2020)), to nanoindentation test (Nix and Gao (1998)), to medicine (Le Guehennec *et al.* (2007)) for production of implants with suitable surface nanotopography and to surface mechanics research dealing with the influence of the surface roughness in thin films materials. The surface roughness can directly influence the material properties such as the elastic characteristics (Mozammel *et al.* (2018)), electronic, magnetic, optical ones (Jiang *et al.* (2008)) and many others (Choe and Steinback (1999)). Thus, considering its practical applications, it is inevitable to understand the surface roughness's influence on the properties of nanomaterials and nanostructures. The surface roughness topic got discrete attention and is commendably discussed in the scientific community due to its significance in the design of novel nanodevices. Due to the imperfection of the preparation process, nanocomposite materials may introduce material interfaces and internal nanorelief peculiarities during fabrication and production. The distribution of internal stresses and the evaluation of the stress-strain state in materials with internal surface nanorelief is still an unexplored area in nanomechanics these days.

The present chapter is broken down focusing on the following sections: (1) Definition of the mechanical problem for in-plane wave motion in general anisotropic solids containing nanoheterogeneities; (2) Reformulation of the defined boundary-value problem via boundary integral equations along the existing boundaries; (3) Verification study of the proposed numerical scheme; (4) Parametric analysis which serves to describe the non-uniform stress distribution in the general anisotropic infinite plane, half-plane and finite solids as a function of the nanorelief geometry, surface elasticity properties, material anisotropy, number, shape and type of nanoheterogeneities and their configuration, their mutual dynamic interactions, their interaction with the solids' boundaries, and type and characteristics of the applied mechanical loads; (5) Finally, the last section presents a list of conclusions and a list of references.

2. Problem formulation by governing partial differential equation

The main goal in this section is to formulate in a general form two-dimensional elastodynamic problems in time domain for infinite, semi-infinite and finite elastic isotropic or anisotropic solids of nanocomposites

with multiple cavities and inclusions arbitrary in number, shape and mutual disposition at nano-scale.

In a Cartesian coordinate system $Ox_1x_2x_3$ consider three different mechanical problems:

- (1) *Problem 1:* Dynamic behavior of an infinite elastic anisotropic solid containing nanocavities and nanoinclusions of arbitrary shape, number, size and configuration under transient or time-harmonic incident plane waves (Fig. 1a)

Consider an anisotropic plane Ω_{inf} under a plane strain dynamic state in the plane $x_3 = 0$ containing a set of M nanoholes (nanocavities) $\Omega_H = \bigcup_{m=1}^M \Omega_H^m$ with boundaries $\Gamma_H = \bigcup_{m=1}^M \Gamma_H^m$ and N elastic nanoinclusions $\Omega_I = \bigcup_{n=1}^N \Omega_I^n$ with boundaries $\Gamma_I = \bigcup_{n=1}^N \Gamma_I^n$ of arbitrary shape, number, size and configuration. The heterogeneities do not intersect each other, and their total surface is denoted as $\Gamma = \Gamma_H \cup \Gamma_I$. The load is an inclined transient or time-harmonic plane longitudinal P or shear SV wave with incident angle θ in respect to the horizontal axis.

- (2) *Problem 2:* Dynamic behavior of a semi-infinite elastic anisotropic solid containing two nanocavities of arbitrary shape, size and configuration under incident time-harmonic plane P waves (Fig. 1b)

The object of study is a homogeneous elastic isotropic or generally anisotropic nano-sheet Ω_0 with a nanorelief boundary Γ_{rel} along its boundary $\Gamma_f = \Gamma_{\text{rel}} \cup \Gamma_{\text{ff}}$, where the flat boundary is denoted by Γ_{ff} . The nano-sheet is subjected to a time-harmonic in-plane P-wave with a fixed frequency ω . The half-plane contains two nanocavities with boundaries Γ_{c1} and Γ_{c2} . The common boundary in the object under study is denoted by $\Gamma = \Gamma_f \cup \Gamma_{c1} \cup \Gamma_{c2}$.

- (3) *Problem 3:* Dynamic behavior of a finite elastic anisotropic solid containing nanocavities and nanoinclusions of arbitrary shape, number, size and configuration under uniform transient loads (Fig. 1c)

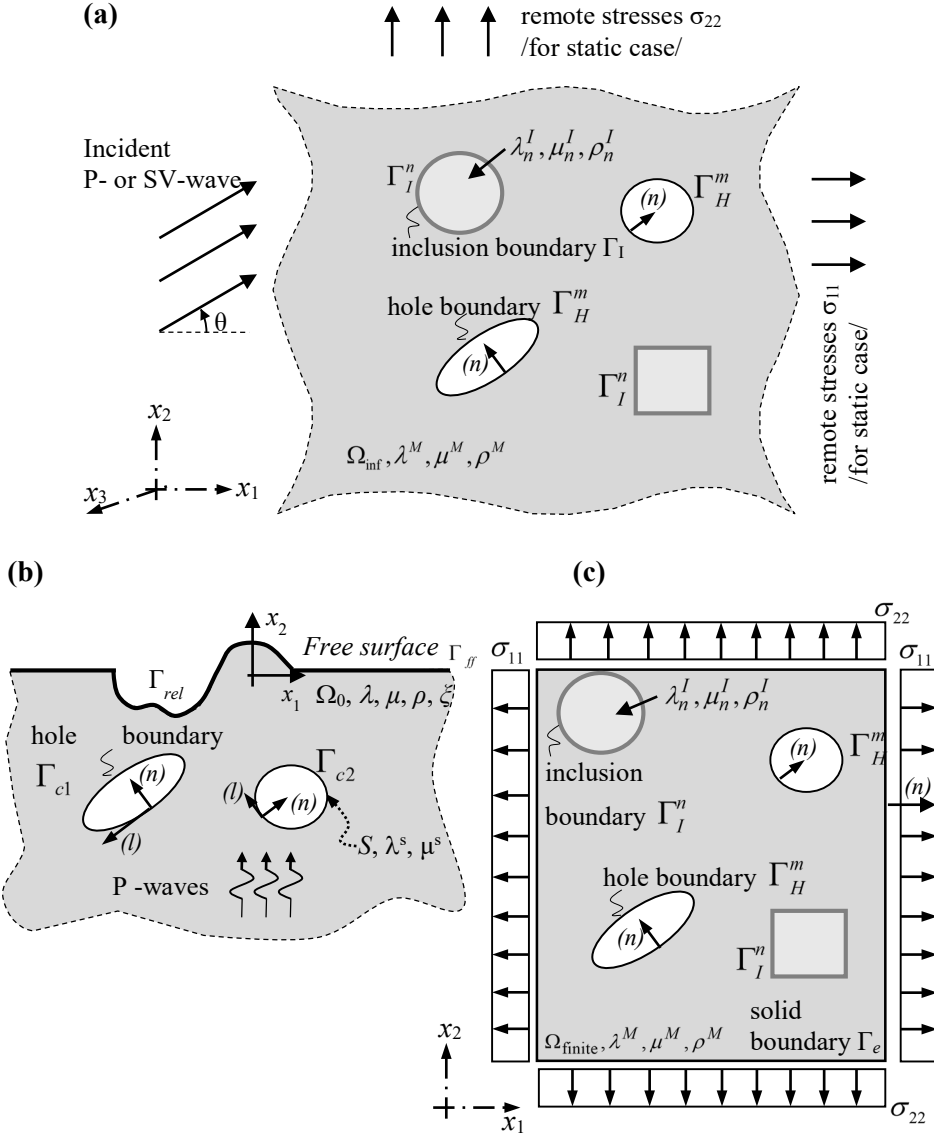


Figure 1: Geometry of 2D elastodynamic problems under consideration in (a) infinite plane; (b) semi-infinite half-plane (nanosheet); (c) finite solid of nanocomposite with nanoimperfections.

Consider a finite anisotropic solid Ω_{finite} with external boundary Γ_e under a plane strain dynamic state in the plane $x_3 = 0$ containing a set of M nano-holes (nanocavities) $\Omega_H = \bigcup_{m=1}^M \Omega_H^m$ with boundaries $\Gamma_H = \bigcup_{m=1}^M \Gamma_H^m$ and N

elastic nano-inclusions $\Omega_I = \bigcup_{n=1}^N \Omega_I^n$ with boundaries $\Gamma_I = \bigcup_{n=1}^N \Gamma_I^n$ of arbitrary shape, number, size and configuration. The heterogeneities do not intersect each other and the total surface of the solid under consideration is denoted as $\Gamma = \Gamma_e \cup \Gamma_H \cup \Gamma_I$. The load is a transient stress pulse rapidly applied along the solid's boundary Γ_e .

It is assumed that the anisotropic material is of monoclinic type, because this is the necessary condition for uncoupling of the 3D problem into two-dimensional ones: in-plane and anti-plane, see Garcia-Sanchez (2005). In this case the only non-zero field quantities are the displacements u_1, u_2 , the stresses $\sigma_{11}, \sigma_{12}, \sigma_{22}$ and the tractions $t_i = \sigma_{ij} n_j$, $i, j = 1, 2$, all dependent on coordinates $\mathbf{x} = (x_1, x_2)$ and time t , where n_j is the outward pointing unit normal vector to the surface under consideration. All elastic inclusions have equal material properties: density ρ^I and stiffness coefficients C_{ijkl}^I , while the solid material properties are ρ^M and C_{ijkl}^M .

The dynamic equilibrium equation in the absence of the body forces, the kinematic relation and the constitutive law for a linear elastic anisotropic solid are

$$\sigma_{ij,j} = \rho \ddot{u}_i, \quad \varepsilon_{ij} = \frac{1}{2} (u_{i,j} + u_{j,i}), \quad i, j = 1, 2, \quad \left\{ \begin{matrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{12} \end{matrix} \right\} = \begin{bmatrix} c_{11} & c_{12} & c_{16} \\ c_{12} & c_{22} & c_{26} \\ c_{16} & c_{26} & c_{66} \end{bmatrix} \left\{ \begin{matrix} \varepsilon_{11} \\ \varepsilon_{22} \\ 2\varepsilon_{12} \end{matrix} \right\}, \quad (1a, b, c)$$

here: $\sigma_{ij} = \begin{cases} C_{ijkl}^M u_{k,l}^M \text{ (matrix);} \\ C_{ijkl}^I u_{k,l}^I \text{ (n-th inclusion).} \end{cases} \quad \rho = \begin{cases} \rho^M; \\ \rho^I. \end{cases}$

In the above $\ddot{u}_i$ is acceleration, ε_{ij} is the strain tensor, comma subscripts denote partial differentiation with respect to the spatial coordinates and the summation convention over repeated indices is implied. In the case of general anisotropy, the angle χ between the coordinate axis Ox_2 and the principal axis of the material symmetry Ox'_2 is $\chi \neq 0; \pi/2$ and in this case six parameters $c_{11}, c_{12}, c_{16}, c_{22}, c_{26}, c_{66}$ characterize the stiffness tensor. Note that the contracted notation of Voigt (1910) is applied to the fourth order stiffness tensor C_{ijkl} , where $C_{ijkl} = C_{jikl} = C_{ijlk} = C_{klij}$, $C_{ijkl} g_{ij} g_{kl} > 0$ for any non-zero real symmetric tensor g_{ij} . If the principal axis of the material symmetry Ox'_2 coincides with the coordinate axis Ox_2 , the material is

orthotropic and it is characterized with the following four independent material constants $c_{11}, c_{12}, c_{22}, c_{66}$, because $c_{16} = c_{26} = 0$. The orthotropic case is transformed into isotropic one if the subsequent relations are true $c_{11} = c_{22} = \lambda + 2\mu$ and $c_{12} = \lambda; c_{66} = \mu$, where λ and μ are Lamé' constants. In the case of the isotropic material the stiffness tensor is $C_{ijkl} = \lambda \delta_{ij} \delta_{kl} + \mu (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk})$.

It is assumed that a quiescent state exists before $t = 0$, which implies that the initial displacements and velocities are zero when transient loads are considered.

The following section discusses the boundary conditions for each mechanical problem.

Non-classical boundary conditions along each interface Γ between a particular inclusion/hole and the surrounding matrix

The mechanical model is based on a combination of the classical elastodynamic theory for the bulk solid presented by the equation of motion (1a) and non-classical boundary conditions discussed below, supplemented with a localized constitutive equation for the solid-nanohole interface Γ_H and solid-nanoinclusion interface Γ_I in the framework of the theory of surface elasticity proposed in Gurtin and Murdoch (1975).

In the Gurtin and Murdoch model it is assumed that the interface between a nanohole Γ_H^m or a nanoinclusion Γ_I^n and its surrounding matrix (denoted by M) is regarded as a thin material surface with own mechanical properties λ^s, μ^s and residual surface tension τ^0 , whose elastic isotropic behavior is described by the following constitutive equation:

$$\sigma_{||}^s = \tau_0 + (\lambda^s + 2\mu^s) \varepsilon_{||}^s, \quad (2)$$

where $\sigma_{||}^s$ and $\varepsilon_{||}^s$ are stress and strain in the tangential direction to the interface boundary.

It is assumed that: (a) the thin interface layer with zero thickness along $\Gamma = \Gamma_H \cup \Gamma_I$ is elastic and isotropic, while the bulk solid is isotropic or anisotropic; (b) λ^s, μ^s for all interface boundaries Γ are one and the same. The residual surface tension τ^0 is often ignored in the case of dynamic

loading because it is defined along the undeformed surface, it is independent from the stress-strain state of the surface and induces only additional static deformation. The following boundary conditions are satisfied in tangential l and normal n directions along the interface boundary Γ (see Mogilevskaya *et al.* (2008), Dong and Pan (2011), Parvanova *et al.* (2016)):

(a) Continuity of the displacement vector along any interface as seen from the side of the inclusion u_i^I and from the side of the surrounding matrix u_i^M in the $Ox_1x_2x_3$ coordinate system:

$$u_i^I = u_i^M = u_i ; i = 1, 2 \quad (3)$$

(b) Interface equilibrium conditions along the thin layer Γ written in terms of the local normal and tangential (n, l) coordinates. These lead to the following relation between tractions along any interface coming from the side of the nanoheterogeneity t_i^I and from the side of the surrounding matrix t_i^M :

$$\begin{Bmatrix} t_1^I + t_1^M \\ t_2^I + t_2^M \end{Bmatrix}_k = \mathbf{f}_k^{sur} + \mathbf{T}_k^{sur} \begin{Bmatrix} u_1 \\ u_2 \end{Bmatrix}_k \quad (4)$$

The matrix $\mathbf{T}_k^{sur}$ and the vector $\mathbf{f}_k^{sur}$ related with the k -th node of the interface under consideration are derived as follows:

$$\mathbf{f}_k^{sur} = \left\{ -\frac{\tau_0}{\rho_s} \begin{Bmatrix} n_1 \\ n_2 \end{Bmatrix} \right\}_k \quad (5)$$

$$\mathbf{T}_k^{sur} = \mathbf{N}_k \begin{bmatrix} \left(-\frac{\alpha}{(\rho_s)^2} + \tau^0 \frac{\partial^2}{\partial l^2} \right) & \frac{-\alpha}{\rho_s} \frac{\partial}{\partial l} - \left(\frac{\tau^0}{\rho_s} \frac{\partial}{\partial l} - \frac{\tau_0}{(\rho_s)^2} \frac{\partial \rho_s}{\partial l} \right) \\ \left(\frac{-\alpha}{\rho_s} \frac{\partial}{\partial l} - \frac{\alpha}{(\rho_s)^2} \frac{\partial \rho_s}{\partial l} \right) + \frac{\tau^0}{\rho_s} \frac{\partial}{\partial l} & \left(\alpha \frac{\partial^2}{\partial l^2} - \frac{\tau^0}{(\rho_s)^2} \right) \end{bmatrix}_k \mathbf{N}_k^T, \quad (6)$$

$$\mathbf{N}_k = \begin{bmatrix} n_1 & -n_2 \\ n_2 & n_1 \end{bmatrix}$$

In the above, $\partial / \partial l$ and $\partial^2 / \partial l^2$ are the first and second tangential derivatives respectively; $n_1 = n_1^I = -n_1^M$; $n_2 = n_2^I = -n_2^M$ are the components of the normal vector as viewed from either side of an interface and ρ_s is the curvature radius for the corresponding interface thin layer Γ . As far as assigning numerical values to the surface constants for single-crystalline materials is concerned,

these have been determined by either atomic simulation (Miller and Shenoy (2000); Shenoy (2002)) or elaborate experiments (Jing *et al.* (2006)). These results indicate that these surface constants depend on the material type and on the surface crystal orientation. Thus, a surface modulus that best captures interface effects at the nanoscale has been defined as $\alpha = K_s = 2\mu^S + \lambda^S$ in the papers by Dong and Pan (2011), Ru *et al.* (2009), Wang *et al.* (2006) and Wang (2009). For real nano-materials, the value of K_s is in the neighborhood of $\pm 10 \text{ N/m}$, and negative values are also possible based on atomistic calculations (see Tian and Rajapakse (2007); Miller and Shenoy (2000)).

In sum, the boundary-value problem (BVP) formulated above must satisfy the governing equation (1a), plus the continuity boundary conditions (3) and the equilibrium boundary condition (4) along each interface Γ between a particular inclusion/hole and the surrounding matrix.

Note that if the membrane interface parameters are $\lambda^S = \mu^S = 0$, the boundary condition (4) transforms into the classical continuity condition $t_i^I + t_i^M = 0$ along the interface between the matrix and inclusion. In the case of a nanohole we have that $t_i^I = 0$ in Eq. (4), respectively $t_i^M = 0$ if $\lambda^S = \mu^S = 0$.

Problem 1: Boundary conditions

The total wave field in an infinite elastic plane (Fig. 1a) is given by the superposition of the incident ('*in*') wave impinges on an inclusion/cavity and a one scattered ('*sc*') by the inclusion/cavity wave. Or, the total displacement is $u_i = u_i^{in} + u_i^{sc}$ and the total traction is $t_i = t_i^{in} + t_i^{sc}$. The boundary conditions (3-4) concern the total displacement and total traction. In the case of an inclusion we have that $u_i^I = u_i^{I,sc}$ and $t_i^I = t_i^{I,sc}$, $u_i^M = u_i^{M,sc} + u_i^{M,in}$ and $t_i^M = t_i^{M,sc} + t_i^{M,in}$. In the case of a nanohole the inclusion traction is zero, $t_i^I = 0$.

Incident wave motion definition

The incident wave motion is the solution of the problem for wave propagation in an infinite plane without any heterogeneity. The incident wave motion solution is available in an analytical form and it is published in many books and papers, among them Achenbach (1973), Manolis *et al.* (2017). Next, the

incident displacement field that develops at field point (x_1, x_2) after passage of a body wave in the elastic isotropic full plane is as follows:

(a) Incident P-wave:

$u_i^{in}(x_1, x_2, \omega) = u_0 \begin{Bmatrix} \cos \theta \\ \sin \theta \end{Bmatrix} e^{-ik_p(x_1 \cos \theta + x_2 \sin \theta)}$, where $u_0 = 1$ is the unit displacement amplitude, while $k_p = \omega/C_p$, $C_p = \sqrt{\lambda + 2\mu/\rho}$ respectively are the P-wavenumber and the phase velocity. In the case of orthotropic material $C_p = \sqrt{c_{22}/\rho}$.

(b) Incident SV-wave:

$u_i^{in}(x_1, x_2, \omega) = u_0 \begin{Bmatrix} \sin \theta \\ -\cos \theta \end{Bmatrix} e^{-ik_s(x_1 \cos \theta + x_2 \sin \theta)}$, where $k_s = \omega/C_s$ and $C_s = \sqrt{\mu/\rho}$ respectively are the SV-wavenumber and the phase velocity. In the case of orthotropic plane $C_s = \sqrt{c_{66}/\rho}$.

The aim of the *Problem 1* is to determine the dynamic stress-strain field at any point of the *infinite nanoheterogeneous elastic plane* and to evaluate the dynamic stress concentration factor (DSCF) along the interface perimeter $\Gamma = \Gamma_H \cup \Gamma_I$.

Problem 2: Boundary conditions

The boundary condition along the boundaries Γ_{rel} , Γ_{c1} , and Γ_{c2} with surface elasticity properties (Fig. 1b) is presented by Eq. (4) where $t_i^I = 0$, while on the flat part Γ_{ff} of the half-plane boundary a traction free boundary condition is satisfied $t_i^M = 0$.

The total wave field in an elastic half-plane is given by the superposition of the free-field (*ff*) wave impinging on a cavity and a scattered (*sc*) by the cavity wave. Or, the total displacement is $u_i = u_i^{ff} + u_i^{sc}$ and the total traction is $t_i = t_i^{ff} + t_i^{sc}$.

Free-field wave motion definition

The free-field wave motion is the solution of the problem for wave propagation in an elastic isotropic/anisotropic half-plane without any heterogeneity. The free-field wave motion solution is available in an analytical form in Manolis *et al.* (2017), Achenbach (1973).

The free field wave motion for displacements u_i^{ff} corresponding to vertically incident P- waves propagating through the orthotropic half-plane in the absence of heterogeneities and relief peculiarities results in the following displacement field at a point $\mathbf{x} = (x_1, x_2)$ (see Garcia-Sanchez (2005)):

$$\begin{pmatrix} u_1^{ff} \\ u_2^{ff} \end{pmatrix} = u_0 \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{ik_p x_2} - \begin{pmatrix} 0 \\ -1 \end{pmatrix} e^{-ik_p x_2}$$

The aim of the *Problem 2* is to determine the wave field at any point inside and along the boundary of *the nanoheterogeneous anisotropic half-plane* and to evaluate the dynamic stress concentration factor (DSCF) along the contours of the nanocavities.

Problem 3: boundary conditions

Along the common boundary $\Gamma = \Gamma_H \cup \Gamma_I$ of nanoholes and nanoinclusions the boundary condition (4) is satisfied having in mind that: (a) in the case of *nanoholes* $t_i^I = 0$ in Eq. (4) and (b) in the case of *nanoinclusions* an additional displacement continuity condition (3) is satisfied along the contact interface between the matrix and inclusions. Along the external boundary Γ_e of the finite bounded solid (Fig. 1c) the following condition holds: $t_j(x_1, x_2, t) = \sigma_{0j} f(t)$, where σ_{0j} is the magnitude of the applied loads in both directions and $f(t)$ is the time history of the transient load.

The aim of *Problem 3* is to determine the dynamic stress-strain field at any point of *the nanoheterogeneous anisotropic finite solid* and to calculate the dynamic stress concentration factor (DSCF) along the common boundary $\Gamma = \Gamma_H \cup \Gamma_I$.

Finally, the three different boundary value problems (BVPs) defined here are presented by the governing equation (1a), along with the initial and boundary conditions discussed for each problem. The goal is to numerically determine the displacement/traction field at any point in an infinite, semi-infinite, or finite elastic isotropic or anisotropic nanocomposite solid containing a set of nanoinclusions or nanoholes, and to calculate the stress concentration factor (SCF) along the perimeter of any nanoimperfection subjected to time-harmonic or transient loading.

It is well known (Kupradze and Gegeliia (1979)) that a system of partial differential equations along with the boundary and initial conditions formulated above may be recast in an integral form. The advantage of

following this path in the Fourier transform domain rather than in the time domain is that the equation of motion becomes an elliptic partial differential equation in the former domain, and as such is more amenable to numerical solutions than its hyperbolic counterpart in time domain. The numerical solution of the transient elastodynamic problems formulated here is obtained by application of direct Fourier transform, BEM numerical procedure in Fourier transform domain, which is based on the fundamental solution derived analytically by the use of Radon transform (Wang and Achenbach (1994), Dineva *et al.* (2005)) and the final solution is obtained by numerical inversion into the time domain.

The governing equation (1a) in the Fourier transform domain becomes:

$$\sigma_{ij,j}(\mathbf{x},\omega) + \rho\omega^2 u_i(\mathbf{x},\omega) = 0 \quad (7)$$

For the aim of simplicity, the same notations for the field variables will be used in the Fourier transform domain. The boundary conditions given above become also frequency dependent in the Fourier transform domain. The common factor $\exp(i\omega t)$ appearing in all the field variables of the problem is omitted.

Finally, the following well-known procedure is used for the solution of the transient problems defined above: (a) application of the direct FFT to *Eq. (1a)* with respect to the time variable and solution of the boundary-value problem in the frequency domain defined by *Eq. (7)*; (b) application of the inverse FFT to the solutions in the frequency domain to obtain solution in time domain.

3. Problem reformulation by boundary integral equations in Fourier domain

The defined BVPs in the frequency domain, together with the boundary conditions can be reformulated via integral equation along the existing boundaries of the solid under consideration. This can be done by the use of the dynamic Betti's reciprocity theorem and the fundamental solution of the elastodynamic equation (7) for a 2D anisotropic material, see Manolis *et al.* (2017). *Problem 1* and *Problem 2* are described by the boundary integral equation (8), having in mind that $\Gamma = \Gamma_H \cup \Gamma_I$ for the *Problem 1* and $\Gamma = \Gamma_{rel} \cup \Gamma_{ff} \cup \Gamma_{c1} \cup \Gamma_{c2}$ for the *Problem 2*

$$C_{ij}u_j^{sc}(\mathbf{x},\omega) = \int_{\Gamma} U_{ij}^*(\mathbf{x},\xi,\omega) t_j^{sc}(\xi,\omega) d\Gamma(\xi) - \int_{\Gamma} T_{ij}^*(\mathbf{x},\xi,\omega) u_j^{sc}(\xi,\omega) d\Gamma(\xi) \quad (8)$$

Problem 3 is reformulated via boundary integral equation (9), where $\Gamma = \Gamma_e \cup \Gamma_H \cup \Gamma_I$:

$$C_{ij}u_j(\mathbf{x},\omega) = \int_{\Gamma} U_{ij}^*(\mathbf{x},\boldsymbol{\xi},\omega) t_j(\boldsymbol{\xi},\omega) d\Gamma(\boldsymbol{\xi}) - \int_{\Gamma} T_{ij}^*(\mathbf{x},\boldsymbol{\xi},\omega) u_j(\boldsymbol{\xi},\omega) d\Gamma(\boldsymbol{\xi}) \quad (9)$$

Here: C_{ij} is the jump term depending on the local geometry at the source point $\mathbf{x}=(x_1,x_2)$, the couple $\mathbf{x},\boldsymbol{\xi}$ presents the position vectors of the source and receiver point $\boldsymbol{\xi}=(\xi_1,\xi_2)$, respectively; $U_{ij}^*(\mathbf{x},\boldsymbol{\xi},\omega)$ is the displacement fundamental solution of the governing elliptic partial differential equation for in-plane wave motion in a generally anisotropic solid, and its corresponding traction is $T_{ij}^*(\mathbf{x},\boldsymbol{\xi},\omega) = C_{ijkl} U_{kl,l}^*(\mathbf{x},\boldsymbol{\xi},\omega) n_k$, see Wang and Achenbach (1994), Dineva *et al.* (2005), Garcia-Sanchez (2005).

The boundary integral equation (8) is written for the scattered wave displacement and traction, which are for: (a) *Problem 1*: $u_i^{sc} = u_i - u_i^{in}$ and $t_i^{sc} = t_i - t_i^{in}$; (b) *Problem 2*: $u_i^{sc} = u_i - u_i^{ff}$ and $t_i^{sc} = t_i - t_i^{ff}$, where u_i and t_i present the total displacement and traction, u_i^{in} and t_i^{in} are the incident wave propagating in the infinite plane, while u_i^{ff} and t_i^{ff} are the free field wave motion displacement and traction in the half-plane discussed above.

All singularities in the kernels related with boundary integral equations (8), (9) are overcome following the detailed descriptions in Garcia-Sanchez (2005). When the static fundamental solutions, as a part of the dynamic ones, are calculated over an element containing the collocation point, the displacement-based kernels exhibit a weak singularity of $O(\ln r)$, while the traction-based kernels exhibit a strong singularity of $O(1/r)$. The integrals with weak singularity are computed using appropriate quadrature rules, while the strongly singular ones are evaluated by the rigid body motion concept. The rigid body motion concept cannot be directly applied to an open polygon geometry. In the case of a half-plane, it is supplemented to enclosed geometry in order to handle the idea of rigid body motion. Since the strong singularities are only in the static part of the traction fundamental solution, the model with additional boundary elements is used once. All regular parts of the integrals are calculated by using numerical integration and standard Gaussian quadrature. The numerical procedure proceeds with discretization of the common boundary Γ with quadratic boundary elements, followed by the nodal collocation procedure. Thus, the following matrix equation system is formed, which gives the total displacement components along the boundary

Γ in terms of the prescribed boundary conditions: $\mathbf{G}\mathbf{t} - \mathbf{H}\mathbf{u} = \mathbf{F}$, where $\mathbf{G}$ and $\mathbf{H}$ are fully populated and nonsymmetric matrices of size $2N \times 2N$, N is the total number of nodes, $\mathbf{u}$ and $\mathbf{t}$ are the displacement and traction vectors at all the nodes, the vector $\mathbf{F}$ describes the applied dynamic load, which is presented by: (a) $\mathbf{F} = \mathbf{G}\mathbf{t}^{in} - \mathbf{H}\mathbf{u}^{in}$ for *Problem 1*; (b) $\mathbf{F} = \mathbf{G}\mathbf{t}^{ff} - \mathbf{H}\mathbf{u}^{ff}$ in the case of *Problem 2*; and (c) $\mathbf{F} = 0$ for the case of *Problem 3*, concerning a finite nanocomposite solid excited along its external boundary.

The formation of local and global influence matrices, after satisfactions of all the boundary conditions, is followed by the formation and solution of the linear algebraic system of equations $\mathbf{A}\mathbf{X} = \mathbf{B}$ with complex coefficients and with respect to the unknown field variables in the frequency domain. Inverse FFT is applied to the solutions in the Fourier domain in order to obtain solutions in the time domain for the cases of applied transient loads.

4. Numerical scheme verification

Before conducting any parametric studies, it is essential to establish the accuracy of the proposed computational discretization technique. The developed and verified numerical procedure is implemented via MATLAB (2024) software and its accuracy and convergence is studied in this section. In all computations the well-known accuracy criterion stating that $\lambda_S / l_{BE} \geq 10$, where l_{BE} is the length of the corresponding boundary element and λ_S is the length of the shear wave propagating inside the solid, is satisfied. The verification of the BEM development is carried out by running several test cases under static, time-harmonic, and transient loading conditions. This section also includes a study to establish the convergence of the results as a function of the mesh refinement.

Test example 1: A nanoscale elliptic cavity in an infinite plate under static loads

An aluminum plate with elastic constants $\lambda^M = 58.17$ GPa and $\mu^M = 26.13$ GPa containing an elliptic hole with semi-axis ratio of $a/b = 1.5$ is subjected to a far-field uniaxial state of loading σ_0 along the Ox_2 axis. A state of plane strain state is assumed to hold. Regarding the cavity interface material properties, we introduce the parameter $R = (a+b)/2$. This particular problem was solved analytically by Tian and Rajapakse (2007a) using the complex variable technique. Fig. 2a summarizes the results of our comparison

study by plotting the hoop stress variation at a fixed observer point on the cavity perimeter with polar angle coordinate of $\varphi = 0$, as a function of the elliptic hole size parameter R (nm) in the absence of the residual interface stress, i.e., for $\tau^0 = 0$. Three different values are examined for the material parameter, namely $K_S = 2\mu^S + \lambda^S = 0; 5.19; -7.92$ N/m, with the first value corresponding to the classical elasticity solution. Next, Fig. 2b plots the normalized hoop stresses versus the position angle φ of the observer point, for a fixed value of $R = 6$ nm and with $\tau^0 = 0$. Finally, Figs. 2c and 2d respectively plot results for the normalized stress pairs $(\sigma_{22}^{sur} R / \tau^0; \sigma_{22}^{cl} / \sigma_0)$ and $(\sigma_{11}^{sur} R / \tau^0; \sigma_{11}^{cl} / \sigma_0)$ along the Ox_1 -axis direction, where σ_{11}^{cl} and σ_{22}^{cl} are the classical elasticity solutions when both parameters $\tau^0 = 0$ and $K_S = 0$, while σ_{11}^{sur} and σ_{22}^{sur} are the stresses caused by a prescribed residual surface stress τ^0 in the absence of far-field loading.

The comparison above demonstrates the high accuracy and favorable convergence characteristics of the present BEM development. Regarding discretization, the basic BEM mesh used for the cavity perimeter consisted of 32 quadratic elements and 64 nodal points.

Test example 2: A nanoscale elliptic inclusion in an infinite plate under static loads

Consider next an infinite plate containing an elliptic inclusion with semi-axes a and b at the nanoscale, and under the influence of a far-field static load of magnitude σ_0 along the Ox_2 axis. The half-radius dimension for the nanoinclusion is again R , while its material parameter values are $\lambda^I = 50.66$ GPa and $\mu^I = 19.0$ GPa. The corresponding material parameter values for the surrounding (infinite) elastic matrix are $\lambda^M = 64.43$ GPa and $\mu^M = 32.9$ GPa, while the surface membrane elastic constant and the residual surface tension at the interface are K_S and $\tau^0 = 0$, respectively. This test example is solved analytically in Tian (2006) by using again the complex potential technique. Fig. 3 plots the present BEM results concurrently with those obtained by Tian (2006), and for three prescribed values of $K_S = -10; 0; +10$ N/m. More specifically, Fig. 3a shows the variation in the non-dimensional tangential stress at the observer point with polar angle $\varphi = 0$ on the interface, versus the inhomogeneity size R and for a fixed ratio of the semi-axes equal to $(a/b) = 1.5$. Similar results are plotted in Fig. 3b when this

ratio is now $(a/b)=3$. Solid lines pertain to results obtained for the surrounding matrix, while dashed lines are results for the inclusion. The comparison clearly demonstrates the excellent agreement achieved between our numerical solution and those obtained by Tian (2006). In terms of details regarding the BEM interface discretization, the meshes used comprised 32 elements for the ellipse with the semi-axis ratio $a/b=1.5$ and 64 elements for the ellipse with the sharper ratio of $a/b=3$. In sum, these are very modest discretization requirements and result in system matrices that correspond to 256 degrees-of-freedom only.

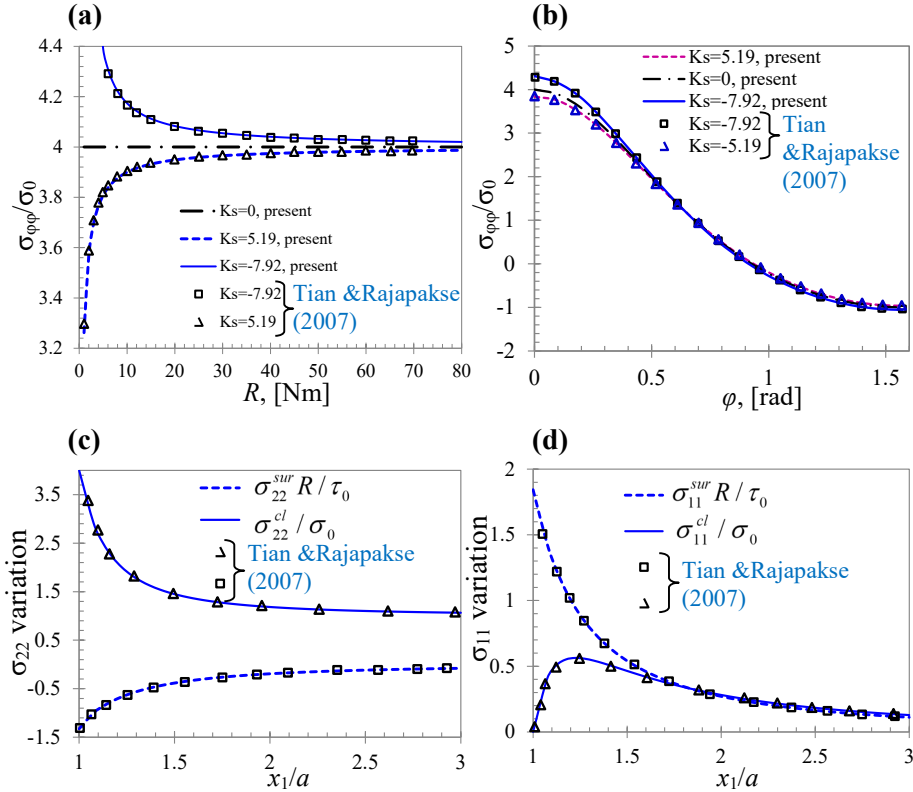


Figure 2: Elliptic nanocavity in the infinite plane under uniaxial static loading σ_0 and residual surface stress $\tau^0=0$: (a) Normalized hoop stress at observer point $\varphi=0$ versus averaged radius $R=(a+b)/2$; (b) normalized hoop stress versus observer point φ at fixed $R=6$ nm; (c) normalized stress $\sigma_{22}^{sur} R / \tau^0$ and $\sigma_{22}^{cl} / \sigma_0$ variation along the x_1 -direction; (d) normalized stress $\sigma_{11}^{sur} R / \tau^0$ and $\sigma_{11}^{cl} / \sigma_0$ variation along the x_1 -direction.

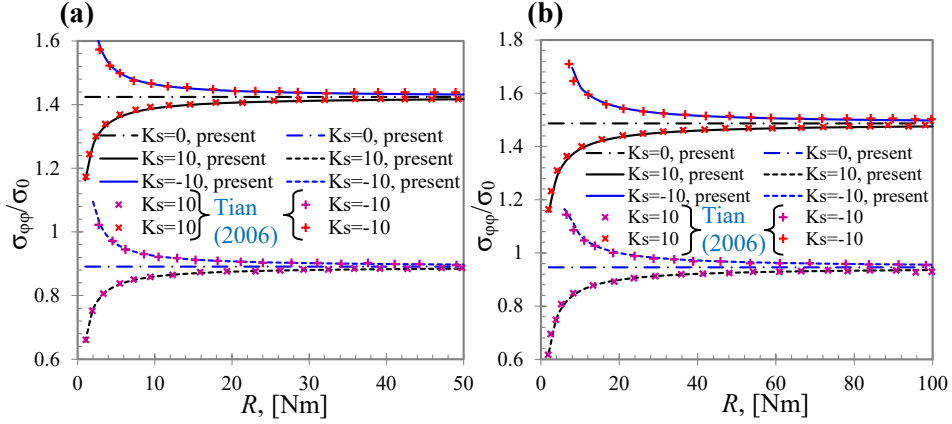


Figure 3: Non-dimensional tangential stress at a fixed polar angle $\varphi=0$ versus nanoinhomogeneity radius R under static uniaxial loading σ_0 along the x_2 -axis and for residual surface stress $\tau^0=0$ at fixed values of the semi-axes ratio: (a) $(a/b)=1.5$; (b) $(a/b)=3$ (Note: Solid lines are for the elastic matrix and dash lines for the inclusion).

Test example 3: A nanoscale circular cavity in an infinite plane under P-waves

The third test example considers surface effects on the diffraction of time-harmonic P-waves with frequency ω by a circular cylindrical nanocavity of radius a_0 placed within an elastic matrix. The following notations are now introduced: (a) the non-dimensional frequency parameter $\Omega = \omega a_0 / C_P$; (b) the dimensionless parameter $s = K_S / (2\alpha_0 \mu^M)$, with K_S previously defined and (c) the dynamic stress concentration factor defined as $\text{DSCF} = |\sigma_{\varphi\varphi} / \sigma_0|$, where $\sigma_0 = -\mu^M u_0 k_S^2$. As previously mentioned, the residual surface tension τ^0 induces an additional static deformation which is neglected in the present dynamic stress analysis. Finally, Poisson's ratio of the elastic medium is $\nu = 0.26$.

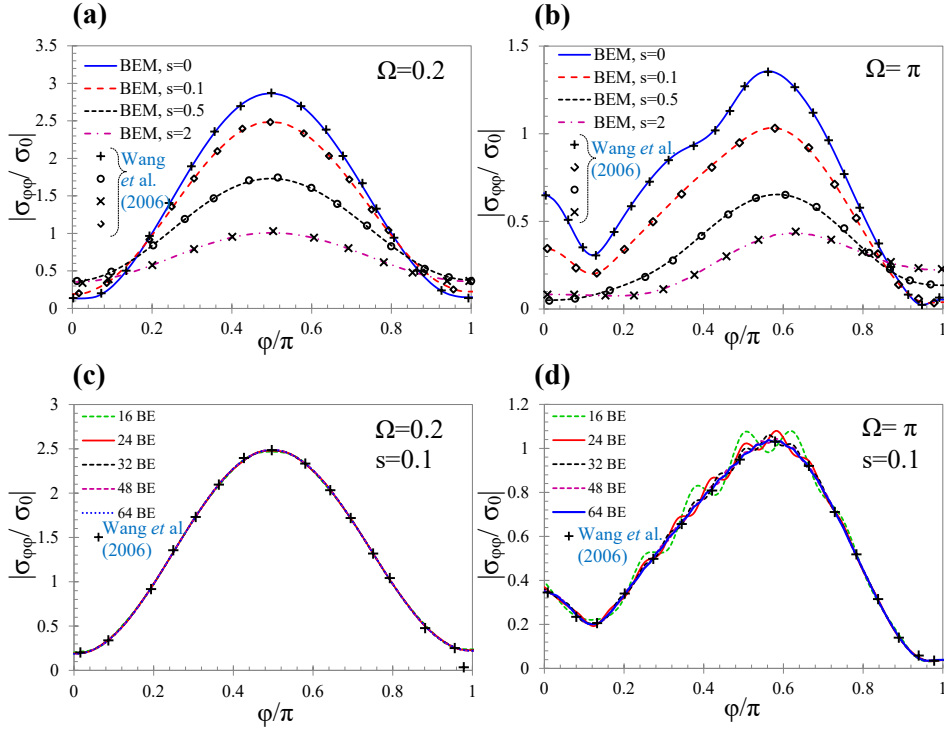


Figure 4: DSCF for a P-wave along the interface boundary of a nanocavity for variable surface parameter s values and at fixed non-dimensional frequency values of: (a) $\Omega=0.2$; (b) $\Omega=\pi$. For a value of $s=0.1$ and variable number of BE used in the cavity contour discretization at fixed non-dimensional frequency values of: (c) $\Omega=0.2$; (d) $\Omega=\pi$.

This particular BVP was solved analytically by Wang *et al.* (2006) using the displacement potential method. Their results are plotted in Figs. 4a and 4b, concurrently with the ones generated by the BEM for comparison purposes. More specifically, DSCF is plotted along the interface boundary at two different dimensionless frequency values of $\Omega = 0.2$ and $\Omega = \pi$, when the incident P-wave is propagating in the positive Ox_1 direction. Despite the fact that the results plotted in Fig. 4 are obtained by two very different computational methods, they are very close to each other as the perimeter is traversed. We first note here that when $s = 0$; $\Omega = 0$, our BEM results degenerate to the classical Kirsch solution of elastostatics, see Muskhelishvili (1977). Also, when only $s = 0$, the BEM results converge to the corresponding solution of the elastodynamic problem with classical boundary conditions and in the absence of surface effects. The BEM mesh used now

comprises 32 elements at the low frequency value $\Omega = 0.2$ and 64 elements at the higher value $\Omega = \pi$.

To justify the use of the above BEM meshes, we continue this example and recompute the DSCF along the cavity's perimeter for a fixed value of $s = 0$, but by varying the number of BE used to model the aforementioned contour. The results are summarized in Fig. 4c and in Fig. 4d for the low frequency value of $\Omega = 0.2$ and the higher one of $\Omega = \pi$, respectively. In the former case, the results are practically identical for all five meshes used, which range from 16 to 64 BE. This is not quite true in the latter case, where the DSCF values coming from the coarser meshes oscillate about the true solution at the crown of the cavity, where maximum values are expected to form. Finally, *Table 1* gives an error difference (as a percentage) between any two consecutive meshes for the DSCF at the cavity's crown, i.e., at $\varphi/\pi=0.5$.

Table 1: Nanocavity impacted by a P-wave: Error (as %) in the DSCF value at the cavity crown ($\varphi/\pi=0.5$) between two consecutive BEM meshes denoted by the number of BE used

Dimensionless frequency Ω	BEM meshes: 16/24	BEM meshes: 24/32	BEM meshes: 32/48	BEM meshes: 48/64
0.2	0.45	0.17	0.12	0.04
π	5.29	2.27	1.77	0.65

Test example 4: A nanoscale circular inclusion in an infinite plane under SV-waves

We consider an infinitely extending, elastic isotropic matrix that contains a circular nanoinclusion of radius a_0 , material properties λ^I , μ^I and density ρ^I . As far as the interface characteristics are concerned, $\tau^0 = 0$ as before. The dynamic excitation comes from a vertically polarized SV-wave with frequency content ω propagating along the Ox_1 axis. This benchmark example was solved by Ru *et al.* (2009) using the wave function expansion method. A comparison between our BEM results and those in Ru *et al.* (2009) is summarized in Fig. 5. More specifically, we compare the dynamic stress concentration factor, now defined as $DSCF = |\sigma_{\varphi\varphi} / \sigma_0|$, at points along the

interface perimeter and at a fixed non-dimensional frequency $\Omega_M = \omega a_0 / C_S$, where the SV-wave velocity is calculated with respect to the matrix material properties. All results in Fig. 5 are plotted for fixed values of the matrix/inclusion stiffness ratio $\mu^I / \mu^M = 0.2$ and at a frequency ratio of $\Omega_I / \Omega_M = 3$, where Ω_I and Ω_M are normalized with the phase velocities of the SV-wave propagating in the inclusion and matrix medium, respectively. Also, Poisson's ratio for both solid phases is $\nu = 0.26$, but different values of the surface parameter are considered, namely $s = 0; 0.1; 0.5; 2.0$. Figures 5a,b are plots for $\Omega_M = 0.2$ and $\Omega_M = \pi$, respectively, where excellent agreement is observed again between these results that are obtained by two very different computational techniques. The BEM mesh comprises 32 elements at the low frequency value $\Omega_M = 0.2$ and 64 elements at the higher value $\Omega_M = \pi$.

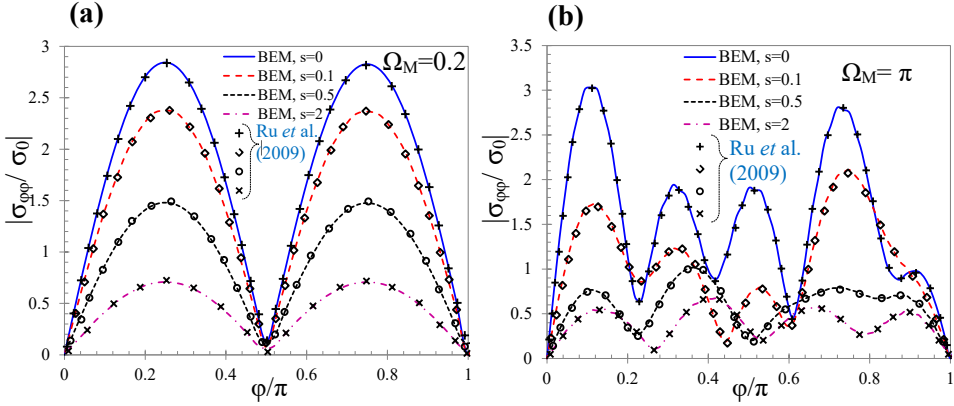


Figure 5: DSCF for an SV-wave along the perimeter of a circular nanoinclusion for different surface elastic parameters s values and at fixed non-dimensional frequency values of: (a) $\Omega_M=0.2$; (b) $\Omega_M=\pi$.

Test example 5: Three nano-scale circular elastic isotropic inclusions in a square elastic isotropic matrix under time-harmonic load

A square elastic isotropic plate with three horizontally arranged circular elastic isotropic inclusions under time harmonic tensile forces of magnitude σ_0 applied in horizontal direction is considered, see Fig. 6(a). The diameter of the inclusions is $d = 2a_0$, where the inclusion radius is a_0 , and the size of the square plate is $10d$. As before, the dimensionless parameter which

captures interface surface elasticity effects is $s = (2\mu^S + \lambda^S) / 2\mu^M a_0$. A constant frequency independent material damping is assumed equal to 5%. The stiffness ratio of inclusion to matrix material is $\mu^I / \mu^M = 0.2$ and their respective densities yield a frequency ratio of $\Omega_I / \Omega_M = 3$, where $\Omega_I = \omega d / C_P^I$ and $\Omega_M = \omega d / C_P^M$, with C_P^I and C_P^M the phase velocities of the P-wave propagating in the inclusion and in the matrix medium, respectively. Poisson's ratio is the same for both inclusion and matrix, equal to $\nu = 0.26$. In order to avoid rigid body motion, four edge nodes belonging to the axes of symmetry are restrained. This numerical example has been presented in Parvanova *et al.* (2016) for the elastic isotropic case. In the current study the fundamental solution for anisotropic material has been used in all the test examples. The case of isotropic material is treated just by setting $c_{11} = c_{22} = \lambda + 2\mu$ and $c_{12} = \lambda$; $c_{66} = \mu$. Additionally, it is assumed that $\tau_0 = 0$. Although, all the material parameters are defined parametrically and any values keeping the given ratios can be assigned, in the current models the geometrical and material parameters, in consistent units [kN], [m] and [t] are: $a_0 = 1$, $\mu_M = 1$, $\mu_I = 0.2$, $\rho_M = 1$, $\rho_I = 1.8$. The respective stiffness tensors for the matrix is $c_{11} = c_{22} = 3.0833$ and $c_{12} = 1.0833$; $c_{66} = 1$ and for the inclusion is $c_{11}^I = c_{22}^I = 0.6167$ and $c_{12}^I = 0.2167$; $c_{66}^I = 0.2$.

The boundary element (BE) mesh of the benchmark models could be found in Parvanova *et al.* (2016) where a comparison with FEM has been made. Three different BE discretizations are considered: **(1)** 32 BE for the matrix contour and 32 BE for each of the inclusion contour; **(2)** 16 BE for the square matrix and 16 BE for each of the inclusion contour; and **(3)** 32 BE for the matrix boundary and 16 BE for inclusion-matrix interface. The normalized dynamic stress concentration factor (DSCF) is defined as $DSCF = \sigma_{\varphi\varphi} / \sigma_0$, where $\sigma_{\varphi\varphi}$ is the hoop or circumferential stress, σ_0 is the magnitude of the applied time-harmonic load. Its distribution along the central nanoinclusion's perimeter at a fixed normalized frequency $\Omega_M = 0.24$ is depicted in Fig. 6(b) for the values of the surface parameter equal to $s=0$; 0.1; 0.5 and 1. The normalized frequency corresponds to the first peak in the DSCF distribution in respect to the frequency at a fixed point $\varphi = \pi / 2$ along the central nanoinclusion. The same set of results but for dimensionless frequency $\Omega_M = 1$ are plotted in Fig. 6(c). The analysis of the results shows that in order to achieve the presented plotting accuracy for low frequencies fine meshes are not necessary. *Models (1)* and *(2)* give identical results with 32/32 and 16/16 BE respectively. For higher frequencies fine meshes on the

matrix contour are necessary. Note that the plotting accuracy in Fig. 6(c) is achieved by *models (1) and (3)* with 32/32 and 32/16 BE along the matrix/inclusion contours.

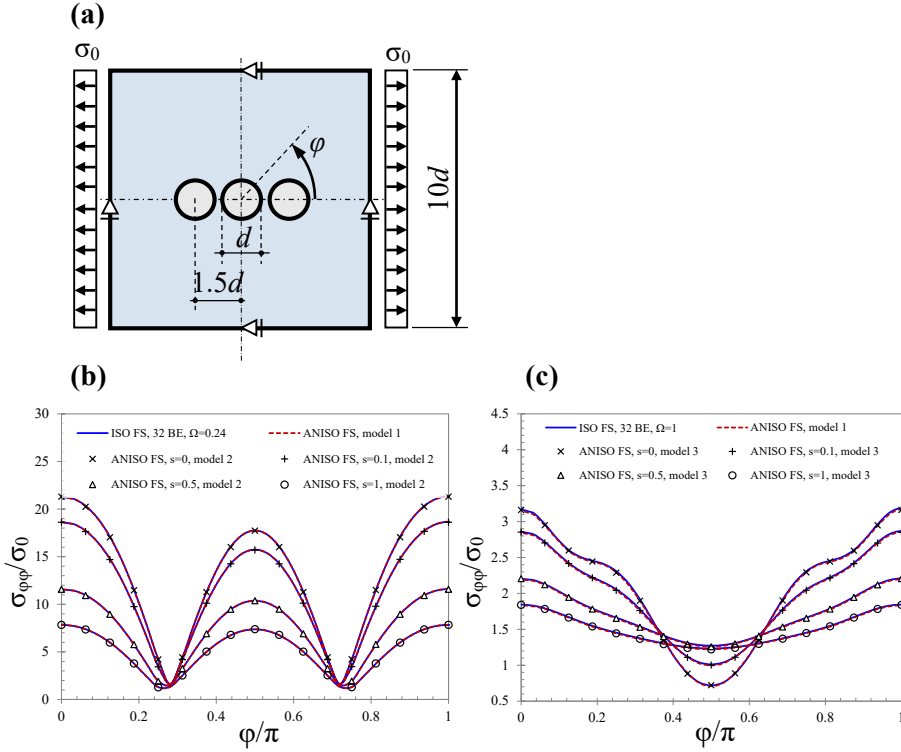


Figure 6: Three elastic isotropic inclusions in a square elastic isotropic matrix: (a) Geometry and loading; DSCF along the central nanoinclusion's perimeter on the matrix side at fixed normalized frequency of (b) $\Omega_M = 0.24$ and (c) $\Omega_M = 1$.

Test example 6: Anisotropic circular inclusion in a square anisotropic matrix under time-harmonic load

The aim of the next test example is to establish the accuracy characteristics of two different numerical methods such as the BEM and the FEM developed herein for heterogeneous domains of finite extent. ANSYS (2024) commercial software which allows solutions involving a solid finite matrix and inclusions with anisotropic structure is used. The surface effect is not implemented in the FEM solutions, so the comparisons here are for surface elasticity parameter $s=0$.

The finite domain is the square matrix from *Test example 5* with a single inclusion in its centre. The anisotropic matrix is LiNaKCsPO3 Glass Fiber. The material stiffness tensor components are as follows $c_{11}=193.946$ MPa; $c_{12}=17.952$ MPa; $c_{22}=39.313$ MPa; $c_{66}=13$ MPa, density is $\rho=2.8$ t/m³, the radius of the inclusion is $a_0=10^{-9}$ m. The inclusion material is assumed 10 times softer, or the respective stiffness tensor or $c_{11}^I=19.3946$ MPa; $c_{12}^I=1.7952$ MPa; $c_{22}^I=3.9313$ MPa; $c_{66}^I=1.3$ MPa, nano-inclusion's density is 1 t/m³. The BEM mesh comprises 48 BE along the matrix contour, 16 of which are used for each of the loaded sides and 8 BE are employed for each of the horizontal edges. For the inclusion-matrix interface 16 BE are used. The respective FE mesh consists of 4332 4-noded plane strain FE with 8 degrees of freedom (PLANE183). 80 FE are located along the inclusion-matrix interface and 40 FE are used per each side of the plate. In order to achieve better accuracy in the DSCF for polar angle $\varphi=\pi/2$ on the matrix side, the FE mesh is refined with 160 quadratic FE along the inclusion-matrix interface and respectively 80 FE per each side of the plate.

The results obtained by the FEM and by the BEM techniques developed here are plotted in Figs. 7, 8. More specifically Fig. 7 plots the normalized horizontal displacement $u_i c_{66} / a_0 \sigma_0$ at points with polar angle $\varphi=0$ and $\varphi=\pi/2$ versus the normalized frequency $\Omega = \omega d / \sqrt{c_{66} / \rho}$. The time harmonic analysis is performed for a frequency range up to $\Omega = 2.333$ divided into 20 equal frequency steps. In all simulations the normalization is with respect to the matrix material parameters.

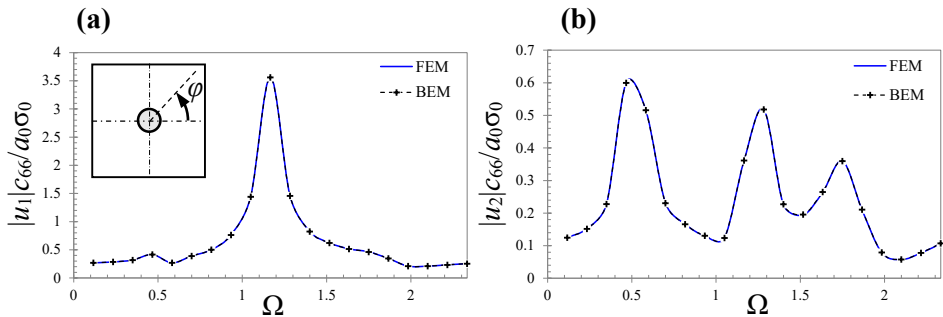


Figure 7: Normalized displacement components versus dimensionless frequency at inclusion-matrix interface for observer point with polar angle (a) $\varphi=0$; (b) $\varphi=\pi/2$.

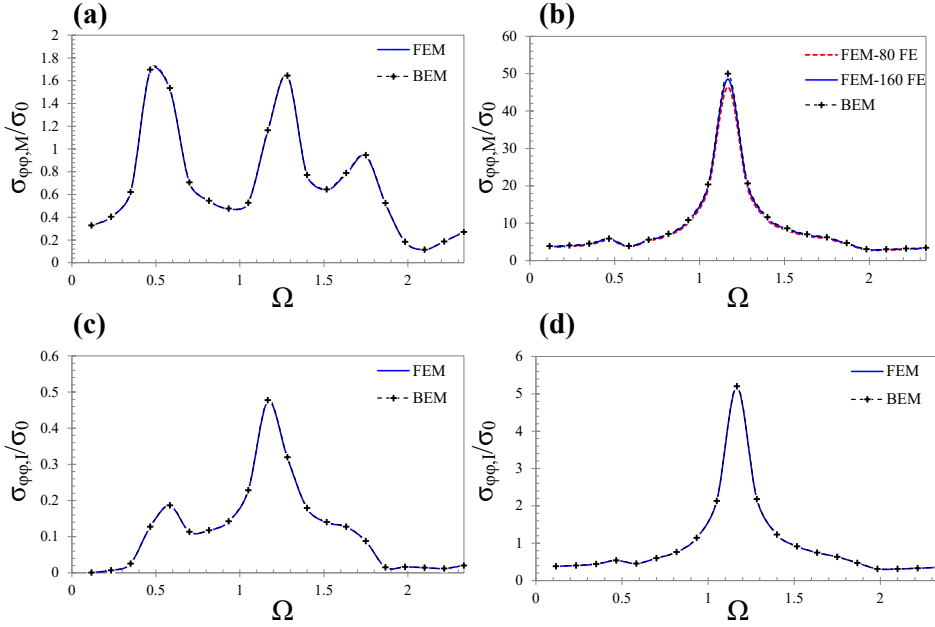


Figure 8: DSCF along inclusion-matrix interface versus dimensionless frequency for observer points with polar angles (a) $\varphi=0$, matrix side; (b) $\varphi=\pi/2$, matrix side; (c) $\varphi=0$, inclusion side; (d) $\varphi=\pi/2$, inclusion side.

DSCFs are depicted in Fig. 8. The hoop stresses from the matrix side are shown in Fig. 8a, b, while those from the inclusion side are presented in Fig. 8c, d. The percentage difference in the extreme displacements with respect to the average values is less than 0.5%. The percentage difference in the maximal hoop stresses with respect to the average values is less than 1% except for the case of $\varphi=\pi/2$ on the matrix side. At this point the percentage difference is 7.4% in the case of the coarse FE mesh (80 quadratic FE on the inclusion-matrix interface) and 2.84% for the fine FE mesh (160 quadratic FE on the inclusion-matrix interface).

In what follows, a convergence study for the case of an anisotropic matrix containing a single anisotropic inclusion is presented. Six different models have been considered in order to investigate the accuracy of the presented numerical technique and to adjust the most effective and optimal BE mesh with respect to the number of BEs. The mesh information for the models is summarized in *Table 2*. The surface effect is neglected in the presented results. The percentage differences between the FEM and BEM solutions for the extreme values of displacements and stresses, calculated with respect to the first model with the finest mesh, are summarized in *Tables 3-5*.

Based on the results presented above the following conclusions could be made: (a) In the case of anisotropic materials, the number of elements along the square plate contour is even more important than the mesh resolution at the contact inclusion-matrix interface; (b) more specifically, the loaded edges require more BEs in order to achieve better accuracy on the contact interface. The results reported in *Tables 3-5* show that differences less than 0.1% with respect to the finest mesh are observed in the third model with 48 BEs for the plate contour, 16 per vertical loaded edges and 8 per horizontal idle edges, and 16 BEs for the contact interface.

Table 2: BE models used in the convergence study

Model	Number of BE
1	64 at matrix contour/16 per side +32 at inclusion-matrix interface
2	32 at matrix contour/8 per side +32 at inclusion-matrix interface
3	48 at matrix contour/16 per loaded edges and 8 per unloaded contours + 16 at contact interface
4	32 at matrix contour/8 per side +16 at inclusion-matrix interface
5	24 at matrix contour/8 per loaded edges and 4 per unloaded contours + 16 at contact interface
6	16 at matrix contour/4 per side +16 at inclusion-matrix interface

Table 3: Percentage differences for $\Omega=0.4666$

Model	$\sigma_{\varphi\varphi,M}/\sigma_0$	difference ,%	$ u_1 c_{66}/a_0\sigma_0$	difference ,%
1	5.880332	-	0.415761	-
2	5.878729	0.03	0.41541	0.08
3	5.877811	0.04	0.41571	0.01
4	5.877469	0.05	0.41536	0.10
5	5.876956	0.06	0.41527	0.12
6	5.857304	0.39	0.414094	0.40

Table 4: Percentage differences for $\Omega=1.1664$

Model	$\sigma_{\varphi\varphi,M}/\sigma_0$	difference ,%	$ u_1 c_{66}/a_0\sigma_0$	difference ,%
1	49.98941	-	3.560316	-
2	49.95549	0.07	3.555272	0.14
3	49.98021	0.02	3.560757	0.01
4	49.96108	0.06	3.554689	0.16
5	50.08954	0.20	3.563612	0.09
6	48.30696	3.37	3.437472	3.45

Table 5: Percentage differences for $\Omega=1.7496$

Model	$\sigma_{\varphi\varphi,M}/\sigma_0$	difference , %	$ u_1 c_{66}/a_0\sigma_0$	difference , %
1	6.242926	-	0.462293	-
2	6.221474	0.34	0.460459	0.40
3	6.238547	0.07	0.461968	0.07
4	6.222752	0.32	0.460343	0.42
5	6.212572	0.49	0.459564	0.59
6	6.097706	2.33	0.447976	3.10

Test example 7: Anisotropic circular inclusion in a square anisotropic matrix under transient dynamic load

The last test example considers again a single anisotropic inclusion in a square anisotropic matrix with geometrical dimensions, material properties all defined in *Test example 6*. The intensity of the transient tensile load applied in horizontal direction is presented by the time-history function $f(t) = F(t)te^{-\beta t}$, where $F(t)$ is the Heaviside step function and the parameter $\beta = 200$. The numerical models and mesh discretization are the same as those described in *Test example 6*. The transient FEM analysis has been performed up to the normalized time $\tau = (t/a_0)\sqrt{c_{66}/\rho} = 323.21$ divided into 300 equal time steps which results in the dimensionless time step $\Delta\tau = 1.077$. The viscous proportional damping is assigned with the stiffness coefficient $2\xi = 0.05\%$. The respective time harmonic BEM analysis has been performed for the normalized frequency range up to $\Omega = 2.916$ divided into 500 equal frequency steps. The corresponding damping in the time harmonic BEM analysis is frequency dependent with the viscoelastic coefficients $c_{ij}^* = c_{ij}(1 + 2i\omega\eta)$ with $\eta = 0.025\%$. The time history BEM responses have been obtained by inverse FFT and the respective time step is $\Delta\tau = 2.155$ or twice larger than that in the transient FEM analysis.

Comparisons for the normalized horizontal displacement at a point with polar angle $\varphi=0$ and the normalized vertical displacement at a point with polar angle $\varphi=\pi/2$ (defined as $u_i c_{66}/a_0\sigma_0$) versus the dimensionless time τ are presented in Fig. 9a. The normalized hoop stress for the same observer points is illustrated in Fig. 9b. In the normalized displacements and hoop stresses the notation $\sigma_0 = \max(f(t))$ is the maximum value of the time-history function.

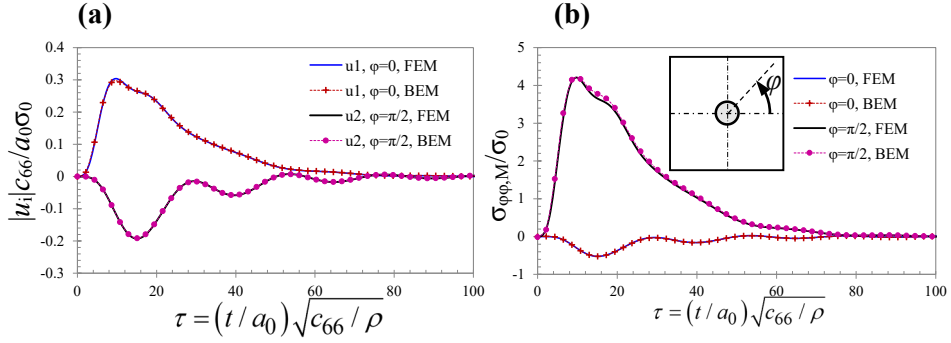


Figure 9: (a) Normalized displacement components and (b) DSCF versus normalized time τ for points belonging to the inclusion matrix interface with the marked polar angles.

All the figures above demonstrate an excellent agreement between the results obtained from different computational techniques. The compared results indicate that the type and density of the BEM discretization meshes used are adequate to achieve satisfactory accuracy and convergence for the planned parametric study, which is presented in the next section.

5. Parametric study

A. Elastic isotropic nanocomposites with different types of nanoheterogeneities under time-harmonic load

A1 Unbounded solids

The aim here is to solve a number of cases involving multiple nanocavities and/or nano-inclusions in an infinite elastic domain, so as to investigate the dependence of the DSCF at the interfaces on the following factors: (a) type, size and shape of the nanoheterogeneity, with the last factor having a direct effect on the surface energy which develops at the interfaces; (b) ratio of the material bulk properties of the matrix to those of the nanoinclusion; (c) surface properties, as quantified by the interfacial material constants and the residual interface tension; (d) dynamic interactions between multiple nanoheterogeneities based on their number and distribution and finally (e) incoming elastic wave's type and its characteristics.

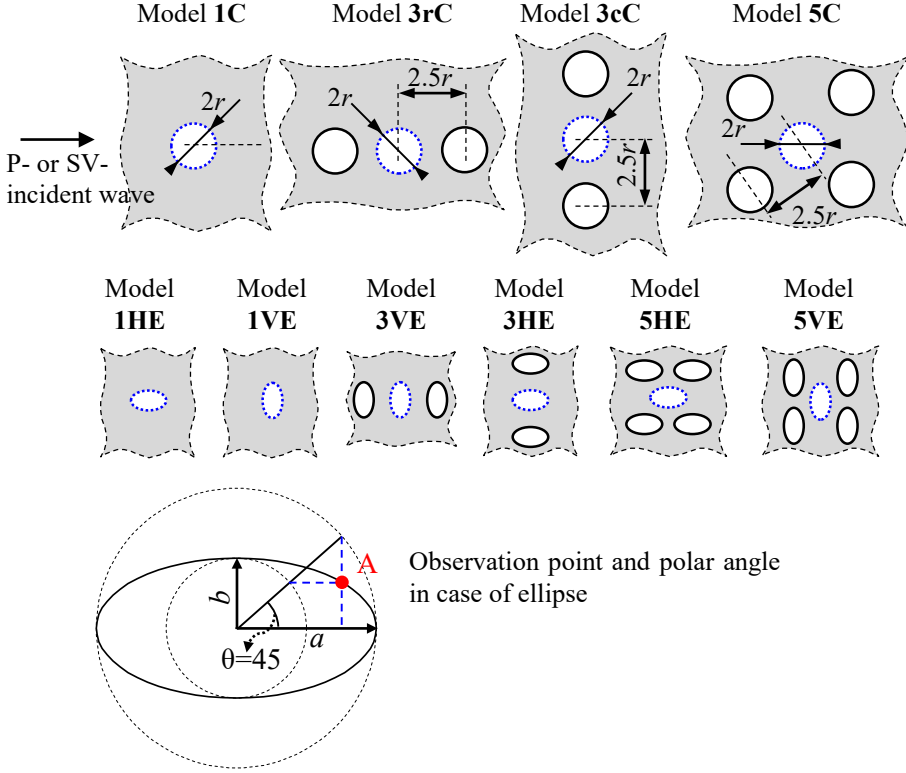


Figure 10: Geometric configuration of the models used in the numerical simulations.

More specifically, four basic configurations are shown in Fig. 10 for three geometrical shapes (circular, horizontally elongated elliptic and vertically elongated elliptic) involving one, three and five nanoheterogeneities. Concurrently shown in Fig. 10 is their geometrical arrangement, as well as the position (using the polar angle along the perimeter) of the observer point in the case of the elliptic shapes. The following abbreviations are now introduced for the aforementioned mechanical models: *C* for circle; *3rC* for three circular cavities arranged in a single row; *3cC* for three circular cavities arranged in a single column; *5C* for five circular cavities; *HE* for horizontally elongated ellipses; and *VE* for vertically elongated ellipses.

The same nomenclature as before is used for the material properties of an inclusion and its surrounding infinite plate, while Poisson's ratio is $\nu = 0.26$ for both solid phases. We now define two ratios, namely $\mu^I / \mu^M = 0.2$ and $\Omega_I / \Omega_M = 3$, where the frequency $\Omega_M = \omega r / C_P^M$ is normalized with the wave number of the P-wave in the matrix and is used for both incident elastic

waves. The radius of the circular nanoheterogeneity is $r=1$ nm, while the averaged radius of the elliptical nanoheterogeneities is $(a+b)/2$ and is again equal to 1 nm. The actual dimensions of the semi-axes for the elliptic shapes are $a=4/3$ nm; $b=2/3$ nm, yielding a ratio $a/b=2$. Next, the center-to-center separation distance between any two neighboring nanoheterogeneities is 2.5 nm. Finally, the surface properties are quantified by the dimensionless parameter $s = (2\mu^S + \lambda^S)/2\mu^M r$. Due to the large difference in the material property values across an interface, a sizeable DSCF value arises around a nanoinclusion, which helps to explain why material degradation and failure is mainly observed at interfaces. This is the reason for investigating stress concentration phenomena near inhomogeneities by researchers in material science. In here, we consider interface effects generated by incident P- and SV- waves and compute the DSCF normalized by the incident wave stress.

The circular nanocavity case

The results of all BEM computations for the normalized DSCF produced by an incident P-wave are plotted versus the dimensionless frequency Ω_M at the observer point with polar angle $\varphi=\pi/2$ in Fig. 11, while those for an incident SV-wave are given for the observer point with polar angle $\varphi=\pi/4$ in Fig. 12. More specifically, this observer point is always placed along the central circular nanoheterogeneity perimeter in all four models denoted with dashed lines in Fig. 10, where both waves are moving along the horizontal direction (incident angle is $\theta=0$). In addition, the results obtained by Ru *et al.* (2009) using the wave function expansion method are also depicted for the case of a single circular cavity (i.e., in Figs. 11a and 12a). As with the other verification examples, an excellent match between these two sets of results is obtained. Before we look at the interference effect generated by the presence of multiple nanoheterogeneities, we make the following general observations: (a) As the vibration frequency increases, the DSCF values decrease, eventually approaching unity. This indicates that the scattered stress field becomes identical to the incident stress field; (b) as the surface parameter s value increases, the DSCF values invariably drop, which indicates that a strong molecular surface action overrides the classical mechanical effects observed at the macroscale; and (c) at high s values, the DSCF distribution becomes nearly flat, irrespective of the value of the exciting frequency, which is again a manifestation of the importance of surface effects at the nanoscale.

Next, the interference effect in the presence of a P-wave shows the following trends, almost independently of the surface parameter s values: (a)

A horizontal arrangement of cavities has minimal impact, as the computed DSCF is smaller compared to the single cavity case; (b) a vertical cavity arrangement, however, significantly alters the results, producing DSCF values that are nearly twice as large as those observed in the previous case; (c) the cross-like arrangement of five cavities is an intermediate situation, where some increase is observed relative to the single cavity case, and this is most noticeable at the higher frequency range and for low parameter s values.

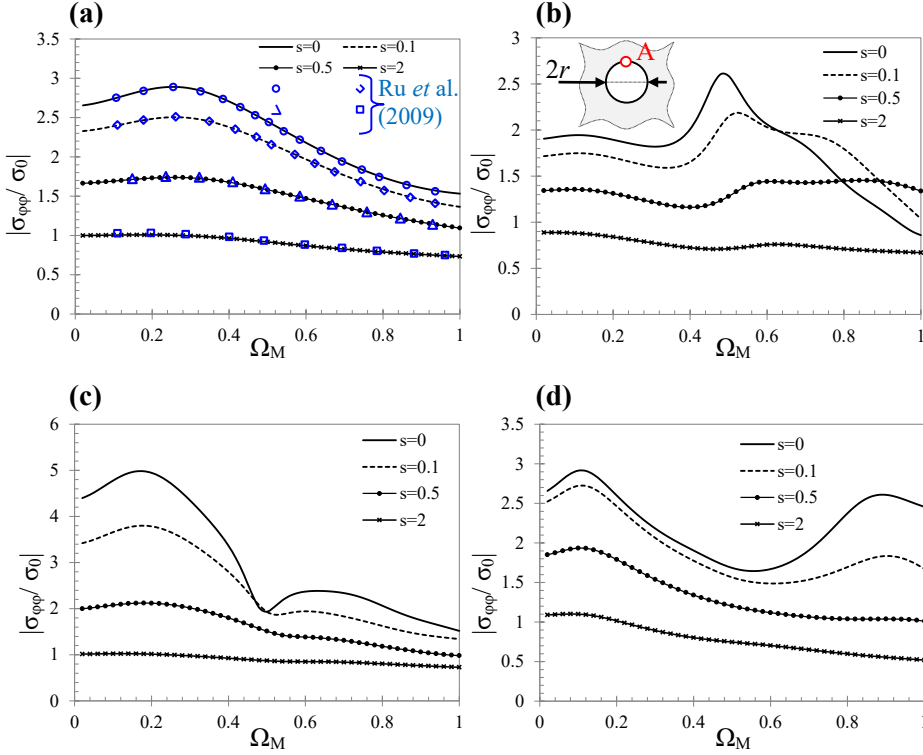


Figure 11: Normalized DSCF versus Ω_M at observer point A ($\varphi=\pi/2$) along the perimeter of the central circular nanocavity at different values of the material parameter s for an incident P-wave($\theta=0$): (a) model 1C; (b) model 3rC; (c) model 3cC; and (d) model 5C.

Finally, when the incident wave is of the SV-type, the situation is quite different: (a) The row-like cavity arrangement mildly amplifies the *DSCF*, somewhere in the order of 15% and for low parameter s values; (b) the column-like cavity arrangement produces high amplification, nearly doubling the DSCF at the higher end of the frequency spectrum and (c) the cross-like arrangement of five cavities produces resonance effects in the

$0.4 \leq \Omega_M \leq 0.6$ frequency band, where the DSCF is now almost an order of magnitude higher for low parameter s values. This last effect is important and is bound to have important repercussions in the design and performance of perforated nanoplates and nanomembranes.

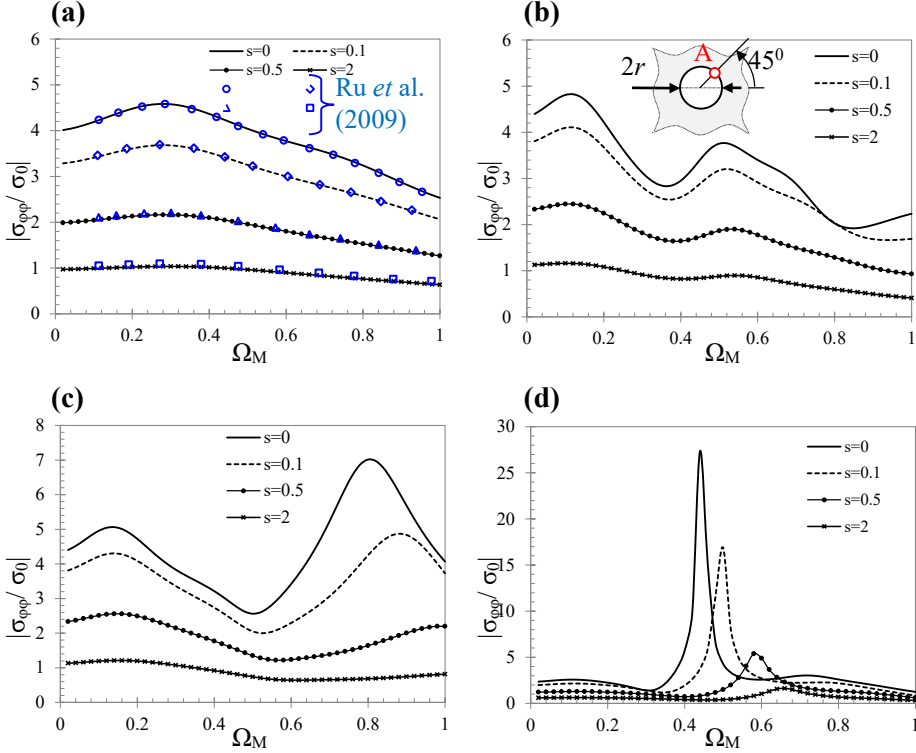


Figure 12: Normalized DSCF versus Ω_M at observer point A ($\varphi=\pi/4$) along the perimeter of the central circular nanocavity at different values of the material parameter s for an incident SV-wave($\theta=0$): (a) model 1C; (b) model 3rC; (c) model 3cC; and (d) model 5C.

The circular nanoinclusion case

We now move on to examine how the replacement of circular nanocavities by circular nanoinclusions affects the DSCF development. We use the same heterogeneity arrangement as before, as well as the same normalized frequency values to plot DSCF along the inclusion perimeter for both P- and SV-incident waves. As previously mentioned, the inclusion/matrix mismatch is quite large, namely $\mu^I / \mu^M = 0.2$. Thus, Figs. 13 and 14 plot the DSCF frequency variation at fixed observer points on the inclusion-matrix interface,

but from the matrix side of the interface and for both P- and SV- waves, respectively.

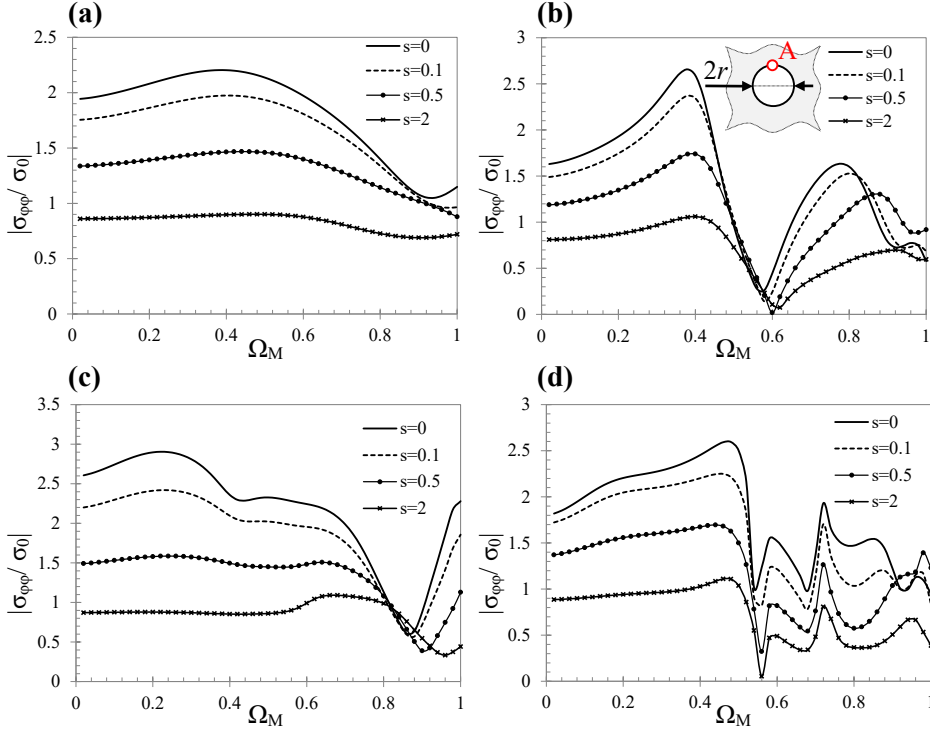


Figure 13: Normalized DSCF versus Ω_M at observer point A ($\varphi=\pi/2$) along the perimeter of the central circular nanoinclusion at different values of the material parameter s for an incident P-wave($\theta=0$): (a) model 1C; (b) model 3rC; (c) model 3cC; and (d) model 5C.

The following observations can now be made: (a) When a single cavity is filled with a soft material, it results in lower DSCF values-especially at relatively low s values, where surface effects are less pronounced; (b) Multiple inclusion arrangements, however, drastically alter the DSCF frequency distribution. While the maximum values observed remain largely unchanged, notable dips (approaching zero) occur at discrete frequency values within the range $0.6 \leq \Omega_M \leq 0.8$. This pattern holds for both types of incident waves, with the exception of the five-inclusion arrangement under SV-waves (Fig. 14d), where resonance effects observed with multiple cavities in Fig. 12d are again present; (c) In summary, the presence of inclusions, as opposed to cavities, tends to be less disruptive to the development of the dynamic stress field's spatial distribution.

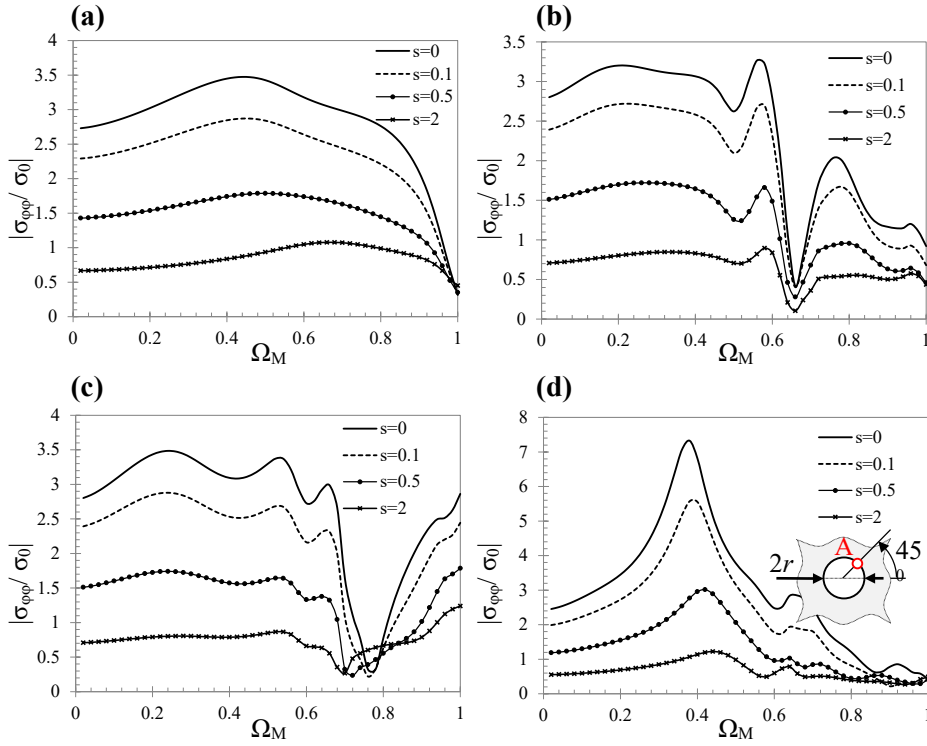


Figure 14: Normalized DSCF versus Ω_M at observer point A ($\varphi=\pi/4$) along the perimeter of the central circular nanoinclusion at different values of the material parameter s for an incident SV-wave($\theta=0$): (a) model 1C; (b) model 3rC; (c) model 3cC; and (d) model 5C.

The elliptic nanocavities

In Fig. 15, we examine the influence of the geometrical shape (horizontally and vertically elongated elliptic cavity boundaries) on the dynamic stress field. This study is carried out in conjunction with multiple cavities ranging from one to three to five, and in four configurations (single, row, column and star arrangements). As before, the normalized DSCF is plotted versus the normalized frequency at an observer point located in the central ellipse with polar angle $\varphi=\pi/2$ when the incident wave is of the P-type. Also, the surface parameter value is fixed at $s=0.1$. When the number of cavities is five, the DSCF distribution looks much like that for a single cavity, which indicates minimal interaction phenomena. Of particular interest is the observation that vertically elongated ellipses reduce the DSCF by approximately 20% on average, compared to the single cavity case, whereas circular and horizontally

elongated ellipses lead to an amplification of the DSCF. With three cavities, however, a spike in the DSCF is observed (the value nearly doubles) for vertically elongated ellipses in the horizontal cavity arrangement, particularly in the mid-frequency range. One reason for this amplification is that the observation point is located at the sharp edge of the ellipse. Although not shown here for the sake of brevity, when inclusions replace the cavities in Fig. 15 and an incident P-wave is applied, the situation changes. Any multiple nanoinclusion arrangement leads to substantially different, and mostly lower, DSCF frequency distributions.

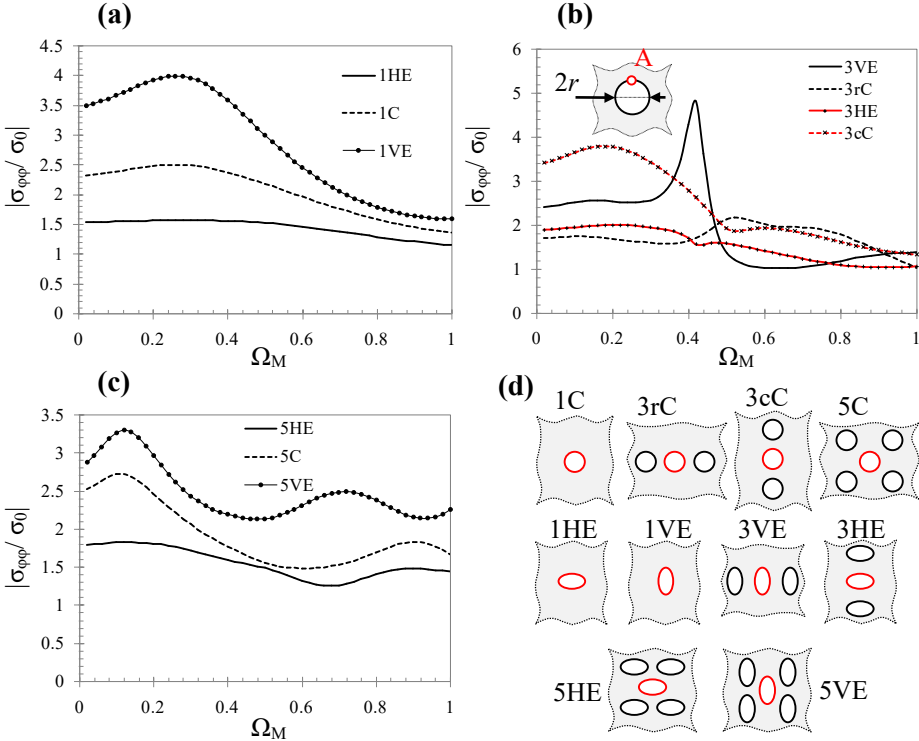


Figure 15: Normalized DSCF versus Ω_M at observer point A ($\varphi=\pi/2$) along the central circular and/or elliptical nanocavities for a fixed $s=0.1$ value due to an incident P-wave ($\theta=0$) and for: (a) single cavity; (b) three cavities; (c) five cavities and (d) are the model layout configurations.

We can conclude that surface effects and the dynamic interaction between multiple nanoheterogeneities-whether cavities or inclusions-clearly lead to multiple wave scattering and diffraction phenomena. More specifically, surface elasticity consistently lowers the DSCF values, regardless of the incident wave frequency, as well as the distance and configuration of the

cavities and inclusions. Finally, a key engineering factor influencing this phenomenon is the ratio of the incident wavelength to the center-to-center separation distance, which affects the non-uniform stress distribution along the matrix interfaces.

A2 Semi-infinite elastic anisotropic solids

The parametric study related with nanoheterogeneities in semi-infinite nano-sheet is conducted regarding the influence of both material anisotropy and surface elasticity on the wave fields that develop in the surrounding medium to the key model parameters. The following non-dimensional parameters are used here: (a) the non-dimensional frequency $\Omega = kd = \omega 2a / \sqrt{c_{66} / \rho}$; (b) the normalized surface elasticity coefficient $s = (\lambda^S + 2\mu^S) / (ac_{66})$; (c) the normalized dynamic stress concentration factor (DSCF) defined as $DSCF = \sigma_{\varphi\varphi} / \sigma_0$, where $\sigma_{\varphi\varphi}$ is the hoop or circumferential stress, normalized by the incident stress σ_0 defined as $\sigma_0 = -c_{66}u_0k^2$ with $k = \omega / C_S$; (d) the normalized displacement components u_i / u_0 , $i=1,2$. In the following numerical models a hysteretic damping ratio $\zeta=2\%$ is assigned. The dynamic time-harmonic excitation is presented by vertically propagating incident plane waves referred as quasi P- (qP) waves as far as they are not purely longitudinal in the anisotropic medium.

The first group of results considers qP- wave scattering by a single circular nanocavity with radius $a=1.10^{-9}$ m and the center point located at the depth $h=-2a$ in a homogeneous elastic anisotropic nano-sheet without any surface relief. Five different material models are considered and their material properties are given in *Table 6*.

Table 6: Material properties of different materials used in the parametric study

Mat. type	stiffness tensor components, [MPa]	ρ , [t/m ³]
IsoMAT-1	$c_{11} = 43.952; c_{12} = 17.952; c_{22} = 43.952; c_{66} = 13$	2.8
AnisoMAT-2	$c_{11} = 81.4505; c_{12} = 17.952; c_{22} = 42.79225; c_{66} = 13$	2.8
AnisoMAT-3	$c_{11} = 118.949; c_{12} = 17.952; c_{22} = 41.6325; c_{66} = 13$	2.8
AnisoMAT-4	$c_{11} = 156.4475; c_{12} = 17.952; c_{22} = 40.47275; c_{66} = 13$	2.8
AnisoMAT-5	$c_{11} = 193.946; c_{12} = 17.952; c_{22} = 39.313; c_{66} = 13$	2.8

Three materials AnisoMAT-2, AnisoMAT-3 and AnisoMAT-4 are chosen between the following limit cases: (a) LiNaKCsPO3 Glass Fiber

denoted as AnisoMAT-5 ($c_{11} = 193.946$; $c_{12} = 17.952$; $c_{22} = 39.313$; $c_{66} = 13$ MPa) and (b) equivalent isotropic matrix material (IsoMAT-1) with Lamé constants $\lambda = c_{12} = 17.952$ MPa and $\mu = c_{66} = 13$ MPa corresponding to the anisotropic one as far as the stiffness coefficients c_{12} and c_{66} are equal. The stiffness tensor of the equivalent isotropic material is then defined as: $c_{11} = c_{22} = \lambda + 2\mu = 43.952$ MPa, $c_{12} = 17.952$ MPa, $c_{66} = 13$ MPa. The difference between AnisoMAT-5 and its isotropic equivalent IsoMAT-1 is only in the c_{11} and c_{22} stiffness components. Note that the three intermediate matrix materials AnisoMAT-2, AnisoMAT-3 and AnisoMAT-4 are with c_{11} and c_{22} stiffness components linearly interpolated between both the limit states.

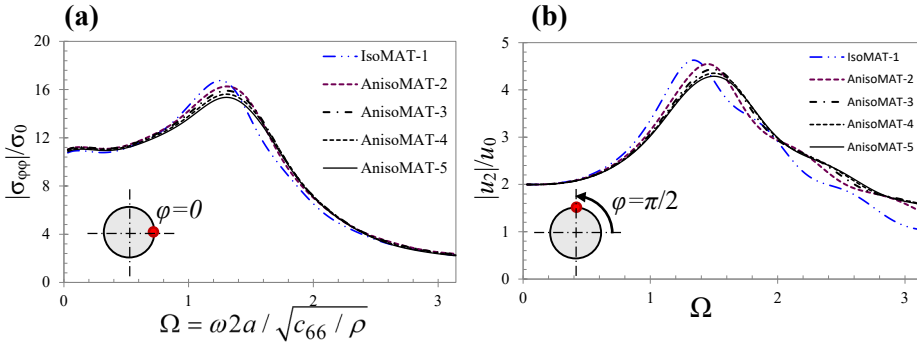


Figure 16: Normalized hoop stresses at marked observer point $\varphi=0$ in (a) and normalized vertical displacement component at point $\varphi=\pi/2$ in (b) versus dimensionless frequency of normal qP-waves for different material types at surface elasticity coefficient $s=0$.

The normalized hoop stresses at the marked observer point $\varphi=0$ and the normalized vertical displacement component at point $\varphi=\pi/2$ versus the dimensionless frequency of a normal qP-wave for different material types at the surface elasticity coefficient $s=0$ are plotted in Fig. 16. Normalized hoop stresses and the normalized vertical displacement versus the polar angle at a fixed dimensionless frequency $\Omega=1.257$, corresponding to the maximal value observed in Fig. 16, are drawn in Fig.17. Fig.18 shows the frequency dependent normalized hoop stresses and the normalized vertical displacement at a variable surface parameter s for IsoMat-1 and AnisoMat-5 materials. In the BE modelling the discretized flat free surface is represented by 20 equal quadrates. BE of total length $\pm 10a$ left and right to the coordinate system origin. The cavity is modelled by 16 BE.

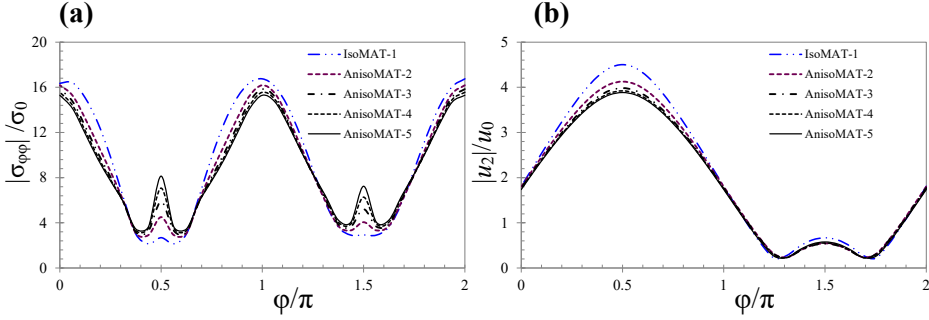


Figure 17: Normalized hoop stresses in (a) and normalized vertical displacement component in (b) versus polar angle at fixed dimensionless frequency $\Omega=1.257$ for different types of materials at surface elasticity coefficient $s=0$.

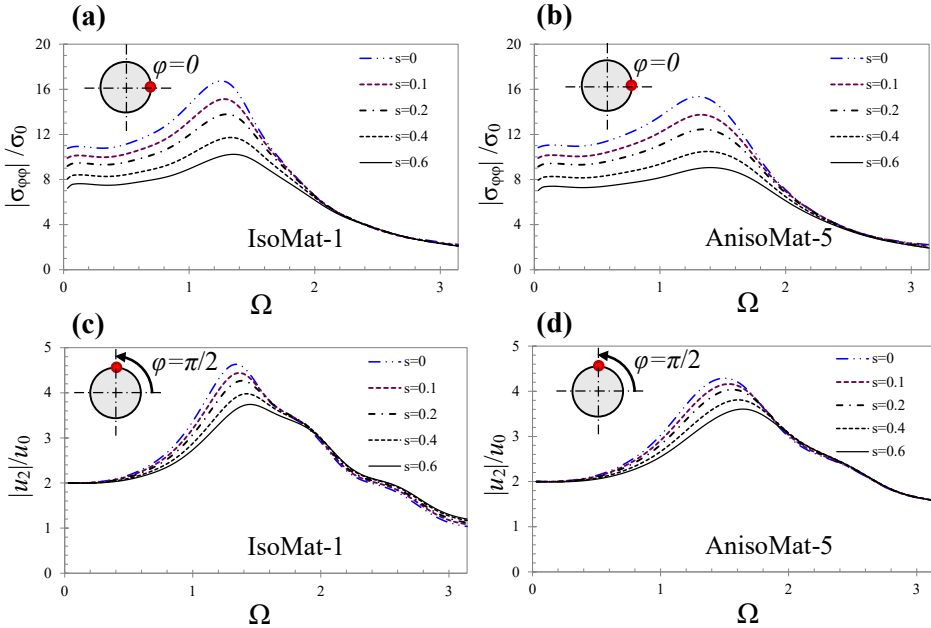


Figure 18: Influence of the surface elasticity coefficient s on the normalized hoop stresses in (a), (b) and normalized vertical displacement component in (c), (d) versus dimensionless frequency for IsoMat-1 and AnisoMat-5 materials.

The second parametric example is a single elliptical cavity buried in a nano-sheet with material type AnisoMAT-5 subjected to normal incident qP-waves. Five different shapes of the ellipse are considered with semi-axis ratio $a/b=2, 1.5, 1, 2/3$ and 0.5 . The semi-axis ratio $a/b=1$ corresponds to a circular cavity, when $a/b>1$ the ellipse is horizontally elongated, ratios $a/b<1$

correspond to vertically elongated ellipses. The averaged radius of the elliptical cavity is $(a+b)/2$ and it is equal to the circular hole radius of 1 nm. The geometry of the problem is presented in Fig. 19 (a). The nodal points of the BE mesh are plotted on the circular cavity model in order to give an impression about the distances between the source and receiver points of the model. The normalized hoop stresses for different cavity shapes, fixed normalized frequency $\Omega=1.257$ and surface elasticity parameter $s=0, 0.2$ and 0.6 are presented in Fig. 19 (b), (c) and (d) respectively. The most unfavorable form which causes largest hoop stresses turns out to be the sharpest horizontally elongated ellipse. The smallest stresses are observed along the vertically elongated elliptical contour with $a/b=0.5$.

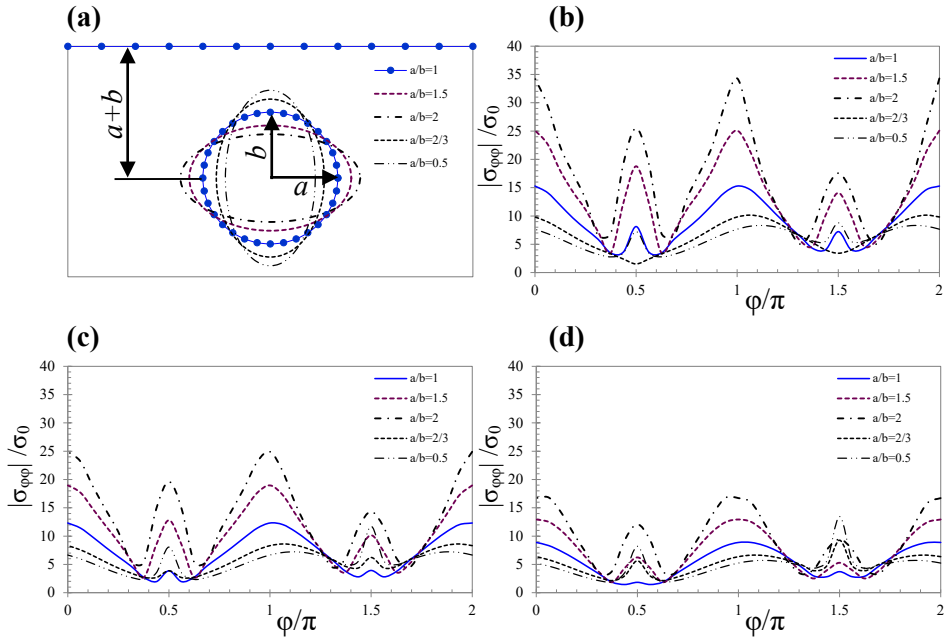


Figure 19: (a) Problem geometry; Normalized hoop stresses for fixed normalized frequency $\Omega=1.257$ and various surface elasticity parameter (b) $s=0$; (c) $s=0.2$; (d) $s=0.6$.

The third group of results concerns qP- wave scattering by two horizontally arranged circular nanocavities with radius $a=1.10^{-9}$ m, the centre point located at depth $h=-2a$ and the separation distance $3a$. As before, the discretized flat free surface is represented by 20 equal quadratic BE of total length $\pm 10a$ left and right to the coordinate system origin both the cavities are modelled by 16 BE. In the plots below, the single nanocavity in the half-plane is referred as *model 1*, the two nanocavities are named *model*

2. Fig.20 presents the frequency-dependent stress concentration at observer points $\varphi=0$ and $\varphi=\pi$ along the left cavity in the case of a single and two cavities for IsoMat-1, AnisoMat-3 and AnisoMat-5 half-planes at $s=0$. The influence of the surface elasticity on the DSCF in the frequency interval under consideration at the point with the polar angle $\varphi=0$ belonging to the left hole of the *model 2* for IsoMat-1 and AnisoMat-5 half-planes is illustrated in Fig.21.

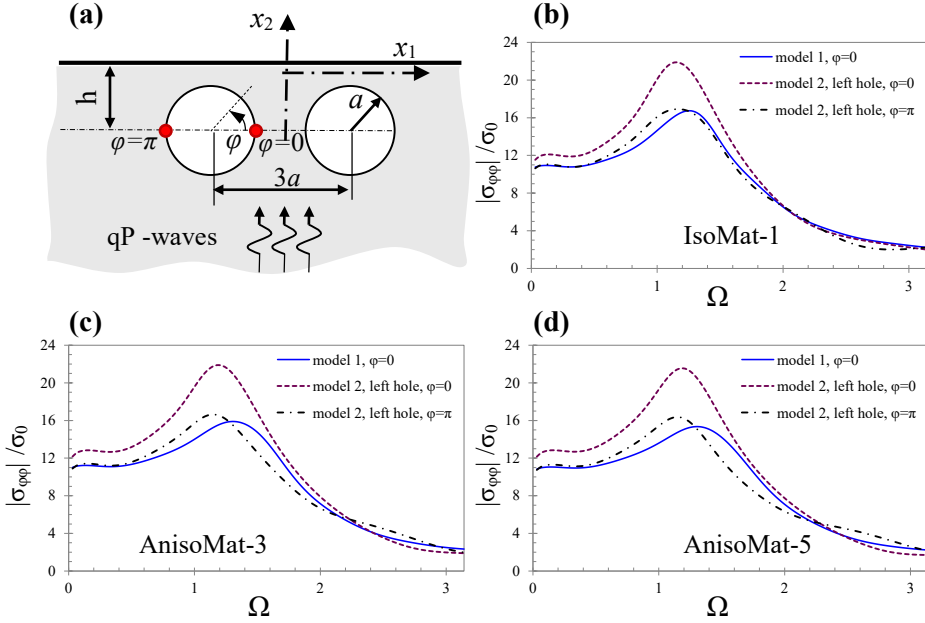


Figure 20: Model geometry in (a); DSCF at $s = 0$ for the marked observer points and IsoMat-1, AnisoMat-3 and AnisoMat-5 materials in (b), (c), (d), respectively.

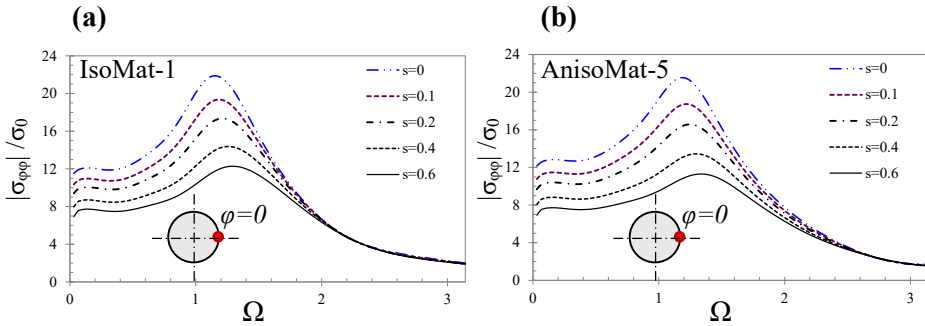


Figure 21: DSCF versus normalized frequency for variable surface parameters s and observer point with polar angle $\varphi=0$ belonging to the left hole of the *model 2* for: (a) IsoMat-1; (b) AnisoMat-5.

The fourth parametric example deals with qP- wave scattering by a semi-circular nanocanyon with radius $a=1.10^{-9}$ m along an elastic anisotropic half-plane, see Fig.22. In all the models below the BE mesh consists of 36 BE, 12 of which are used for the relief peculiarities. As before the discretized free surface is $\pm 10a$ left and right to the coordinate system origin. The normalized vertical displacement components along the half-plane free surface for the depicted material types and fixed dimensionless frequencies $\Omega=2.702$ and $\Omega=5.56$, in the absence of surface elasticity effect, are shown in Fig. 23.

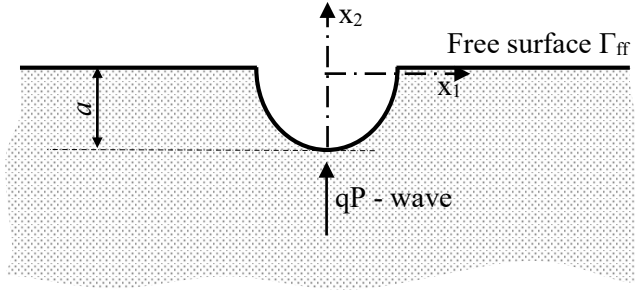


Fig. 22: Layout of the problem.

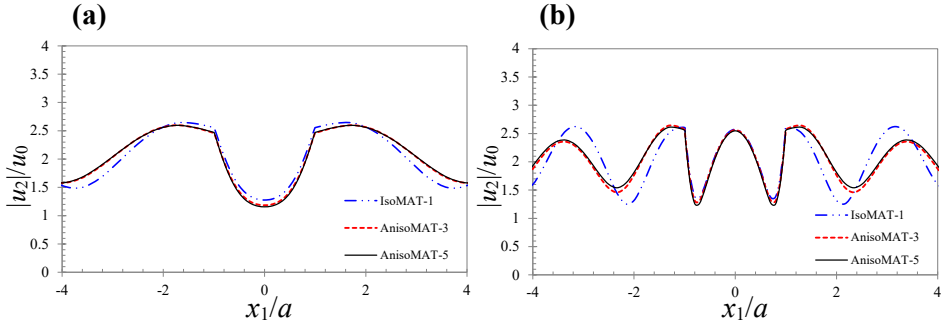


Figure 23: Normalized vertical displacement component along the free surface of semi-circular nanocanyon at $s = 0$ for different types of materials and for fixed dimensionless frequency: (a) $\Omega=2.702$; (b) $\Omega=5.56$.

In the next numerical simulation, the shape of the canyon varies from a horizontally elongated to a vertically elongated semi-ellipse. The averaged radius of the elliptical nanorelief is $(a+b)/2$ and it is equal to the semi-circular nanocanyon radius of 1 nm. The elliptical canyons are horizontally or vertically elongated depicted as *model 1* and *model 2* respectively. The semi-circular shape is plotted as *model 0*. The actual dimensions of the semi-axes for the elliptic shapes are $a=4/3$ nm; $b=2/3$ nm, yielding a ratio $a/b=2$ for the

horizontally elongated canyon. For the vertically elongated semi-elliptical canyon the same dimensions are $a=2/3$ nm; $b=4/3$ nm, with ratio $a/b=1/2$, see Fig. 24.

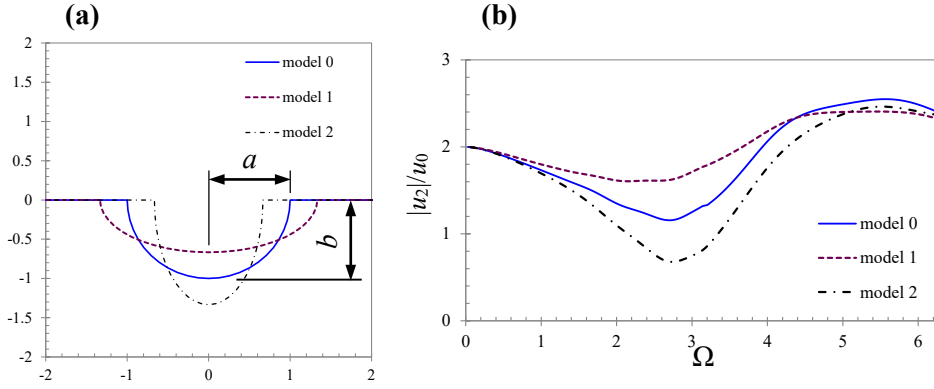


Figure 24: Geometry of the different canyon shapes in (a); Vertical displacement component at bottom of the canyon versus dimensionless frequency for different canyon models at $s = 0$ in (b).

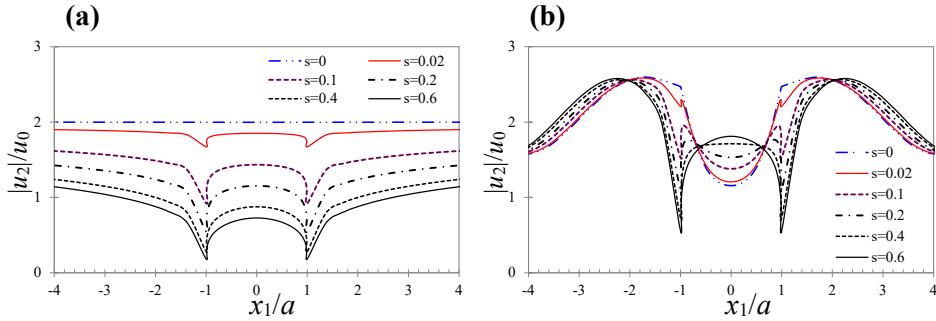


Figure 25: Normalized vertical displacement components along the free surface of a semi-circular canyon (*model 0*) for variable s and fixed dimensionless frequency: (a) $\Omega=0.03$; (b) $\Omega=2.702$.

Figs. 24-35 concern a half-plane with anisotropy of the material AnisoMat-5. The vertical displacement at bottom of the nanocanyon with a semi-circular, horizontally or vertically elongated elliptic shape versus the dimensionless frequency at $s=0$ is depicted in Fig.24b. The frequency range in the time harmonic analysis of all canyon models is up to $\Omega = 6.28$ divided into 200 equal frequency steps. The normalized vertical displacements along the free surface of an anisotropic half-plane with a nanocanyon having different shapes for different surface elasticity coefficients and at fixed

frequencies are presented in Figs. 25, 27, 28. The normalized vertical displacement at the bottom of the nanocanyon with different shapes versus the frequency for variable surface parameter s is shown in Fig.26. Fig.29 illustrates the distribution of the vertical displacement along the free surface of different canyon models for the fixed dimensionless frequency $\Omega=2.702$ and the surface parameters $s=0.02$ and $s=0.2$.

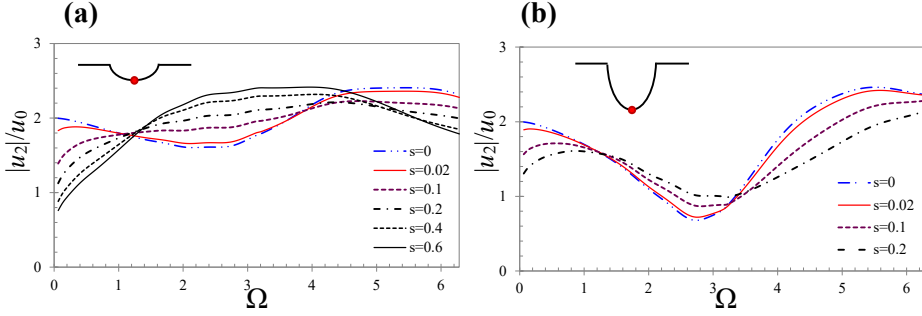


Figure 26: Normalized vertical displacement component at the bottom of the nanocanyon versus dimensionless frequency for variable surface parameter s in the following cases: (a) horizontally elongated semi-elliptical canyon (*model 1*); (b) vertically elongated semi-elliptical canyon (*model 2*).

The next set of results concerns qP- wave scattering by a semi-circular nanohill with radius $a = 1.10^{-9}$ m along an elastic anisotropic half-plane, see the problem geometry in Fig.30a.

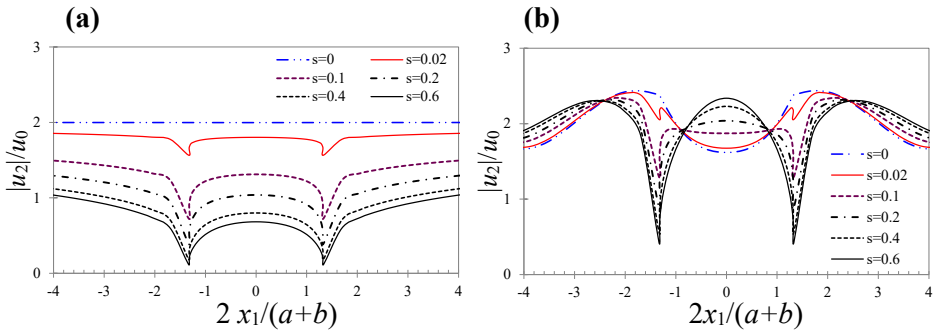


Figure 27: Normalized vertical displacement components along the free surface of horizontally elongated semi-elliptical canyon (*model 1*) for variable s and fixed dimensionless frequency: (a) $\Omega=0.03$; (b) $\Omega=2.702$.

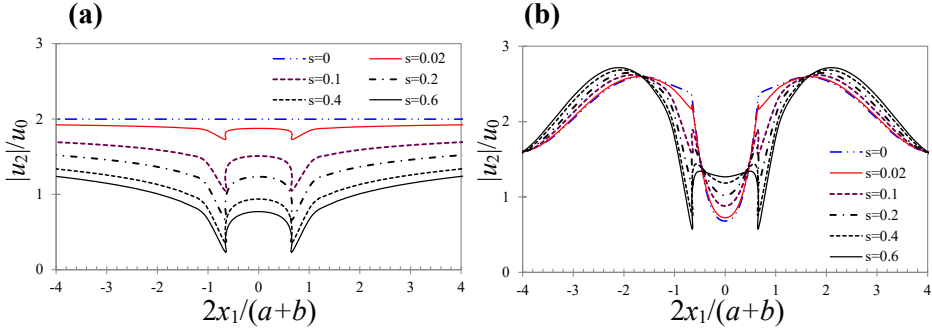


Figure 28: Normalized vertical displacement components along the free surface of vertically elongated semi-elliptical canyon (*model 2*) for variable s and fixed dimensionless frequency: (a) $\Omega=0.03$; (b) $\Omega=2.702$.

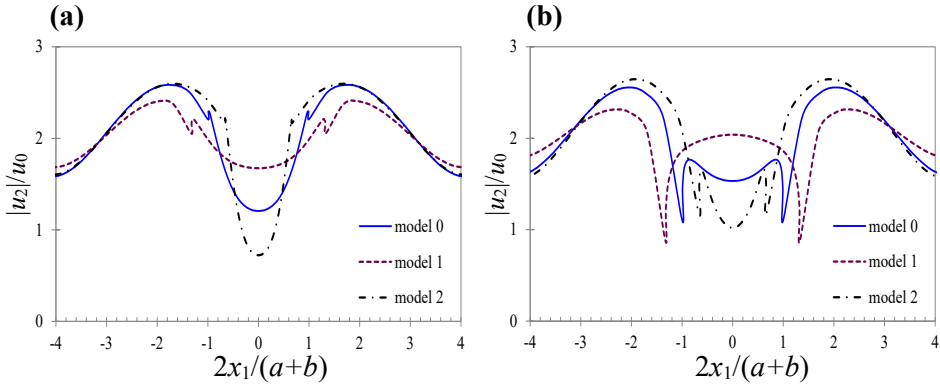


Figure 29: Normalized vertical displacement components along the free surface of different canyon models for fixed dimensionless frequency $\Omega=2.702$ and surface parameter: (a) $s=0.02$; (b) $s=0.2$.

The vertical displacement component at the top of the nanohill versus frequency of the incident wave for different hill models without surface effect is shown in Fig.30b. The time harmonic analysis in case of a nanohill is performed for a frequency range up to $\Omega=6.28$ divided into 100 equal frequency steps. The normalized vertical displacements along the free surface of the nanohill with different geometry for variable s and fixed frequencies are given in Figs. 31, 33, 34. Normalized vertical displacement at the top of the horizontally and vertically elongated semi-elliptical nanohill versus the dimensionless frequency and variable surface parameter s is presented in Fig.32. Fig.35 reveals the influence of the nanohill geometry on the vertical displacement along the free surface of the anisotropic half-plane for a fixed surface parameter $s=0.2$ and the dimensionless frequency: (a) $\Omega=0.063$; (b) $\Omega=2.702$. The influence of the material anisotropy is shown in Fig.36.

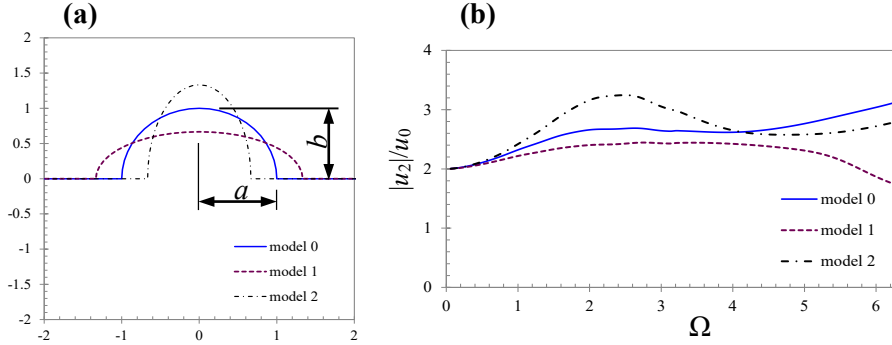


Figure 30: Geometry of the different hill shapes in (a); Vertical displacement component at top of the nanohill versus dimensionless frequency for the different hill models without surface effect in (b).

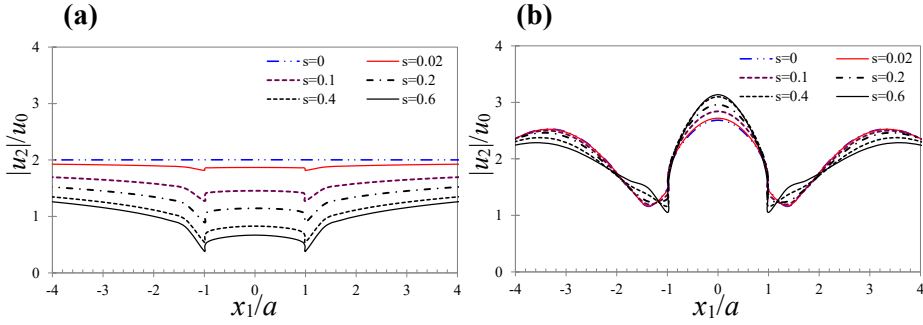


Figure 31: Normalized vertical displacement components along the free surface of semi-circular nanohill (*model 0*) for variable s and fixed dimensionless frequency: (a) $\Omega=0.063$; (b) $\Omega=2.702$.

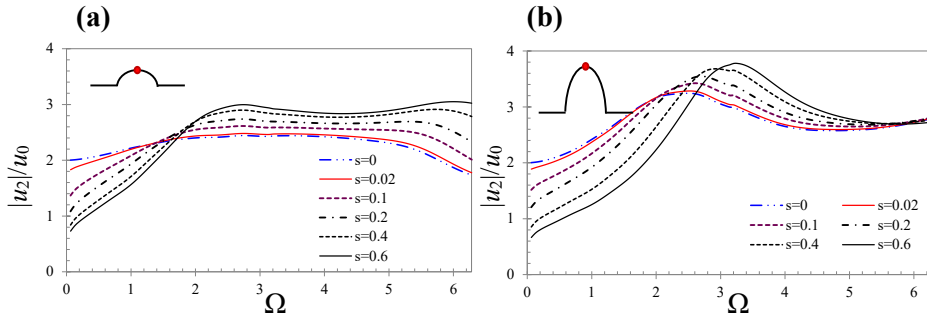


Figure 32: Normalized vertical displacement component at the top of the nanohill versus dimensionless frequency and variable surface parameter s for: (a) horizontally elongated semi-elliptical hill (*model 1*); (b) vertically elongated semi-elliptical hill (*model 2*).

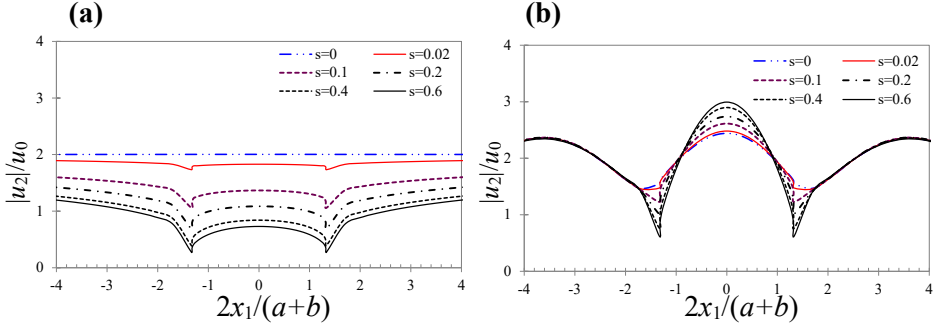


Figure 33: Normalized vertical displacement components along the free surface of horizontally elongated semi-elliptical hill (*model 1*) for variable s and fixed dimensionless frequency: (a) $\Omega=0.063$; (b) $\Omega=2.702$.

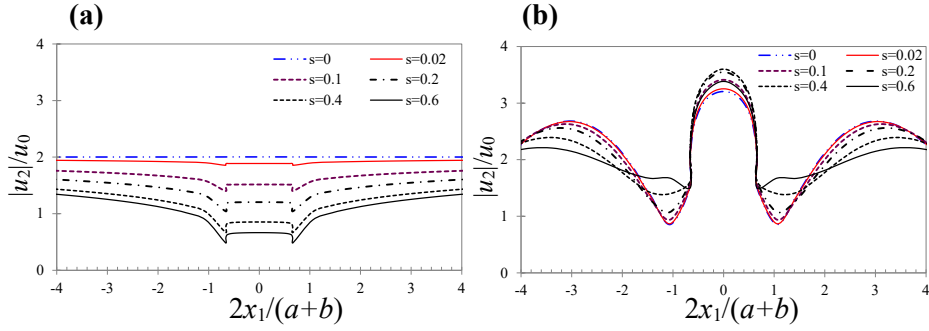


Figure 34: Normalized vertical displacement components along the free surface of vertically elongated semi-elliptical hill (*model 2*) for variable s and fixed dimensionless frequency: (a) $\Omega=0.063$; (b) $\Omega=2.702$.

The last parametric example concerns the nanotopography of a semi-circular canyon followed by a semi-circular hill, as shown in Fig. 37a. The BE mesh here consists of 48 BE, 24 of which are used for the relief peculiarity, respectively 12 for each canyon and hill shapes. The discretized flat free surface is again measured $\pm 10a$ left and right to the surface middle point. The normalized vertical displacement at the bottom of the canyon, central point of the free surface, and top of the hill versus the dimensionless frequency of the incident wave and variable surface parameter s are depicted in Fig. 37b-d. The normalized vertical displacements along the relief peculiarity and part of the flat free surface for variable s and fixed frequencies are given in Fig. 38.

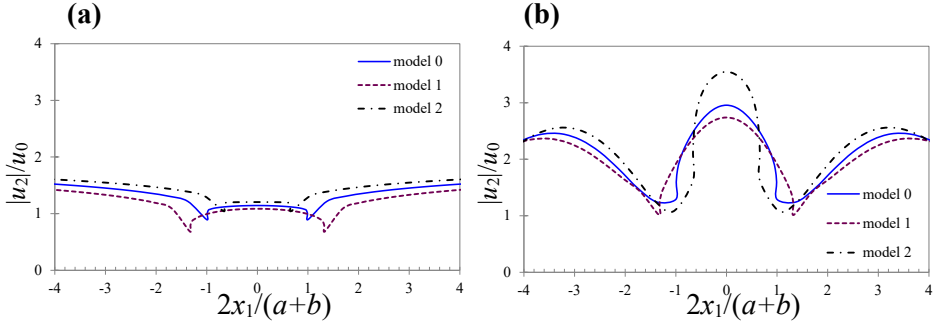


Figure 35: Normalized vertical displacement components along the free surface of different nanohill models for fixed surface parameter $s=0.2$ and dimensionless frequency: (a) $\Omega=0.063$; (b) $\Omega=2.702$.

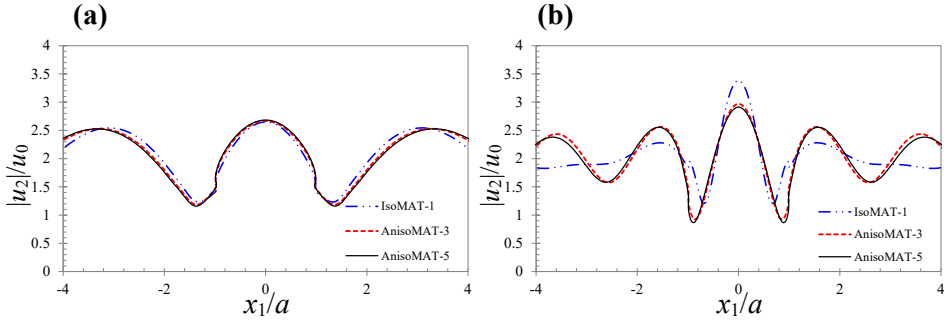


Figure 36: The normalized vertical displacement components along the free surface of semi-circular nanohill for different types of materials at fixed dimensionless frequency: (a) $\Omega=2.702$; (b) $\Omega=5.56$.

The following conclusions can be drawn from the numerical results presented above:

(a) Figs. 16-21 illustrate the wave field in an anisotropic half-plane without nanorelief but containing one or two nanocavities. It can be seen that the influence of both material anisotropy and surface elasticity depend on the frequency of the incident wave and position of the observer point. Figs.18 and 21 show the following effects: (*) with the increase of the surface parameter s the dynamic response parameters decrease and thus the effects at the nanoscale are clearly demonstrated. This picture is clearer when the observer point is at $\varphi=0$ and the frequency is $\Omega=1.257$, corresponding to the peak values in Fig.18a; (**) The material anisotropy shifts the dynamic response peak to the higher frequencies. This can be seen when Figs. 18a,c are compared with Figs. 18b,d. The same trend persists in the case of two

nanocavities, see Figs. 21a, b; (***) the dynamic interaction between both nanocavities is visible in Fig.20. Due to this dynamic interaction the response peak is shifted to the lower frequency. The percentage differences between the peak amplitudes for the case of single and two cavities at point $\varphi=0$ for different materials is as follows – 30.6%, 37.7% and 40.3% for IsoMat-1, AnisoMat-3 and AnisoMat-5 respectively, see Figs. 20b,c,d. The percentage differences are calculated with respect to the isotropic material.

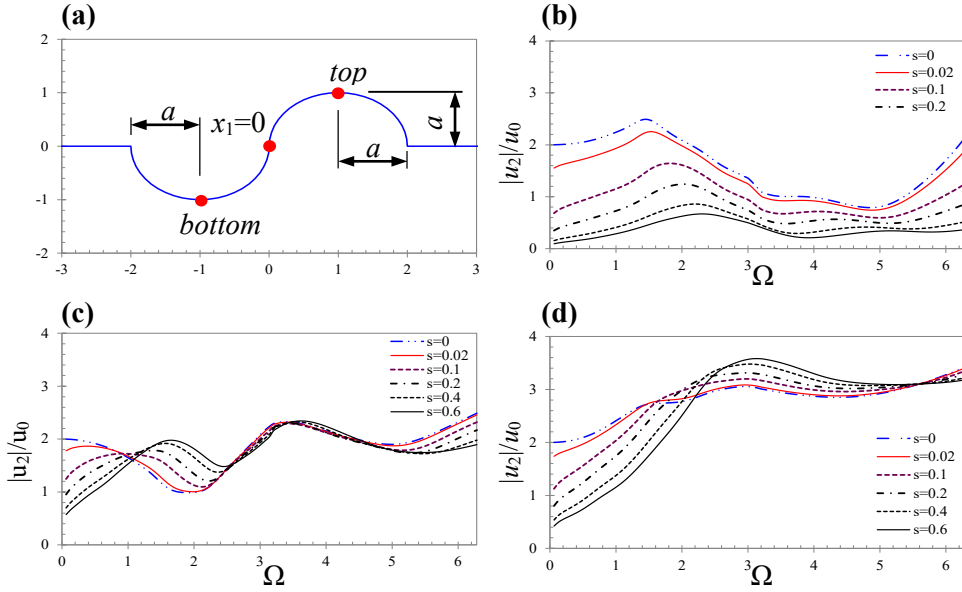


Figure 37: (a) Problem geometry; Normalized vertical displacement component versus dimensionless frequency and variable surface parameter s for: (b) point at $x_1=0$; (c) top of the hill; (d) bottom of the canyon.

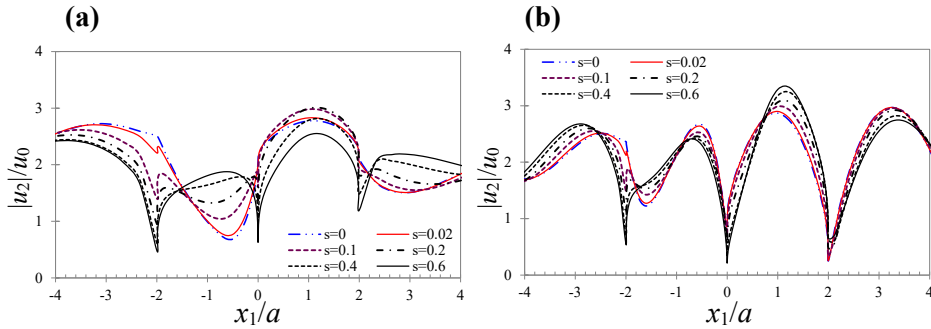


Figure 38: Normalized vertical displacement components along the free surface for variable s and fixed dimensionless frequency: (a) $\Omega=2$; (b) $\Omega=4$.

Figs. 23-29 present the scattered displacements and stress concentration fields in an anisotropic half-plane with a semi-circle and a semi-elliptical nanocanyon subjected to a time-harmonic normal qP-wave. The anisotropic material in Figs. 24-29 is AnisoMat-5. The sensitivity of the wave field to the material anisotropy and to the shape of the canyon is shown in Figs. 23-24, respectively. The minimal displacement amplitude in the frequency interval under consideration is obtained for the vertically elongated canyon at the frequency $\Omega=2.765$, while for semi-circle and horizontally elongated canyons this occurs at the frequencies $\Omega=2.702$ and 2.136 , respectively (although, for a horizontally elongated canyon the dip point is not clearly pronounced), see Fig.24. The percentage difference between displacement amplitudes for horizontally and vertically elongated canyons at fixed frequency $\Omega=2.765$ is 58.3%, calculated with respect to the higher amplitude of the vertically elongated canyon. The combined influence of the nano-canyon shape, the incident wave frequency and the surface elasticity properties, along the free surface for fixed frequency, is demonstrated in Figs. 25, 27, 28, 29. These figures clearly illustrate the geometrical profile of the nanocanyon at the lower frequency $\Omega=0.03$. At a fixed frequency $\Omega=2.702$, fixed surface elasticity coefficient $s=0.02$ and fixed position at the bottom of the canyon at $2x_1/(a+b)=0$, the percentage difference between the corresponding displacement amplitudes for horizontally and vertically elongated nanocanyons is 56.8%, calculated with respect to the higher amplitude of the vertically elongated canyon, see Fig. 29a.

(c) Figs. 30-36 show the scattered displacements and stress concentration fields in an anisotropic half-plane with a semi-circle and semi-elliptical nanohill subjected to the time-harmonic normal qP-wave. The anisotropic material in Figs. 30-35 is AnisoMat-5. Figs 31, 33, 34, 35 reveal how the shape of the nanohill and surface elasticity can change the scattered wave field in the anisotropic half-plane. While the tendency for decreasing the dynamic response with increasing the surface elasticity coefficient persists, here in contrast to the case of the canyon, the maximal displacement amplitudes occur in the case of the vertically elongated nanohill, see Fig.35. The influence of the material anisotropy can be seen in Fig.36b.

(d) The displacement results in Fig. 38a follow the surface relief geometry and the position of the canyon bottom, the top of the hill and all the rid points can be seen. The surface elasticity tendency is clearly demonstrated in Fig. 37b, while the rest of the figures show that this tendency can vary in the different frequency intervals of the incident wave.

B Multiple nano-inclusions in a finite domain under time-harmonic and transient loads

The next set of results examines the influence of the nano-inclusions' configuration on the dynamic stress-strain state. Four different models of anisotropic nano-inclusions in a finite anisotropic solid are considered in order to illustrate the influence of the heterogeneity arrangement (see Fig. 39a): (a) a single central inclusion; (b) three nano-inclusions in a vertical line; (c) three nano-inclusions in a horizontal line; (d) five inclusions. The diameter of the nano-inclusion is d , the size of the square plate is $10d$. The intensity of the time harmonic tensile load applied in horizontal direction is σ_0 . The matrix material is anisotropic LiNaKC₃PO₃ Glass Fiber with the respective stiffness tensor and density defined in the last row of *Table 6*. The inclusions are anisotropic with stiffness tensor 10 times softer than the matrix material and density $\rho_I = 1 \text{ t/m}^3$. The time harmonic analysis is performed for a frequency range up to $\Omega = 2.916$ divided into 50 equal frequency steps. A constant hysteretic material damping is assigned equal to 5%.

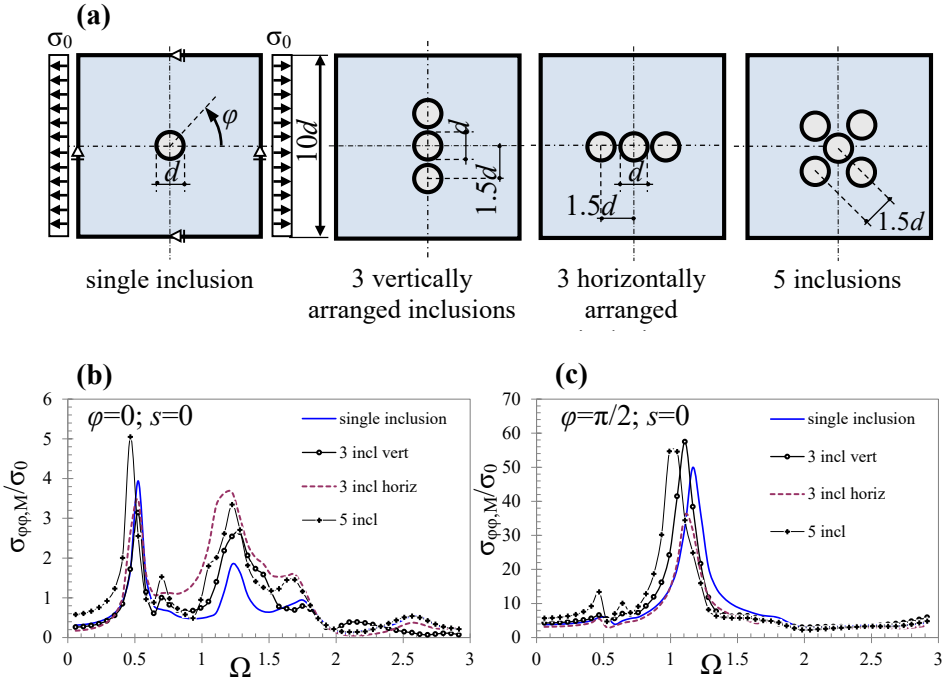


Figure 39: (a) Inclusion configurations; Normalized hoop stresses along central inclusion-matrix interface measured on the matrix side versus normalized frequencies and different inclusion patterns for points with polar angles: (b) $\varphi=0$; (c) $\varphi=\pi/2$.

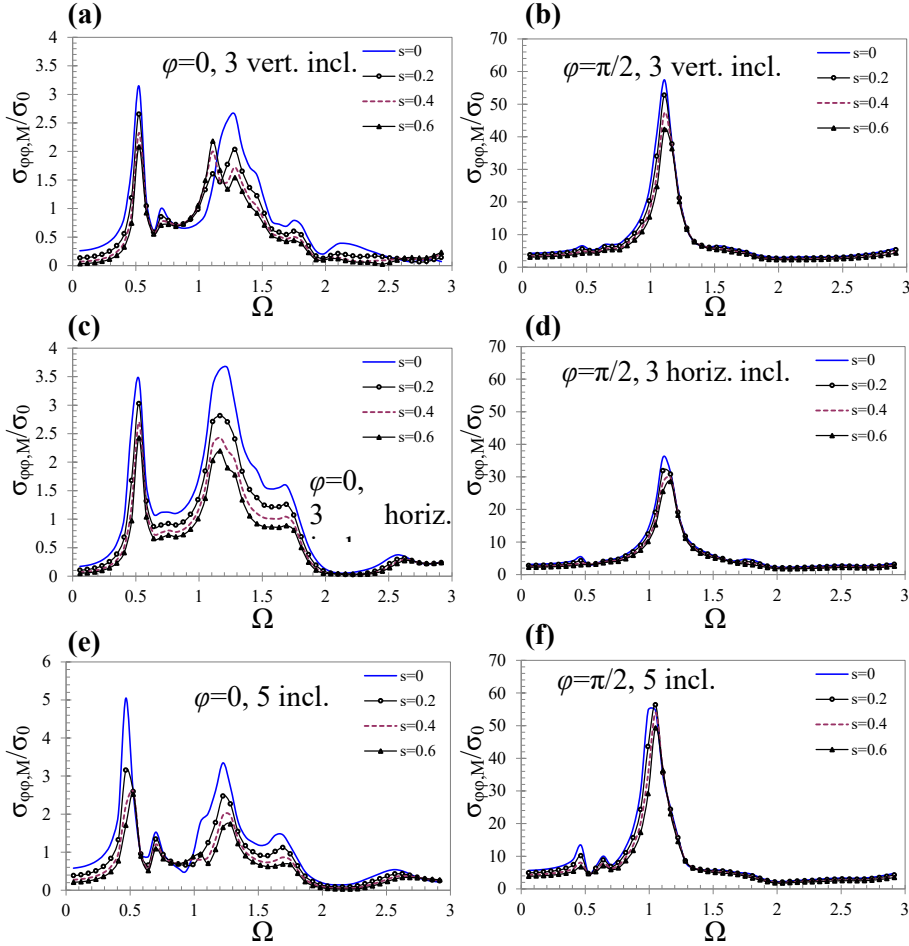


Figure 40: DSCF along central inclusion-matrix interface measured on the matrix side for different surface parameters versus dimensionless frequency and (a),(b) 3 vertically arranged inclusions, $\varphi=0$ and $\varphi=\pi/2$; (c),(d) 3 horizontally arranged inclusions, $\varphi=0$ and $\varphi=\pi/2$; (e),(f) 5 inclusions, $\varphi=0$ and $\varphi=\pi/2$.

The normalized hoop stresses $\sigma_{\varphi\varphi,M} / \sigma_0$ for observer points at the central inclusion-matrix interface on the matrix side versus the normalized frequency $\Omega = \omega d / \sqrt{c_{66} / \rho}$ are depicted in Fig. 39 b,c. The observer points are with the polar angles $\varphi=0$ and $\varphi=\pi/2$ and the results are obtained for the single inclusion model, three inclusions in a vertical line, three inclusions in a horizontal line, and five inclusions. The surface elasticity parameter is set to $s=0$. The influence of the surface elasticity parameter

$s = (\lambda^S + 2\mu^S) / (2c_{66}a_0)$ is illustrated in Fig. 40 where the DSCF versus the normalized frequency for the same observer points is presented. The subplots in Fig 40a, b are for three inclusions in a vertical line, the subplots in Fig. 40c,d are related with the horizontal inclusions arrangement, and finally the subplots in Fig. 40e,f are for the five inclusions model.

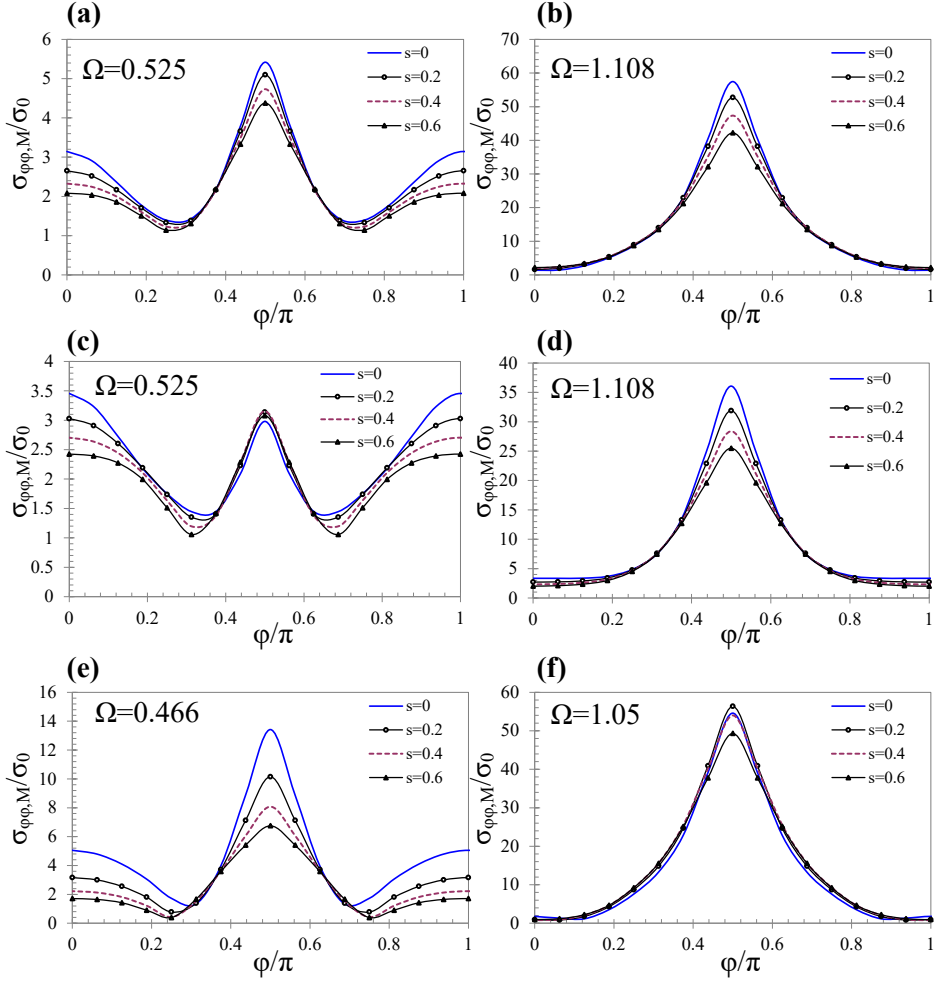


Figure 41: Normalized hoop stresses at inclusion-matrix interface measured on the matrix side for fixed normalized frequencies and different inclusion arrangements: (a), (b) 3 vertically arranged inclusions; (c), (d) 3 horizontally arranged inclusions; (e), (f) 5 inclusions.

The importance of the observer's location is illustrated in Figure 41. The normalized hoop stresses along the central inclusion-matrix interface on the matrix side at fixed normalized frequencies corresponding to the first and second peaks as observed in Figure 40, are given in Figure 41. The presented results are for multiple nanoinclusions models and different values of the surface elasticity parameter s varying from 0 to 0.6.

Figures 39-41 illustrate the complex nature of the wave field within the finite anisotropic solid containing multiple anisotropic nanoinclusions. The dynamic stress-strain state is highly sensitive to both the number and the geometric configuration of the nanoinclusions. The scattered and diffracted wave field results from the interplay between the inclusions' number and geometry, along with other key factors of the model, such as the applied load frequency, the observer's position, and the surface elasticity phenomenon.

The obtained results show that the case of five inclusions gives higher values of the stress resonance peak at the observer point $\varphi=0$, see Figure 39, than the cases of the single and three horizontal/vertical nanoinclusions. However, Figure 39b for the observer point at $\varphi=\pi/2$ reveals that the geometrical configuration of three vertical nanoinclusions provokes a maximal stress peak. Figure 41 illustrates that the stresses, corresponding to the frequency of the second peak, developed in the case of three vertically arranged nanoinclusions are higher than those developed in a solid with five or three horizontally arranged heterogeneities.

The following section examines the influence of the nanoinclusion pattern on the time-history responses of a finite anisotropic solid. Here, three different inclusion arrangements are presented namely: a single central inclusion; three nano-inclusions in a vertical line; three nano-inclusions in a horizontal line (see Fig. 39a). The transient tensile load intensity applied in horizontal direction is defined by the time-history function $f(t) = F(t)t e^{-\beta t}$, where $F(t)$ is the Heaviside step function and the parameter $\beta = 200$. Two types of damping are applied: viscous proportional damping with the viscoelastic coefficients $c_{ij}^* = c_{ij}(1 + 2i\omega\eta)$ with $\eta = 0.025\%$ and a hysteretic frequency independent damping of 5%. The time harmonic BEM analysis is performed for the normalized frequency range up to $\Omega = 2.916$ divided into 500 equal frequency steps followed by inverse FFT in order to get time-history solutions. The respective time step is $\Delta\tau = 2.155$.

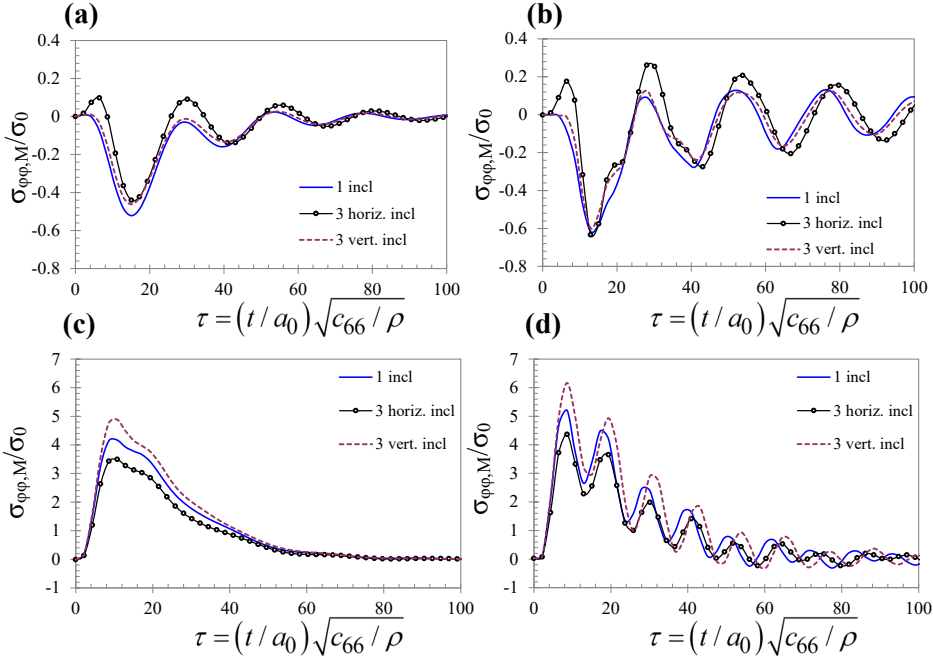


Figure 42: Normalized hoop stresses measured on the matrix side of the nanoinclusion-matrix interface versus normalized time τ for different inclusions' configuration and damping type: (a) $\varphi=0$ and viscous damping 0.025%; (b) $\varphi=0$ and hysteretic damping 5%; (c) $\varphi=\pi/2$ and viscous damping 0.025%; (d) $\varphi=\pi/2$ and hysteretic damping 5%.

The normalized DSCF for different inclusions arrangements and both types of damping versus the normalized time are plotted in Fig. 42. All plots are for inclusions with no surface effect. The DSCF for a point with the polar angle $\varphi=0$ from the matrix side is portrayed in Fig. 42a, b for the case of viscous and hysteretic damping, respectively. The same set of results for the second observer point with the polar angle $\varphi=\pi/2$ is depicted in Fig. 42c, d. The influence of the surface effect in case of a single nano-inclusion and both types of damping is illustrated in Fig. 43. The DSCF of the point with polar angle $\varphi=0$ is presented in Fig. 43a, b for different values of normalized surface elasticity parameter in case of viscous and hysteretic damping. The dimensionless hoop stresses for the second observer point with polar angle $\varphi=\pi/2$ and both damping types are portrayed in Fig. 43c, d.

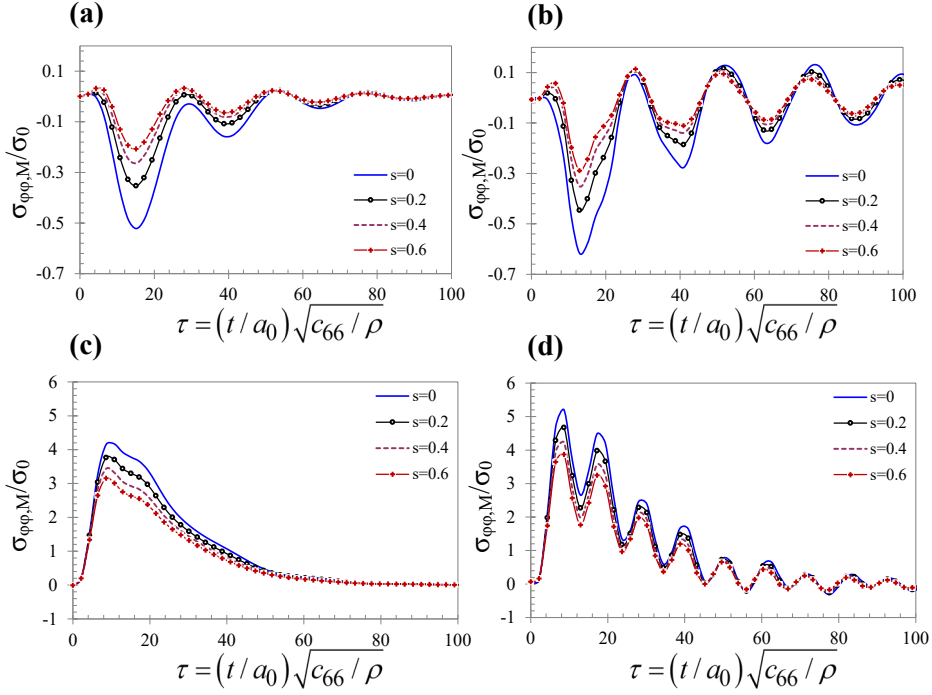


Figure 43: Normalized hoop stresses measured on the matrix side of the nanoinclusion-matrix interface versus normalized time τ for single inclusion model at points with polar angles: (a) $\varphi=0$ and viscous damping 0.025%; (b) $\varphi=0$ and hysteretic damping 5%; (c) $\varphi=\pi/2$ and viscous damping 0.025%; (d) $\varphi=\pi/2$ and hysteretic damping 5%.

Fig. 44 presents the DSCF for multiple nano-inclusions arranged in a vertical and horizontal line for a varying surface elasticity parameter and viscous frequency dependent damping. The subplots in Fig. 44a, b are for the three inclusions arranged in a vertical line and both observer points with polar angles $\varphi=0$ and $\varphi=\pi/2$ respectively. The same set of results for the horizontally patterned inclusions are portrayed in Fig. 44c,d. Fig. 45 is analogous to Fig. 44 but in case of hysteretic damping.

Figure 42 reveals that the highest dynamic stress values occur at point $\varphi=\pi/2$ for the case of three vertically arranged nanoinclusions, for both types of damping. In contrast, at $\varphi=0$, the configuration with three horizontally arranged nanoinclusions represents the more critical setup.

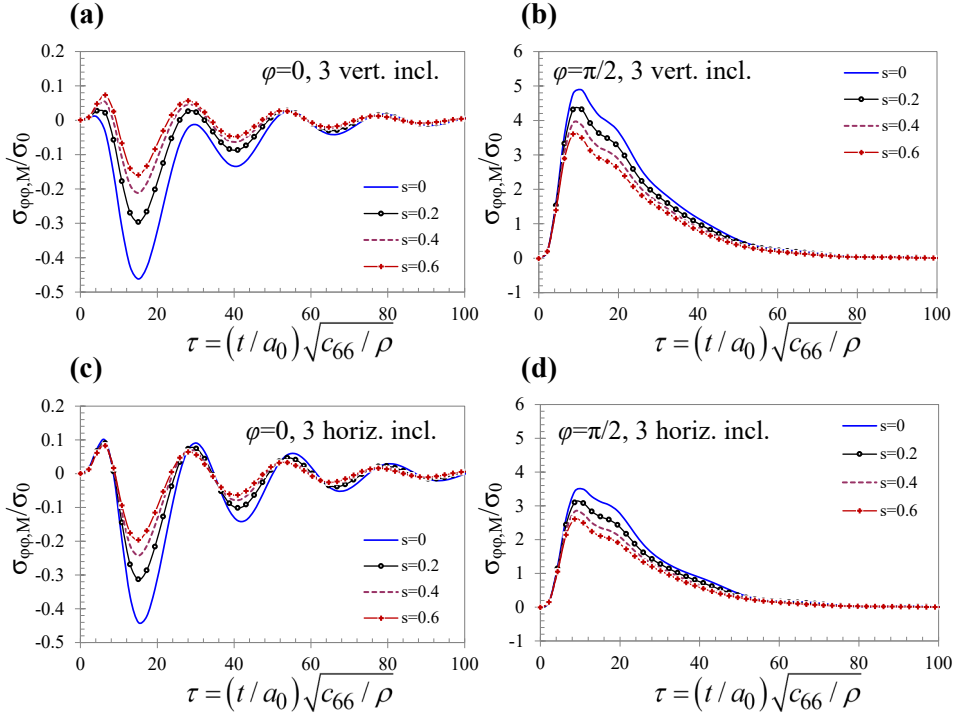


Figure 44: Normalized hoop stresses measured on the matrix side of the nanoinclusion-matrix interface versus normalized time τ in the case of viscous damping 0.025%, for 3 horizontal and vertical inclusion patterns and at points with polar angles: (a) $\varphi=0$, 3 vertical inclusions; (b) $\varphi=\pi/2$, 3 vertical inclusions; (c) $\varphi=0$, 3 horizontal inclusions; (d) $\varphi=\pi/2$, 3 horizontal inclusions.

Figures 43-45 confirm the previously observed trend that, as the surface elasticity increases, the resulting stresses decrease. This trend is independent of the material damping type or the geometric configuration of the multiple nanoinclusions.

6. Conclusions

The in-plane elastodynamic behavior of finite, semi-infinite, and infinite elastic solids, whether isotropic or anisotropic, containing multiple elastic anisotropic nanoimperfections of arbitrary number, material properties, and geometric configurations is analysed using boundary integral equations within the framework of the Gurtin-Murdoch surface elasticity model. The proposed numerical scheme is validated and applied in a comprehensive

parametric study. The key parameters influencing the dynamic stress-strain response are examined in detail. The type of anisotropic material significantly impacts the time-harmonic behavior of the nanoheterogeneous matrix. Both the resonance frequencies and stress amplitudes are strongly dependent on the material anisotropy for a fixed surface parameter value. The influence of the surface parameter and material anisotropy on the normalized hoop stresses is most prominently observed in the plots at fixed frequencies. The timing and magnitude of the response peaks vary significantly across different anisotropic materials, even when the other model parameters remain constant. Additionally, the dynamic stress-strain state in both the frequency and time domains is highly sensitive to the number and geometric configuration of the nanoinclusions. The dynamic interaction between inclusions is demonstrated through the analysis of various models of the nanoheterogeneities' arrangement.

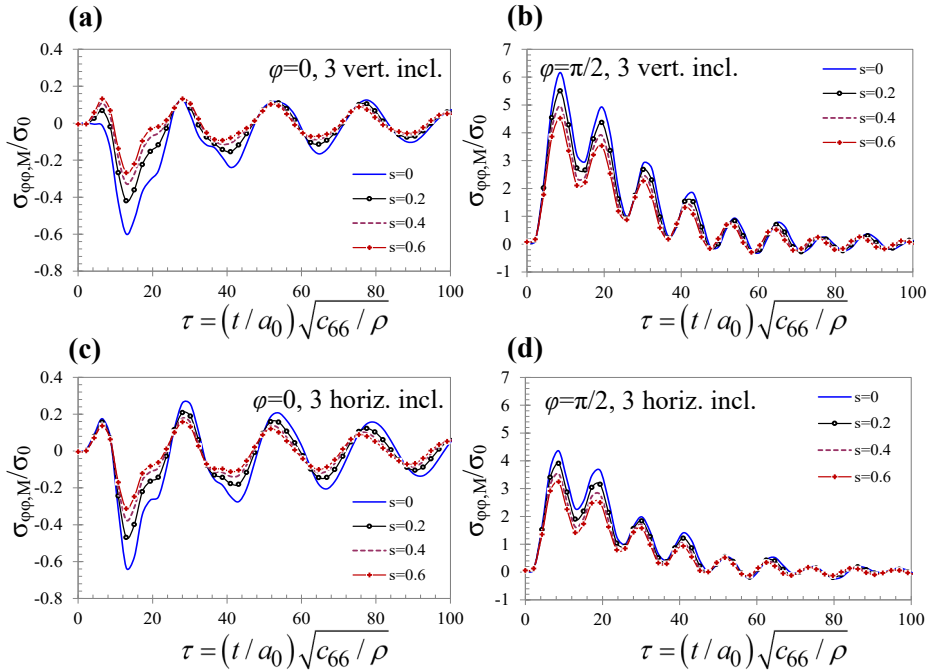


Figure 45: Normalized hoop stresses measured on the matrix side of the nanoinclusion-matrix interface versus normalized time τ in the case of hysteretic damping 5%, for 3 horizontal and vertical inclusion patterns and at points with polar angles: (a) $\varphi=0$, 3 vertical inclusions; (b) $\varphi=\pi/2$, 3 vertical inclusions; (c) $\varphi=0$, 3 horizontal inclusions; (d) $\varphi=\pi/2$, 3 horizontal inclusions.

The scattered wave field and the non-uniform stress distribution within the nanoheterogeneous anisotropic solid result from the interplay of various key parameters. This study focuses on highlighting the significance of the surface elasticity parameter, which, along with other important factors, governs the dynamic response of the solid. In fact, as surface effects become more pronounced, the DSCF values decrease at higher surface elasticity parameters, indicating that the surface elasticity enhances the strength of the interface itself.

In conclusion, the hybrid approach, combining the classical elastodynamic theory with non-classical boundary conditions from surface elasticity theory, has the potential to quantify size effects at the nanoscale. The methodology developed here, along with the numerical results obtained, is highly relevant for material science, non-destructive testing of nanostructural components, and computational nanomechanics.

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Notations list

Notation	Meaning
$\Omega_{\text{inf}}, \Omega_{\text{finite}}$	Infinite or finite isotropic/anisotropic plane
Ω_0	Half-plane domain
Ω_H	Nanoholes domain
Ω_I	Nanoinclusions domain
Γ	Total boundary of the model
Γ_H	Total interface of all nanoholes
Γ_I	Total interface of all nanoinclusions
Γ_{rel}	Nanorelief boundary of the half-plane
Γ_{ff}	Flat boundary of the half-plane
Γ_f	Boundary of the half-plane
Γ_e	External boundary of the finite domain
$u_i, i=1,2$	Displacement components
$u_i^{in}, i=1,2$	Incident displacement components
$u_i^{sc}, i=1,2$	Scattered displacement components
$u_i^{ff}, i=1,2$	Free-field displacement components
$t_i, i=1,2$	Traction components
$t_i^{in}, i=1,2$	Incident traction components
$t_i^{sc}, i=1,2$	Scattered traction components
$t_i^{ff}, i=1,2$	Free-field traction components
$x_i, i=1,2$	Space coordinates
ω	Circular frequency in [rad/s]
t	Time variable in [s]
$\sigma_{ij}, i, j=1,2$	Stress components

$n_j, j = 1, 2$	Outward pointing unit normal vector
ρ	Density in [t/m ³]
ρ^I, ρ^M	Inclusion and matrix density in [t/m ³]
C_{ijkl}^I, C_{ijkl}^M	Inclusion and matrix stiffness tensor coefficients
$\ddot{u}_i, i = 1, 2$	Acceleration components
$\varepsilon_{ij}, i, j = 1, 2$	Strain components
$c_{11}, c_{12}, c_{16}, c_{22}, c_{26}, c_{66}$	Stiffness matrix components in [MPa]
λ, μ	Lame' constants in [MPa] or [GPa]
ν	Poisson's ratio
λ^S, μ^S	Mechanical properties at the nano-surface interface in [N/m]
$\sigma_{ll}^S, \varepsilon_{ll}^S$	Stress and strain in the tangential direction to the nano-surface interface
τ^0	Residual surface tension
$\partial / \partial l, \partial^2 / \partial l^2$	First and second tangential derivatives
ρ_s	Curvature radius for the nano-interface
α, K_s	Nano-surface modulus in [N/m]
θ	Incident wave angle with respect to the horizontal axis
k_p, k_s	P- and SV- wavenumber
C_p, C_s	P- and SV- wave phase velocity in [m/s]
σ_{0j}	Magnitude of the applied loads
$f(t)$	Time history of the transient load
DSCF	Dynamic stress concentration factor
i	Imaginary unit
x, ξ	Position vectors of the source and receiver point
$U_{ij}^*(\mathbf{x}, \xi, \omega)$	Displacement fundamental solution
$T_{ij}^*(\mathbf{x}, \xi, \omega)$	Traction fundamental solution
G, H	Influence matrices
u, t	Displacement and traction vectors
F	Dynamic load vector
λ_S	SV-wavelength
l_{BE}	Length of the boundary element
φ	Polar angle
a, b	Semi-axis of the elliptical nano-inclusion
R	Characteristic (average) radius of the elliptical nano-inclusion

a_0	Nanocavity radius
r	Heterogeneity radius
d	Heterogeneity diameter
Ω	Dimensionless frequency
s	Dimensionless surface parameter
$\sigma_{\varphi\varphi}$	Circumferential stress
τ	Dimensionless time
ξ, η	Damping coefficients

PART II. OPTIMIZATION OF NANOCOMPOSITES

Chapter 5. Optimization of nanocomposites

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Anotation

This chapter explores, summarizes, and analyzes various optimization methods used to enhance the design, properties, and manufacturing processes of nanocomposite structures (NCs). It examines different types of nanocomposites and the key factors subject to optimization, including NC geometry, loading conditions, environmental influences, and manufacturing techniques. A detailed discussion is provided on the numerical techniques and optimization methods, along with examples of their application to NCs. These methods include the response surface method, decision tree method, machine learning algorithms, artificial neural networks, differential evolution algorithms, the finite element method, genetic and evolutionary algorithms, topological optimization, adaptive optimization, and more. Additionally, the chapter presents the authors' contributions to the performed optimization approaches for nanocomposites.

1. Key concepts

Nanocomposites

The field of nanocomposite materials is rapidly evolving and holds significant potential to influence various aspects of society. These materials offer remarkable possibilities by enabling the development of substances with enhanced or unique properties through precise control of composition, structure, and phase interactions at the nanoscale. Nanocomposites consist of a matrix—such as a polymer, metal, or ceramic combined with nanoparticles

or nanoscale fillers (typically under 100 nanometers in at least one dimension), leading to improvements in mechanical, thermal, electrical, or optical characteristics (Bryning *et al.* 2005; Kashiwagi *et al.* 2005; Zhang *et al.* 2005).

The incorporation of nanoscale reinforcements greatly enhances the performance of nanocomposites compared to traditional materials (Moradi *et al.* 2015; Hosseini *et al.* 2014; Zare and Garmabi, 2014; Norouzi *et al.* 2015; Hobbie *et al.* 2009; Xie *et al.* 2011). This makes them highly appealing for various industries, including automotive, aerospace, healthcare, packaging, and energy storage. By offering superior properties, nanocomposites contribute to improved performance, sustainability, and efficiency across these applications.

Types of nanocomposites

Depending on the nature of the matrix and the type of nanofillers used, nanocomposites can be classified into several categories. Here's a detailed breakdown of the main types of nanocomposites:

- **Polymer-Based Nanocomposites** – Polymers reinforced with nanofillers such as carbon nanotubes, graphene or similar 2D nanomaterials, or nanoclays. These materials exhibit improved strength, flexibility, and barrier properties.
- **Metal-Based Nanocomposites** – Metals infused with nanoparticles like ceramic or carbon nanostructures, which enhance conductivity, hardness, and wear resistance.
- **Ceramic-Based Nanocomposites** – Ceramic matrices reinforced with nanoscale particles to improve toughness, thermal stability, and durability.

Common nanofillers used in nanocomposites

Nanofillers play a crucial role in enhancing the properties of nanocomposites by improving their mechanical strength, thermal stability, electrical conductivity, and other functional characteristics. These fillers, typically ranging in size from 1 to 100 nanometers, are dispersed within a matrix material (polymer, metal, or ceramic) to create advanced composites with superior performance. The most commonly used nanofillers in nanocomposites are following.

- Carbon Nanotubes (CNTs) – Enhance mechanical strength and electrical conductivity.
- Graphene – Improves thermal conductivity, mechanical properties, and electrical performance.
- Nanoclays – Enhance flame resistance and barrier properties.
- Metallic Nanoparticles (e.g., Silver, Gold, Copper) – Provide antibacterial properties and improve electrical conductivity.
- Silica Nanoparticles – Increase hardness and thermal resistance.

In recent years, the polymer nanocomposites have garnered significant research attention due to their enhanced properties, which stem from the synergistic combination of a polymer matrix with organic or inorganic nanomaterials. These materials offer unique design possibilities, making them highly advantageous for developing multifunctional materials tailored for specific applications.

Polymer nanocomposites consist of two distinct phases: a continuous polymer matrix and a dispersed nanoreinforcement phase, typically ranging from 1 to 100 nm in size. The matrix, usually a thermosetting or thermoplastic polymer, plays a crucial role in evenly distributing applied loads to the embedded nanoreinforcements (Díez-Pascual *et al.* 2012). Various nanomaterials, commonly referred to as nanofillers or nanoreinforcing agents, are incorporated to improve the properties of the polymeric matrix. Based on their composition, these nanofillers can be classified into three main categories, as illustrated in Figure 1: (1) **organic**, which includes dendrimers, micelles, liposomes, polymer nanoparticles (NPs), and ferritin; (2) **inorganic**, comprising metal nanoparticles (Ag, Au, Cu), metal oxide nanoparticles (e.g., Fe₃O₄, ZnO, MgO, TiO₂), and mesoporous silica; and (3) **carbon-based**, which includes fullerenes, quantum dots, carbon nanotubes, graphene, and its derivatives (Khan *et al.* 2019).

The nanomaterials can also be classified based on their dimensions, as described by Pokropivny and Skorokhod (2007). They are categorized as: 0D when all their dimensions are smaller than 100 nm, such as fullerenes, quantum dots (QDs), and metallic nanoparticles (NPs); 1D when two dimensions are smaller than 100 nm, such as carbon nanotubes (CNTs); 2D when only one dimension is at the nanoscale, such as graphene; 3D when none of their dimensions are confined to the nanoscale, such as dendrimers. It has to be noted, that 3D bulk material is made up of individual blocks that are in the nanometer scale (1–100 nm), so 3D nanomaterials have three arbitrary dimensions above 100 nm (Mekuye and Abera, 2023).

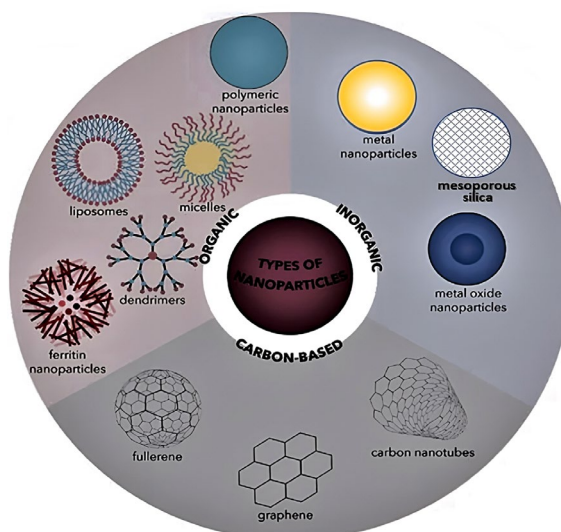


Figure 1: The primary types of nanomaterials can be classified based on their composition into three categories: organic, inorganic, and carbon-based, as outlined by Champa-Bujaico *et al.* (2022).

Recently, various carbon allotropes have been utilized as nanofillers in polymer nanocomposites, including fullerenes (Giacalone and Martin, 2006), quantum dots (QDs) (Xu *et al.* 2004), carbon nanotubes (CNTs) (Iijima, 1991), graphene (G) (Novoselov *et al.* 2004), and its derivatives, graphene oxide (GO) and reduced graphene oxide (rGO) (Figure 2).

The method used to synthesize carbon-based nanomaterials significantly depends on their purity and quality, thereby influencing the final properties of the composite (Díez-Pascual, 2021a).

Braga & Magalhães (2015) demonstrated that the addition of 19 wt% glass fiber enhanced the tensile strength, Young's modulus, and impact strength of epoxy resin. Hydroxyapatite (HA) and graphene oxide (GO) have been identified as effective fillers for improving the mechanical, electrical, and thermal properties of epoxy (Baradaran *et al.* 2014; Zhang *et al.* 2008; Mebarki *et al.* 2014; Stankovic *et al.* 2015; Zhao *et al.* 2004). Li *et al.* (2008) found that the tensile strength of PLA/HA composites increased with 5–10 wt% of nanoparticles.

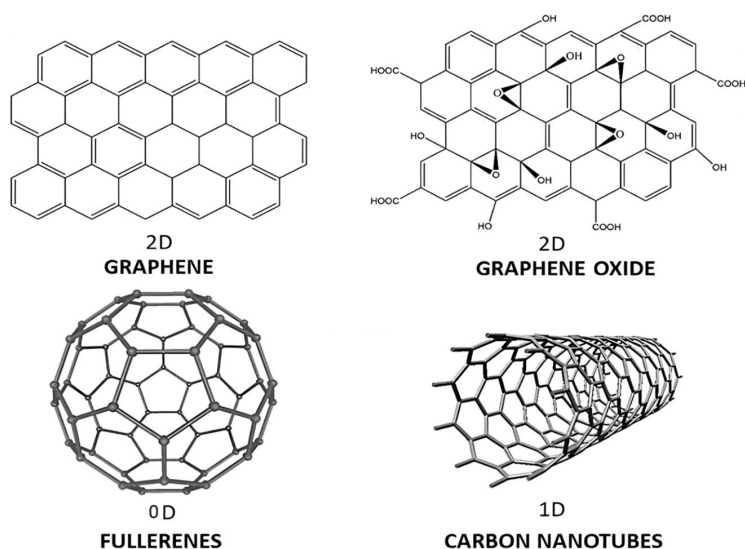


Figure 2: The structural representation of carbon-based nanomaterials includes 2D graphene (G) and graphene oxide (GO), 0D fullerenes, and 1D carbon nanotubes (CNTs) (Champa-Bujaico *et al.* 2022).

Moreover, the simultaneous incorporation of multiple nanoparticles can lead to synergistic effects, enhancing the physical and mechanical properties of reinforced nanocomposites. Maazouz *et al.* (1993) observed synergistic effects on fracture toughness when hybrid rubber and glass beads were added to an epoxy matrix. Osorio *et al.* (2011) filled epoxy resin with HA and carbon nanotubes, finding synergistic effects on the mechanical properties, with improvements of up to 87% and 82%, respectively. Huang *et al.* (2014) studied the effects of GO and CNT on polypropylene, enhancing Young's modulus and the glass transition temperature (T_g). Zhao *et al.* (2004) incorporated HA and carbon fiber into epoxy resin, reporting significant increases in impact and flexural strength.

Additionally, other studies have shown that the combination of HA and GO improves compressive and flexural strength (Harichandran and Selvakumar 2018; Nadeem and Sadaf 2017). Fereidoon *et al.* (2014) used a blend of silica (SiO_2) and HA nanoparticles in a polypropylene (PP) matrix, demonstrating that tensile strength increased by 6.47% for PP- SiO_2 , 26.57% for PP-HA, and 22.85% for PP-HA- SiO_2 . The experimental results show that the presence of nanoparticles helps to resist bending load and improved stress transfer between epoxy polymer/HA/GO (Balguri *et al.* 2017).

Interface

The optimal design of a nanocomposite involves the even distribution of individual nanoparticles within a polymer matrix. Achieving a uniform dispersion of nanoparticles is a critical factor in unlocking the full potential for property enhancement (Müller *et al.* 2017; Bitinis *et al.* 2011). A well-dispersed nanofiller leads to a larger interface between the nanomaterial and the polymer chains, which can result in better properties compared to traditional polymer composites containing macro- or micro-fillers. The reinforcing effect of the nanofiller depends on various factors, such as the type of nanofiller, its concentration, the aspect ratio, geometry, size, orientation, and distribution (Luceño-Sánchez *et al.* 2021; Díez-Pascual, 2021b). Evaluating the dispersion of the nanofiller in the polymer matrix is essential, as the mechanical and thermal properties are closely related to the resulting morphology. Three primary nanocomposite morphologies have been identified (Figure 3) (Alexandre and Dubois, 2000): phase-separated, intercalated, and exfoliated. In a phase-separated morphology (Figure 3a), the polymer does not intercalate between the nanofillers, resulting in a composite with properties similar to traditional composites. An intercalated structure (Figure 3b) occurs when a single extended polymer chain is inserted between the nanofillers, creating an ordered arrangement. In an exfoliated structure (Figure 3c), the nanofiller is fully and uniformly dispersed within the continuous polymer matrix. A notable characteristic of these nanocomposites is that significant property improvements can be achieved even with low nanofiller concentrations (typically 1–10 wt.%) (Díez-Pascual, 2019).

Interphase region

The interphase region in nanocomposites refers to the area between the nanofiller and the polymer matrix. This region plays a crucial role in determining the overall properties of the nanocomposite, as it influences the interaction between the filler material and the surrounding polymer matrix. The characteristics of the interphase region, including its composition, thickness, and structure, are critical to enhancing the performance of nanocomposites.

One reason for the improvement in properties is the large interphase region, which results from strong chemical and geometric interactions between the particle surface and the polymer chains close to the particle, as well as the high surface-to-volume ratio of the nanoinclusions. For instance, if a composite contains 5 wt% of 40 nm particles that are perfectly dispersed,

the total interfacial surface area would be approximately $3.5 \text{ m}^2/\text{cm}^3$. As shown in Figure 4, the interphase area extends beyond the layer of matrix chains directly attached to the filler surface due to the cooperative nature of the macromolecular network, significantly expanding the interphase domain into the matrix (Ciprari *et al.* 2006).

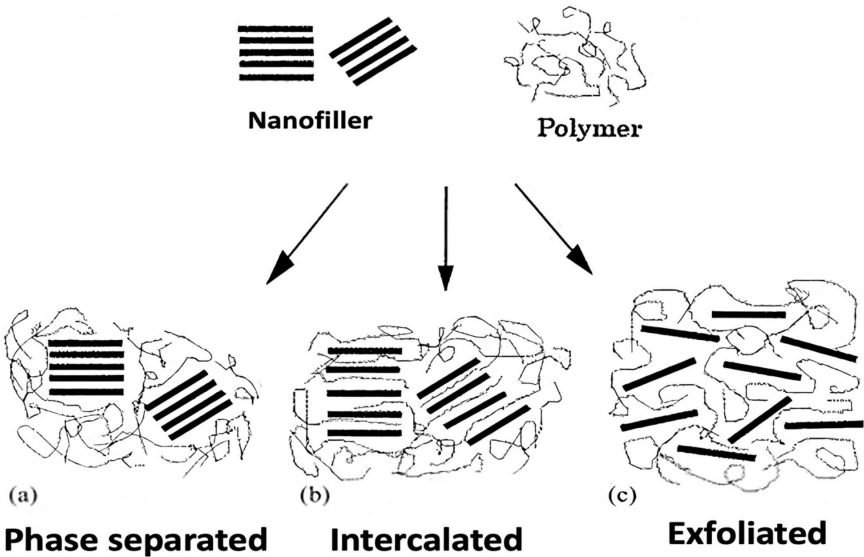


Figure 3: The potential structures of polymer nanocomposites: (a) phase separated - In this arrangement, the polymer does not intercalate between the nanofillers, resulting in distinct phases within the composite, (b) intercalated - Here, a polymer chain is inserted between the nanofillers, creating an ordered structure. and (c) exfoliated - In the exfoliated structure, the nanofillers are uniformly and completely dispersed throughout the continuous polymer matrix (Champa-Bujaico *et al.* 2022).

Parameters for optimization of nanocomposite structures

The optimization of nanocomposite structures involves several parameters that must be carefully considered to achieve the desired mechanical, thermal, and chemical properties. These parameters influence the overall performance and durability of the nanocomposite structures, especially when they are subjected to static and dynamic loading conditions. Below are the key parameters for the optimization of nanocomposite structures:

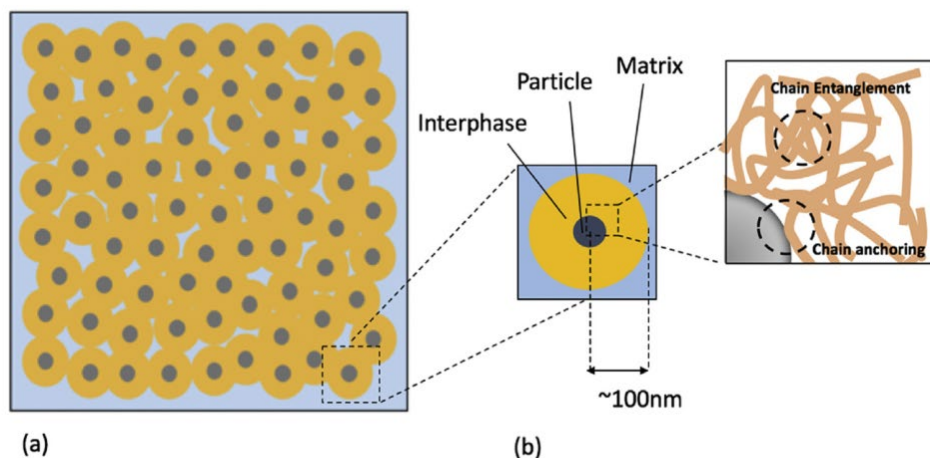


Figure 4: Interphase configuration: (a) A diagram illustrating the interphase region in a nanocomposite sample. (b) A diagram showing the extended interphase structure, where yellow chains are directly attached to or chemically interacting with the nanofiller. Blue chains are influenced by the filler indirectly through interactions with the yellow chains. The cooperative interactions among the chains extend the interphase zone, which can persist up to approximately 100 nm from the particle surface. Note: the figures are not to scale (Wang *et al.* 2018).

Material composition

The mechanical properties are influenced by several factors: 1) The type of nanofiller (such as graphene, carbon nanotubes, or nanoclays, etc.) (Champa-Bujaico *et al.* 2022); 2) The concentration of both nanofiller and polymer (Champa-Bujaico *et al.* 2022); 3) The ratio of nanoparticles in hybrid nanocomposites (Dadrasi *et al.* 2019); 4) The type of matrix, whether thermosetting or thermoplastic polymer (Champa-Bujaico *et al.* 2022); 5) The type of adhesive, whether rigid, flexible, or toughened (Akpınar *et al.* 2017).

Akpınar *et al.* (2017) studied adhesively bonded composite joints under tensile and bending moment loads. Their findings showed that composite joints reinforced with carbon fibers as the adhesive demonstrated much higher resistance to failure loads, depending on the type of adhesive used. Additionally, the research revealed that the incorporation of nanoparticles into the adhesive increased both the tensile and four-point

bending failure loads of the composite joint, with variations depending on the type of adhesive and nanoparticles used.

Structural characteristics of the nanofiller

The structural characteristics of the nanofiller play a critical role in determining the overall performance and properties of nanocomposites. These characteristics influence the interaction between the nanofiller and the polymer matrix, as well as the mechanical, thermal, and electrical properties of the resulting material. A detailed understanding of the structural aspects of nanofillers can help in optimizing the design of nanocomposites for various applications. They are following:

1). **Size of the nanofiller.** The size of the nanofiller is one of the most important structural characteristics because it directly impacts the surface area and interaction with the polymer matrix.

2). **Aspect ratio.** The aspect ratio refers to the ratio of the length to the diameter (or thickness) of the nanofiller. Nanofillers with a high aspect ratio, such as carbon nanotubes (CNTs) and fibers, have a larger surface area for interactions with the polymer matrix and can significantly influence the properties of the nanocomposite.

3). **Shape and Morphology.** The shape and morphology of nanofillers also play a significant role in the mechanical and physical properties of nanocomposites.

4). **Surface Characteristics.** The surface characteristics of the nanofiller play a crucial role in determining how well the filler interacts with the polymer matrix. These characteristics include surface energy, functional groups, and surface roughness.

5). **Crystallinity and Structure.** The crystallinity and internal structure of the nanofiller are important factors that influence the overall performance of the nanocomposite. These factors affect properties such as mechanical strength, thermal stability, and electrical conductivity.

6). **Surface Chemistry and Functionalization.** The surface chemistry of nanofillers plays a significant role in their interaction with the polymer matrix. The surface can be modified by functionalizing it with specific chemical groups to enhance its compatibility with the polymer.

7). **Dispersion and Distribution.** The dispersion of nanofillers within the polymer matrix is critical to achieving the desired properties in nanocomposites. A proper dispersion leads to better interactions between the filler and the matrix, maximizing the performance of the composite.

Nanocomposite structures geometry refers to the configuration, shape, and structure of the adhesive joints that bond distinct materials together. The geometry of the nanocomposite plays a significant role in determining the mechanical performance, including strength, durability, and resistance to failure under different loading conditions (e.g., tensile, shear, bending). In the context of nanocomposite structures, the geometry involves several factors, including the adhesive type, filler material, shape and dimensions of the nanocomposite structure, and the interaction between the adhesive and the composite matrix. A detailed understanding of the nanocomposite structure's geometry is essential for optimizing the properties and performance of nanocomposite-based structures in applications such as aerospace, automotive, and medical fields.

Key factors influencing nanocomposite structure's geometry include:

1). **Layers Thickness:** The thickness of the layers in the structure plays a crucial role for delamination in the nanocomposite structures (Kirilova *et al.* 2023; Boyadjiev *et al.* 2024).

2). **Overlap Length:** The overlap length is the distance over which the adhesive bonds two materials. In the case of nanocomposite structures, a larger overlap length improves the transfer of loads between the bonded parts and increases nanocomposite structure's strength. However, longer overlaps may lead to higher material usage and weight, so optimization is essential for balancing strength and efficiency (Akpinar *et al.* 2017; Bavi *et al.* 2013).

3). **Bonding Area:** A larger bonding area, especially when the nanofillers are well-dispersed, helps to distribute the stresses more evenly across the adhesive layer, resulting in improved mechanical performance. The properly designed composite structure's geometry ensures that the adhesive effectively engages the entire bonding surface (Bavi *et al.* 2013).

4). **Edge Effects:** Sharp edges or discontinuities in the adhesive composite joint can act as stress concentrators, leading to premature failure. Filletting or rounding of the edges can help to distribute stress more uniformly, reducing the risk of failure at the edges (Bavi *et al.* 2013).

5). **Interface properties** – adhesion between nanoparticles and the polymer matrix is very important (Wang *et al.* 2018);

6). **Interfacial shear strength** is commented in (Formica *et al.* 2018);

7). **Compatibility between the polymer and nanofiller** is discussed in (Champa-Bujaico *et al.* 2022).

Formica *et al.* (2018) have applied differential evolution algorithm coupled with an ad hoc finite element implementation of a nonlinear 3D mesoscale theory for determination of the optimal set of material parameters

that can give rise to the best hysteretic damping capacity of carbon nanotube (CNT) nanocomposites. According to the 3D mesoscale theory, the hysteresis is due to the shear stick-slip between the nanotubes and the polymer chains of the hosting matrix. The amount of energy dissipated through the CNT-matrix stick-slip depends on the nanocomposite constitutive parameters such as the elastic mismatch, the nanofiller content/distribution, and the CNT-matrix interfacial shear strength.

Loading conditions and environmental factors

The performance of nanocomposite materials is influenced not only by their internal structure and design but also by the external conditions under which they are used. These include loading conditions (such as the type, magnitude, and direction of applied forces) and environmental factors (such as temperature, humidity, and exposure to chemicals). Understanding these factors is critical in optimizing the design, processing, and application of nanocomposites, particularly when they are used in structural, aerospace, automotive, or biomedical applications.

1). Static, dynamic, and impact loads (Soltannia and Taheri, 2015; Kirilova *et al.* 2017). 2). Working temperature and humidity (Petrova *et al.* 2022; Malekinejad *et al.* 2023). 3). Frequency of cyclic loads (Mishnaevsky, 2022; Silva *et al.* 2022).

Soltannia and Taheri (2015) conducted an experimental study to examine the impact of nano-reinforcements on the mechanical behavior of adhesively bonded single-lap joints using composite adhesives, under varying levels of loading (deformation). Their results demonstrated that the nano-reinforced composite structures showed high resistance in impact loading tests. The nanoparticles were dispersed in the material using a mechanical stirrer and a three-roll mill. The findings revealed that the nano-reinforced joints exhibited enhanced hardness and strength.

Kirilova *et al.* (2023) conducted a theoretical investigation on the effects of geometry and axially applied mechanical loads on delamination in a three-layer tungsten disulphide (WS_2)/SU-8/poly(methyl methacrylate) (PMMA) nanocomposite. The study applied a two-dimensional stress-function method and minimized strain energy to derive two analytical solutions for the interface shear stress (ISS) in the middle layer, considering two nanostructures with thinner and thicker PMMA layers.

Several studies indicate that environmental factors like temperature and humidity can affect the volume and performance of adhesives in bonded joints, potentially leading to degradation of polymer-based adhesives and

reduced service life. Although some research has focused on the effects of these factors individually and has resulted in predictive models to help engineers to design reliable adhesive joints, the combined effect of temperature and moisture is still not fully understood (Viana *et al.* 2017). Ulus *et al.* (2022) found that incorporating Nylon 6.6 nanofibers modified with graphene nanoplatelets (GNPs) into water-aged aluminum-composite adhesively bonded single lap joints could enhance the adhesive performance.

Humfeld and Dillard (1998) explored the behavior of adhesive joints subjected to temperature cycles. They found that, at high temperatures, thermal stresses tend to relax quickly due to the viscoelastic nature of the adhesive. However, when the joint cools to ambient temperature, residual stresses are reintroduced and become locked in due to reduced mobility of the polymer chains. With each cycle, the residual stresses increase, leading to adhesive cracking and eventual joint failure. Additionally, the optimal design parameters, such as adhesive thickness, overlap length, materials, and manufacturing processes, may vary depending on the intended application of the joint (Gualberto *et al.* 2021).

Understanding how adhesive joints react to dynamic loading, impact forces, and fatigue is an area of growing interest (Fernandes *et al.* 2023; Gollins *et al.* 2020a, 2020b). Numerous studies on the dynamic behavior of adhesive joints have provided valuable insights into their resilience and failure mechanisms under different loading rates (Li *et al.* 2022). These studies are crucial for structures subjected to cyclic loading or impact events, such as in automotive crash scenarios or components in wind turbines (Mishnaevsky, 2022; Silva *et al.* 2022).

Production process

The production process of nanocomposites involves incorporating nanofillers (such as nanoparticles, nanotubes, or nanowires) into a matrix material (typically a polymer, metal, or ceramic) to enhance the properties of the composite. The process must ensure that the nanofillers are well-dispersed within the matrix to achieve the desired performance improvements. Several methods are available for the production of nanocomposites, and each method varies depending on the type of matrix material, the intended application, and the properties that need to be enhanced.

Common methods for producing polymeric nanocomposites include melt-blending, compression molding, solution processing, resin transfer molding, and in-situ polymerization (Díez-Pascual, 2022). The choice of production technique is influenced by the specific application of the final product. Residual stress and strain are other factors that influence the

mechanical properties of nanocomposites (Meijer *et al.* 2000). Effective stress transfer from the continuous phase to the dispersed phase is essential for the strength and stiffness of the composite, and this transfer depends on the differences in the elastic modulus and Poisson's ratio between the phases (Haque and Ramasetty, 2005). The coefficient of thermal expansion of both the matrix and reinforcement must also be considered, as any mismatch can lead to the formation of thermal residual stresses (McCartney, 1989). A key consideration in preparing nanostructure-reinforced adhesives is ensuring that the carbon nanostructures are evenly dispersed throughout the adhesive, preventing aggregation of the nanostructures (Akpinar *et al.* 2017).

2. Methods of optimization of nanocomposites

Optimizing nanocomposites involves improving their mechanical, thermal, electrical, and other functional properties by carefully managing factors such as composition, processing methods, dispersion of nanofillers, and interfacial interactions. Achieving peak performance requires a careful balance between material design, processing conditions, and the specific needs of the application.

To successfully optimize and design these materials, all processing factors must be considered together. Modeling the intricate relationships between the influencing parameters, both input and output, presents a significant challenge.

Over the past two decades, materials science has experienced a major shift, moving from the creation of basic computational techniques for developing new materials to more sophisticated methods that enhance result reliability through a combination of computational predictions and experimental validation.

Several approaches have been developed for modeling and optimizing the mechanical properties of the nanocomposites in question, as outlined below:

Response surface method

The Response Surface Method (RSM) is a set of mathematical and statistical techniques used to investigate the relationships between multiple input variables (design factors) and one or more output variables (responses). RSM involves conducting a series of carefully designed experiments to identify an optimal response, which is an approximation of the experimental

model. This simplified model is sufficient for estimation and practical application, even when limited information about the process is available. Techniques like RSM help in developing models that identify the optimal operational factors (Dadrasi *et al.* 2019).

Decision tree method

The decision tree is a data mining technique used to extract valuable insights from datasets and identify patterns in the data. It is widely employed in various applications due to its simplicity, low ambiguity, and effectiveness in handling missing values. This method can accommodate both discrete and continuous variables. Decision trees utilize recursive partitioning, similar to classification trees, where errors are measured using mean-square error, though this can be customized and minimized during the training process. The terminal nodes in a decision tree represent the mean value of the outcomes, which serves as the predicted output value (Hastie *et al.* 2009).

Machine learning applied to polymeric nanocomposites

Machine learning (ML) is a branch of artificial intelligence focused on creating algorithms that allow computers to learn from past data to predict future outcomes. ML algorithms are commonly used in biology and chemistry (Webb, 2018; Xu and Jackson, 2019), which has prompted materials scientists to investigate their potential in designing new materials with enhanced properties and broader applications (Liu *et al.* 2020). By combining experiments and computer simulations, a large volume of data is generated, making it possible to apply ML algorithms in materials science to predict properties and design novel materials. ML can be particularly useful in predicting the characteristics and properties of nanocomposites.

Classification of machine learning methods

In general, machine learning can be classified into three types: **(1) supervised learning**; **(2) unsupervised learning**; and **(3) reinforcement learning**.

In **supervised learning**, labeled data samples are provided to the machine learning system for training, which then predicts the output based on this data (Riedmiller, 1994). Essentially, an algorithm learns the mapping

function from input to output: $y = f(x)$ (Zhang and Zhou, 2014). The objective is to approximate the mapping function so accurately that, when new input data (x) is given, the corresponding output (y) can be predicted. After training and processing, the model is tested with sample data to verify if it accurately predicts the output. This approach is called "supervised learning" because the algorithm's learning process is akin to a student learning under an instructor's guidance. The learning phase concludes when the algorithm achieves an acceptable level of performance. Common examples of supervised learning algorithms include linear regression, random forest, spam filtering, and support vector machines (Zhang and Zhou, 2014).

In the ***unsupervised learning***, a machine operates without supervision. It is provided with a set of data that is neither labeled, classified, nor categorized, and the algorithm must work with this data independently (Barlow, 1989). The goal is to transform the input data into new features or group similar objects based on patterns. Since there is no predefined outcome, the machine seeks to extract valuable insights from large datasets. The unsupervised learning can be divided into two main types of algorithms: clustering and association (Figueiredo and Jain, 2002). The clustering problems involve identifying inherent groupings within the data, such as segmenting customers based on purchasing behavior. The association rule learning, on the other hand, focuses on discovering patterns that describe large sections of data, like people who buy item X are likely to buy item Y. The popular unsupervised learning algorithms include k-means for clustering tasks and the apriori algorithm for association rule learning.

The ***reinforcement learning*** is a feedback-based machine learning approach where a learning agent receives rewards for correct actions and penalties for incorrect ones. The agent learns autonomously from this feedback and works to improve its performance, with the ultimate goal of maximizing reward points. In the reinforcement learning, the agent interacts with and explores its environment. An example of this is a robotic dog that learns to move its limbs through reinforcement.

Of the three types of learning mentioned, supervised learning is the most commonly applied in the field of polymeric nanocomposites. Algorithms in this category typically follow a six-stage process, as outlined in Figure 5.

- ***Data Acquisition***: The data must be collected systematically, either from published articles, technical reports, or through personal experimental data. It's important to note that some data sources or published studies may not report all the relevant variables.

- **Data Preparation:** Once suitable data is gathered, it undergoes preprocessing, which involves formatting, cleaning, and sampling. Formatting ensures the data is structured and enhances its quality. Key materials and process variables that impact the behavior being modeled should be carefully reviewed. This includes nano-filler parameters like type, concentration, shape, and size, as well as matrix parameters such as nature, concentration, the manufacturing process used to create the nanocomposites, and properties like density, thickness, and porosity. Some irrelevant attributes are removed during the cleaning stage to maintain consistency and ensure the quality of the data. Incorrect data can compromise the accuracy of machine learning models. The sampling step selects a subset of the data that will be used for training (Xu and Goodacre, 2018). Converting raw data into relevant attributes for input features in the selected algorithm is essential for making accurate predictions, and this process is called feature engineering (Langley, 1994).

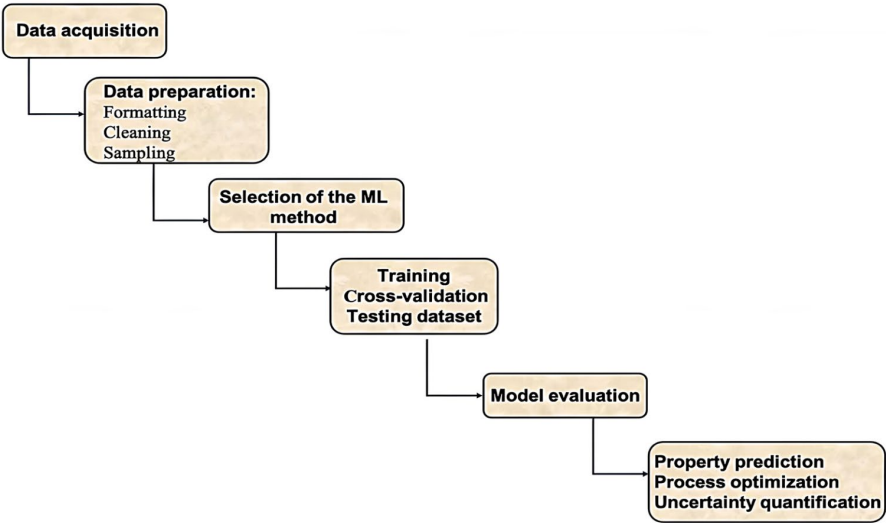


Figure 5: Scheme of the six-stage approach for the implementation of ML algorithms (Champa-Bujaico *et al.* 2022).

- **Selection of the ML Method:** After preparing the data, the next step is to establish a hypothesis function ($h(x)$) that maps the input parameters (x) to the output (y) and choose an appropriate machine learning algorithm. Depending on the type of data and whether the problem is related to classification or regression, a suitable algorithm is selected. For classification problems, algorithms like K-nearest neighbor (KNN), decision trees, neural networks, naïve Bayes, and support vector machines (SVM) are commonly

used (Sharma *et al.* 2013). For regression tasks, algorithms such as linear regression, support vector regression, neural networks, Gaussian processes, and ensemble methods are typically applied (Pardalos and Xue, 1999).

- **Training:** The chosen algorithm is trained using the processed data, which is divided into three subsets: training, cross-validation, and testing datasets. The model learns to process the data using the training dataset. The cross-validation dataset is used for parameter tuning and to prevent overfitting issues.

- **Model Evaluation:** This step is critical in the model development process. Even if the training data error is very small, a model can still be inaccurate. To evaluate the model's performance, a test dataset is used, which forms the basis for making final predictions. After this, the best model is selected, and the hypothesis function is assessed.

Property prediction, process optimization and uncertainty quantification

Machine learning (ML) has been used in polymeric nanocomposites to predict material properties, optimize processes, analyze microstructures, and quantify uncertainties in materials and their properties due to complex manufacturing processes. One of the key applications of ML is optimization. This process involves a repeated training of various models, which can be computationally expensive and challenging for complex simulations. An optimization algorithm works by iterating through different models to find potential solutions until a satisfactory result is achieved. An optimization problem is defined by three main components: (1) variables, which are the parameters the algorithm adjusts; (2) constraints, which are the limits or boundaries for these parameters; and (3) the objective function, which represents the goal the algorithm strives to achieve.

There are two types of optimization algorithms that can be applied: deterministic and stochastic. Deterministic algorithms use specific instructions to find solutions while ignoring uncertainties in the variable space (Sun, 2013). In contrast, stochastic algorithms are probabilistic, modeling uncertainties through appropriate probability distributions (Pedro *et al.* 2018). A newer approach, called robust optimization, is used to explicitly model and minimize uncertainty by employing a set-based deterministic description of uncertainties (Chatterjee *et al.* 2017).

Optimization methods can be significantly enhanced in terms of both effectiveness and efficiency by incorporating machine learning (ML) algorithms (Sakar *et al.* 2019). For example, Salah *et al.* (2020) optimized the process parameters and predicted the absorption index of polycarbonate (PC)/CNT nanocomposites using a multilayer perceptron network approach. Khanam *et al.* (2016) optimized the thermal conductivity, crystallization temperature, degradation temperature, and tensile strength of linear low-density polyethylene (LLDPE)/graphene nanoplatelets (1–10 wt%) nanocomposites processed in a twin-screw extruder, with screw speeds and feeder speeds of 50, 100, and 150 rpm. The properties were predicted using an artificial neural network (ANN). The first three properties increased with higher screw speeds and graphene content. The tensile strength reached its peak at 4 wt% and 150 rpm, which were found to be the optimal conditions for stress transfer from LLDPE's amorphous chains to the graphene nanoplatelets. Yusoff *et al.* (2019) predicted the rheological properties of nanosilica/polymer-modified bitumen using multilayer perceptron neural network models and achieved excellent agreement with experimental data, with an R value of 0.978. More recently, Kosicka *et al.* (2022) applied various optimization algorithms to predict the mechanical properties of epoxy-based nanocomposites reinforced with alumina (5–25 wt%). Using Python programming and available libraries, a neural network predicted properties like Young's modulus, maximum stress, maximum strain, and hardness for the nanocomposites.

Computational analyses of polymer nanocomposites often encounter uncertainties due to variations in material properties, measurement inaccuracies, limitations in experimental set-ups, environmental factors, and inaccurate geometrical features (Karsh *et al.* 2019). Uncertainties in parametric inputs, initial and boundary conditions, as well as computational and numerical uncertainties from inherent assumptions, approximations, and model inaccuracies, can cause significant deviations from deterministic values or the anticipated material behavior. These deviations can alter the overall performance of the nanocomposite. To ensure the reliability of simulation results and assess risks when making final product decisions, it is essential to quantify these uncertainties (Hammer and Villmann, 2007). In this context, Doh *et al.* (2021) applied the Bayesian inference approach to quantify the uncertainty in the electrical conductivity of polymer/CNT nanocomposites. The correlation between CNT conductivity and the phase transition parameter, along with the critical exponent, plays a significant role in the electrical conductivity of the composite during uncertainty quantification.

Yu *et al.* (2019) proposed a design strategy to enhance the toughness of nanocomposite materials through the use of artificial intelligence (AI), implemented with the innovative ‘AutoCompDesigner’ algorithm. This algorithm combines a machine learning predictor with an AI-enhanced genetic algorithm, allowing for the discovery of novel material designs across a broad solution space. By leveraging a deep convolutional neural network trained on a dataset of hundreds of thousands of soft and brittle material combinations obtained from finite element analysis, the researchers were able to predict the properties of new graphene nanocomposites without relying on traditional simulations. Furthermore, they examined the physical mechanisms that contribute to improved material performance and demonstrated how AI can identify optimal designs with minimal sampling.

Artificial neural network (ANN)

The neural networks are a favored algorithm among material science researchers for analyzing data-intensive aspects. These mathematical tools, inspired by the biological nervous system, are used to solve a variety of problems by identifying underlying relationships in available data (Anderson and McNeill, 1992). In the human brain, millions of neurons are interconnected through a network that processes the flow of information to generate meaningful outputs. Similarly, neural networks consist of multiple neurons that act as processors working in parallel and organized into different layers. The first layer, known as the input layer, collects all relevant information (preprocessed data). The intermediate (hidden) layer, composed of many discrete nodes, performs the computations (Wanas *et al.* 1998). The final layer, called the output layer, delivers the predictions. A basic architecture of an artificial neural network (ANN) is depicted in Figure 6. According to Aleksander and Morton (1990), an ANN is a massively parallel-distributed processor made up of simple processing units, naturally capable of storing experimental knowledge and making it accessible for use. It mirrors the brain in two ways: (1) The network acquires knowledge from its environment through a learning process, and (2) the strength of the connections between neurons, or synaptic weights, is used to store the knowledge.

The Artificial Neural Networks (ANNs) are particularly effective for applications where large datasets are available, but finding an accurate solution is challenging due to multiple mathematical approaches, or when the dataset is incomplete, noisy, or complex. Some properties of polymer nanocomposites, such as fatigue, wear, and creep, are well-suited for ANN

analysis (Lynch *et al.* 2001). ANNs are especially useful in polymeric nanocomposites when only material composition and testing conditions are provided as input data. They can help to model the relationship between manufacturing parameters and material performance, forming the basis for optimization in computer processing. The required number of training data can be reduced by optimizing the ANN architecture and selecting the appropriate input parameters. Common predictor functions used in ANNs include multilayer perceptrons (MLPs) and radial basis functions (RBFs), which help minimize prediction errors (Moradkhani *et al.* 2004). The typical architecture for output computation and error minimization is feedforward (FF) with backward propagation (BP). In FF architecture, no loops are formed throughout the network, meaning that units in successive layers do not receive feedback. In BP, synaptic weights are adjusted by backpropagating errors, and weights are updated after each record passes through the network. One complete iteration, or "epoch," occurs when all records have processed through the network, after which the process repeats. Mathematical equations, called activation functions, link the weighted sums of each layer to the succeeding layer, producing the output.

The architecture of an ANN model can be mathematically expressed as:

$$Y=F(x); Y=A(W.x+B_i)+B_0 \quad (1)$$

where Y is the output vector, x is the input vector, A is the activation function (sigmoid, tanh, softmax, softplus etc.), W is the matrix that contains the synaptic weights, B_i is the column vector of biases from the input layer to the hidden layer and B_0 is the column vector of biases from the hidden layer to the output layer.

Matos *et al.* (2019) utilized an artificial neural network (ANN) to explore the potential of epoxy/CNT nanocomposites for creating damage-detecting sensors. They employed the finite element method (FEM) to generate extensive data for the ANN, which was then used at a macroscopic scale to predict the conductivity of the nanocomposites in response to multiaxial strain up to 1%.

Khanam *et al.* (2016) applied an ANN to optimize various properties of polyethylene/graphene nanoplatelet composites, including thermal conductivity, crystallization temperature, degradation temperature, and tensile strength, in relation to process parameters. The nanocomposites, with varying nano-filler content, were processed in a twin-screw extruder at different screw and feeder speeds (50, 100, and 150 rpm). The tensile strength peaked at 4% wt graphene nanoplatelets and a feeder speed of 150 rpm.

Esmacili and Dashtbayazi (2014) used an ANN to model the mechanical alloying process for synthesizing Al/SiC nanocomposite powders, followed by optimization using a genetic algorithm. The ANN model predicted the nanocomposite properties, such as crystallite size and lattice strain of the aluminum matrix, while the optimization aimed to identify the maximum lattice strain and minimum crystallite size achievable by adjusting the process variables.

Thongvigitmanee and May (2002) applied an ANN to model thin-film integral capacitors for next-generation electronic packaging applications using polymer-ceramic composites. Their model considered factors such as ceramic particle size, ceramic volume fraction in the polymer matrix, polymer cure time and temperature, surfactant percentage, and ultrasonic mixing time. These models were used to determine process optimization via genetic algorithms to find the optimal combination of polymer/ceramic materials and process conditions that would achieve the desired electrical properties.

Genetic algorithm method

An alternative method for optimizing the properties of polymer nanocomposites is the genetic algorithm (GA). Developed by John Holland (1992), the GA has since been extensively studied and refined. It is a bio-inspired approach based on the principles of species evolution (Eiben and Smith, 2003), where individuals better suited to their environment have a greater chance of surviving and reproducing, thus passing on their advantageous traits to future generations. In this context, each individual represents a potential solution to the optimization problem at hand, with the individual's genetic makeup corresponding to the values of the parameters that define the solution encoding. In the case of polymer nanocomposites, each individual in the population represents a unique nanocomposite design. The algorithm operates in parallel, managing a population of individuals that compete to evolve and reach the next generation.

The genetic algorithm is considered as an evolutionary algorithm because it operates through the progression of successive stages for a population of solutions. The survival probability of an individual is determined by its degree of adaptation, which makes the algorithm non-greedy. This means that, in addition to the genetic traits, other factors—such as random events—can also help an individual to survive and thrive in later generations, even if they are not the most optimized at the outset.

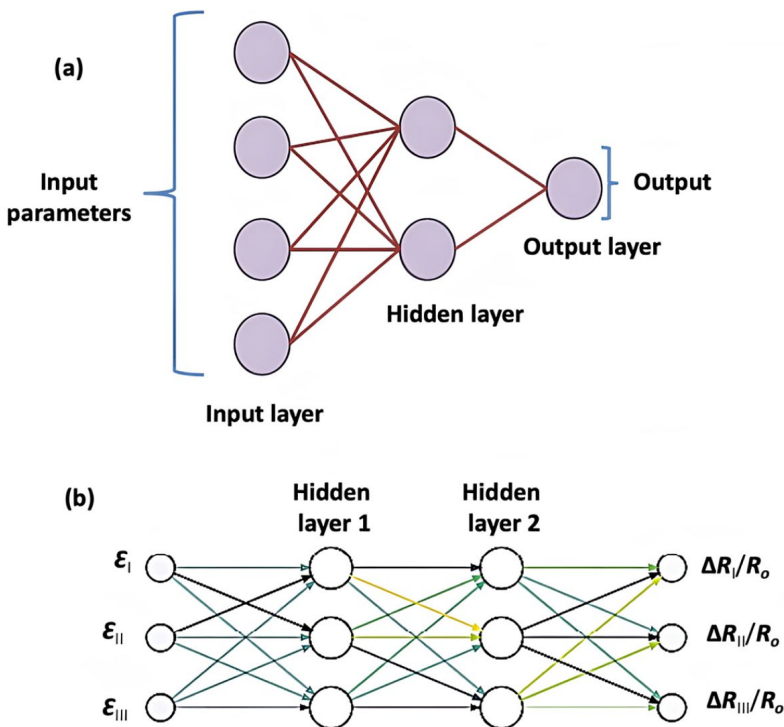


Figure 6: (a) Diagram showing the basic architecture of an artificial neural network (ANN), which consists of input, hidden, and output layers. The input layer receives the preprocessed data, the hidden layer computes the correlations, and the output layer generates the predicted results. (b) Example of an ANN used to predict the electro-mechanical response of polymer/CNT nanocomposites (Champa-Bujaico *et al.* 2022).

The adaptation of an individual in a genetic algorithm is assessed using an evaluation or fitness function, which measures one or more desirable properties in the nanocomposite. A higher quality in these properties translates to a greater likelihood of survival within the population. Depending on the problem at hand, optimization may involve either maximizing or minimizing this function. For nanocomposite design, the objective could be to maximize properties like material strength, thermal conductivity, electrical conductivity (García-Carrillo *et al.* 2022), or hydraulic performance (Han *et al.* 2019). In other cases, the goal is to minimize a cost function, such as minimizing the potential energy of Au-Ag bimetallic nanoparticles (Shao *et al.* 2018) or reducing the friction factor while maximizing heat transfer (Miandoab *et al.* 2022). Alternatively, the objective might be to classify

samples based on their structure (Zhang *et al.* 2020), with the fitness function being defined as classification accuracy, which needs to be maximized. The evaluation function enables the distinction between individuals, identifying the one with the highest or lowest fitness value, based on whether the function aims for maximization or minimization.

The implementation of a genetic algorithm involves three fundamental operators (Araujo *et al.* 2019): the selection operator, which is responsible for choosing individuals to form the population of a generation and/or determining which individuals will produce offspring; the crossover or recombination operator, which generates new individuals from progenitor ones; and the mutation operator, which, with a low probability, induces significant changes in the composition of certain individuals. The effects of mutation can be either detrimental to an individual's survival or, conversely, highly beneficial, depending on the outcome.

Figure 7 illustrates the basic flowchart of a genetic algorithm. The process begins with a set of randomly generated individuals that form the initial population, representing a collection of random solutions to the problem. As these solutions are random, their fitness values are expected to be far from the optimal ones. If the algorithm's termination conditions are not met, it moves on to the next generation. During each generation, the population undergoes parent selection, crossover, and mutation operations. The resulting new individuals are then evaluated, and the selection of survivors for the next generation takes place. If the stopping conditions are still not satisfied, a new generation begins.

Genetic algorithms (GA) are widely used for global optimization and have been applied in exploring polymer spaces (Kim *et al.* 2021). They perform a structured search based on procedures inspired by natural evolution. In each iteration, the parameter vectors (genotypes) within a population undergo updates through selection, crossover, and mutation to generate offspring, followed by the evaluation of the objective function value. GA has been utilized to predict the thermal and optoelectronic properties of both neat polymers and fiber-reinforced composites (Ponticelli *et al.* 2020). Despite its significant potential, the application of GA to polymeric nanocomposites remains limited (Moghri *et al.* 2014; He *et al.* 2019).

Rabothata *et al.* (2021) applied a genetic algorithm (GA) to optimize both the design parameters and mechanical properties (elastic modulus and strength) of polymeric nanocomposites. The algorithm, implemented in Matlab, proved to be quite effective in finding the optimal property values. Mairpady *et al.* (2021) combined an artificial neural network (ANN) with a GA to optimize the concentration of nanofillers and compatibilizing agents in injection-molded high-density polyethylene (HDPE) bionanocomposites

containing nanoTiO₂ or cellulose nanocrystals. They successfully optimized mechanical properties such as Young's modulus, tensile strength, and fracture strength, achieving minimum errors and regression values above 95%. This study highlights the potential of optimizing nanofiller content and types in polymeric matrices to enhance mechanical durability.

Dadrasi *et al.* (2019) conducted both experimental and theoretical studies on the flexural and compressive properties of epoxy-based hybrid nanocomposites reinforced with hydroxyapatite nanoparticles and graphene oxide nanoplates. The test samples were prepared using a design of experiment based on a central composite design. The experimental results were modeled using response surface methodology, artificial neural networks, and decision tree methods. To identify the optimal nanoparticle content for achieving maximum flexural and compressive properties, a genetic algorithm was employed. The results showed a 60.48% improvement in flexural strength for the sample reinforced with 3.5 wt% HA compared to neat epoxy. Furthermore, the flexural modulus increased by 74.54% in the sample containing 7 wt% HA and 0.25 wt% GO. The compressive strength rose by 66% in the sample with 0.25 wt% GO, while the compressive modulus increased by 212% in the sample containing 1.02 wt% HA and 0.43 wt% GO, compared to pure epoxy. Using a genetic algorithm, the optimal values for flexural strength, flexural modulus, and maximum compressive strength for nanocomposites with different HA and GO compositions were determined. Based on these findings, the authors concluded that GO plays a key role in enhancing the mechanical properties of the nanocomposites.

Boyadzhiev *et al.* (2024) applied an optimization method that combines a genetic algorithm (Shopova and Vaklieva-Bancheva, 2006) with a deterministic optimization scheme to find the optimal layer thicknesses, length, and mechanical loading conditions for an axially loaded graphene/MoS₂/PET nanocomposite, ensuring it operates safely without delamination. The study includes two distinct analytical solutions (Case 1 and Case 2) for calculating the interface shear stress (ISS) in the middle layer of the structure. These solutions are derived from the two-dimensional stress-function method and the minimization of strain energy. For optimization, a theoretical delamination criterion based on the ISS model is used as the criterion for evaluating the interface layer. The results from optimization showed that at the obtained optimal values of layer thicknesses, length, and mechanical loading, the model ISSs confirmed and fulfilled the model criterion in graphene/MoS₂/PET.

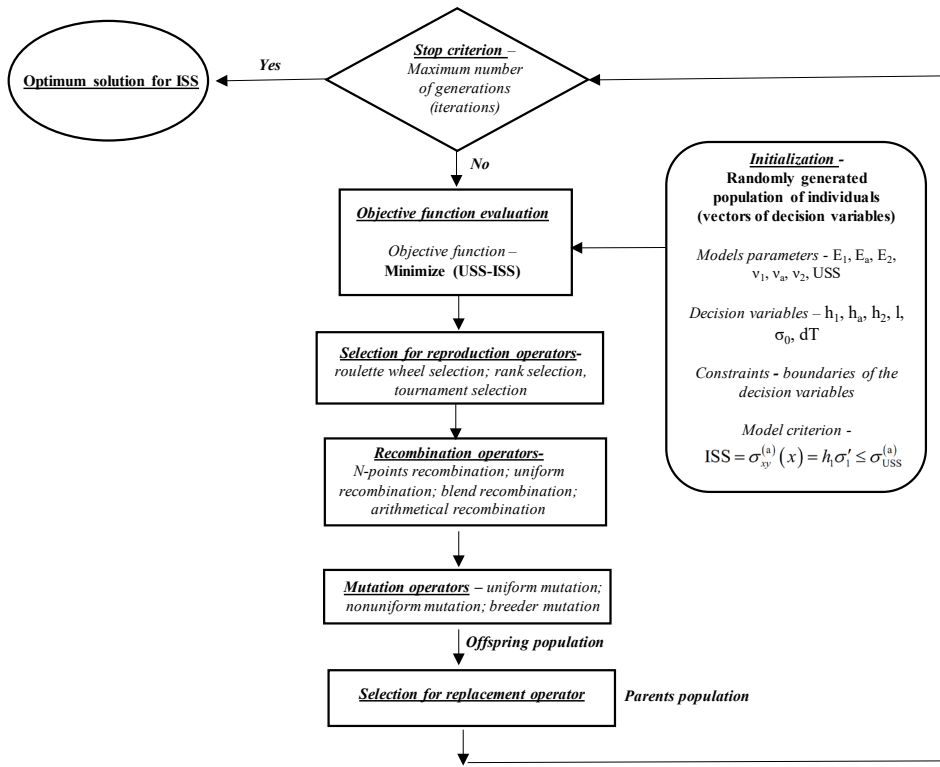


Figure 7: Flowchart of the genetic algorithm used in (Petrova *et al.* 2024; Boyadzhiev *et al.* 2024; and Kirilova *et al.* 2024).

The obtained optimal interval of values for thickness of adhesive coincides well with available literature data (Yu *et al.* 2014). The proposed method in Boyadzhiev *et al.* (2024) is applied also in Petrova *et al.* (2024) for hBN/PMMA nanocomposite and in Kirilova *et al.* (2024) - for WS₂/SU-8/PMMA. The value obtained by Gou and Ke (2019) value for the thickness of interfacial layer value for boron nitride nanotubes (BNNT)/PMMA is in our optimal interval for this value (Petrova *et al.* 2024). The results for optimal WS₂ length in Kirilova *et al.* (2024) coincide very well with results of Wang (2017) for an optimal WS₂ flake length needed to assure a full reinforcement in WS₂ nanocomposites (40 μm). Also, the optimal thickness of the interfacial layer in the same structure (Kirilova *et al.* 2024) is very close to the same value, used in Kim *et al.* (2014) for WS₂/PVA nanocomposite (0.5 nm).

Differential Evolution (DE)

Differential Evolution (DE) is a stochastic, population-based optimization algorithm that falls under the category of evolutionary algorithms (EAs). It is especially efficient for tackling complex, nonlinear, and multimodal optimization challenges. DE operates by maintaining a population of candidate solutions (individuals) that evolve across multiple generations. Rather than relying on traditional genetic operations, DE generates variation through differential mutation and crossover. The algorithm assesses the fitness of offspring solutions and keeps the best-performing ones for the next generation. DE is simple to implement with few or a minimal number of control parameters and proves to be highly robust across a diverse array of optimization problems.

The Differential Evolution algorithm includes the following steps:

- *Initialization:* 1). A population of N candidate solutions is randomly initialized within the problem's search space. 2). Each individual (solution) is represented as a vector of parameters.
- *Differential mutation:* 1). A mutant vector is generated for each individual by adding a weighted difference of two or more randomly selected individuals. 2). Common mutation strategy:

$$v_i = x_{r1} + F(x_{r2} - x_{r3}) \quad (2)$$

where F is a scaling factor and x_{r1} , x_{r2} and x_{r3} are randomly selected individuals.

- *Crossover(recombination):* A trial vector is created by combining elements of the mutant vector and the original individual using a crossover probability CR .
- *Selection:* 1). The trial vector is compared to the original vector based on an objective function. 2). The better-performing solution is retained for the next generation.
- *Termination:* The process repeats until a stopping criterion is met (e.g., reaching a maximum number of iterations or achieving a desired fitness value).

Storn and Price (1997) used Differential Evolution (DE) to find the optimal material parameters that maximize the damping ratio of CNT nanocomposites. This approach is useful for multi-dimensional optimization tasks, such as determining the optimal values for the interface shear stress

(ISS), CNT volume fraction, Young's modulus of the host matrix, and the hysteresis shape parameter. Unlike other optimization methods, DE does not require a gradient function, making it suitable for cases where the objective function is non-differentiable.

Formica *et al.* (2018) applied a DE method in combination with a custom finite element implementation of a nonlinear 3D mesoscale theory to optimize the hysteretic damping capacity of CNT nanocomposites. The theory models the energy dissipation caused by shear stick-slip between the nanotubes and the polymer chains of the matrix. In this case, the dissipated energy depends on various nanocomposite parameters, including elastic mismatch, nano-filler content and distribution, and CNT-matrix interfacial shear strength. The objective function is defined as the area under the damping ratio curve versus the strain amplitude over the strain range of interest. The DE process begins with an initial population of individuals representing the variables involved in the optimization. Each individual has an associated fitness value based on the objective function. The algorithm operates by creating a new population from the previous one, comparing fitness values, and selecting the better individuals. The DE process stops when the best fitness is within a certain threshold or when the maximum number of iterations is reached. As a result, the optimized material parameters that maximize the damping capacity of the nanocomposite were determined.

Finite Element Analysis (FEA)

Finite Element Analysis (FEA) is a powerful numerical tool used to simulate and optimize engineering problems. By breaking down complex structures into smaller elements, it provides accurate insights into stress, deformation, temperature, and fluid behavior. While FEA requires expertise in meshing, boundary conditions, and solver selection, it remains an indispensable tool for design validation, failure analysis, and product optimization in various industries.

Fundamentals of the Finite Element Method (FEM)

FEA is based on the Finite Element Method (FEM), which follows these steps:

Step 1: Discretization (Mesh Generation)

- The geometry of the structure is divided into smaller, finite elements (mesh).
- These elements can be 1D (beams, bars), 2D (triangles, quadrilaterals), or 3D (tetrahedrons, hexahedrons).
- The finer the mesh, the more accurate the solution, but it increases computational cost.

Step 2: Selection of Element Type & Shape Functions

- Each element has specific shape function that describe how displacements, strains, and stresses vary within it.
- Common elements include linear, quadratic, or higher-order elements.

Step 3: Formulation of Governing Equations

- The physical problem is converted into mathematical equations.
- Governing equations depend on the type of problem:
 - Structural Mechanics: Uses equilibrium equations and Hooke's Law.
 - Heat Transfer: Uses conduction and convection equations.
 - Fluid Dynamics: Uses Navier-Stokes equations.

Step 4: Assembly of Global System of Equations

- The equations for all elements are assembled into a global stiffness matrix.
- This matrix represents the entire system and links all elements together.

Step 5: Application of Boundary Conditions and Loading

- Essential boundary conditions (fixed supports, forces, temperatures) are applied.
- External forces, pressures, or temperature changes are defined.

Step 6: Solving the System of Equations

- A system of algebraic equations is solved using numerical methods such as:
 - Gaussian elimination
 - Iterative solvers (e.g., Conjugate Gradient Method)
- The result gives displacements, stresses, strains, or temperatures at each node.

Step 7: Post-Processing and Interpretation of Results

- The solution is visualized using contour plots, deformed shapes, stress distributions, and animations.

The results are analyzed to check for failure, safety, and optimization opportunities.

Types of FEA Analysis

➤ **Structural Analysis**

Used to determine **stresses, deformations, and failure modes** in structures.

- Static Analysis: Finds stress and strain under static loads.
- Dynamic Analysis: Evaluates time-dependent behaviors (e.g., vibration, impact).
- Nonlinear Analysis: Accounts for material plasticity, large deformations, and contact problems.

➤ **Thermal Analysis**

Analyzes heat conduction, convection, and radiation effects.

- Steady-State Thermal Analysis: Studies temperature distribution under constant conditions.
- Transient Thermal Analysis: Examines temperature changes over time.

➤ **Fluid Dynamics (CFD – Computational Fluid Dynamics)**

Solves Navier-Stokes equations to study fluid flow, pressure distributions, and heat transfer.

- Laminar vs. Turbulent Flow: Determines fluid behavior.
- Multiphase Flow: Simulates interactions between liquids, gases, and solids.

➤ **Electromagnetic Analysis**

Used for electrical and magnetic field simulations.

- Applications: Antenna design, transformers, motors, waveguides.

Advantages of Finite Element Analysis

- **Handles Complex Geometries:** Suitable for irregular shapes and real-world structures.
- **Accurate and Reliable:** Provides precise results by refining the mesh.
- **Reduces Physical Prototyping Costs:** Saves time and money in design testing.

- Applicable to Multiple Domains: Used in mechanical, civil, aerospace, and biomedical engineering.
- Identifies Weaknesses Before Manufacturing: Helps to prevent failure in real-world applications.

Applications of FEA

- Automotive Industry: Crash testing, chassis strength, vibration analysis.
- Aerospace Engineering: Aircraft structural analysis, aerodynamics, fatigue analysis.
- Civil Engineering: Bridge design, earthquake resistance, foundation stability.
- Biomedical Engineering: Prosthetic design, bone stress analysis, cardiovascular simulations.
- Manufacturing: Welding simulations, machining stress analysis, product optimization.

Limitations of FEA

- Computationally Intensive: Large, complex models require high processing power and time.
- Mesh Sensitivity: Poor meshing can lead to inaccurate results.
- Requires Expert Knowledge: Needs proper selection of boundary conditions and solver settings.
- Simplifications and Assumptions: Real-world complexities may not be fully captured.

Finite Element Analysis (FEA) simulations are well-suited for studying complex, non-homogeneous material systems because they allow for explicit configuration of all relevant material phases. This makes FEA an effective tool for analyzing the behavior of nanocomposites, as it can incorporate important factors like nanofiller dispersion and interphase properties. FE models have been developed to analyze various behaviors of polymer nanocomposites, including thermal and mechanical properties (Deng *et al.* 2012; Wood *et al.* 2016), as well as dielectric behavior (Huang *et al.* 2014; Zhao *et al.* 2017), and to investigate the impact of the interphase on these properties.

Wang *et al.* (2018) developed and tested a model for two types of polymer nanocomposite response data: viscoelastic and dielectric

simulations. For both cases, they created finite element models to simulate the composite properties based on the given microstructures obtained from Scanning Electron Microscope (SEM) or Transmission Electron Microscope (TEM) images (Huang *et al.* 2014; Deng *et al.* 2012). The FEA setup is shown in Figure 8. Microstructure dispersion data were directly obtained from TEM images (Figure 8a). A binary image representing the filler and matrix phases was generated using a previously developed Niblack analysis algorithm (Niblack, 1985). The binary image was then characterized to identify geometric descriptors, which were used to reconstruct the equivalent 3D microstructure, assigning each point in the FEA model to a material constituent (filler, interphase, matrix) (Figure 8c). The geometric data for the filler and matrix were directly extracted from the original image, while the interphase region between the filler and particle was modeled as an extended layer around each particle. The interphase thickness was assumed to be 50 nm, based on previous studies on filler-filler spacing and experimental measurements (Cheng *et al.* 2015). The FEA model was then executed in the appropriate software to obtain the frequency-dependent viscoelastic or dielectric response.

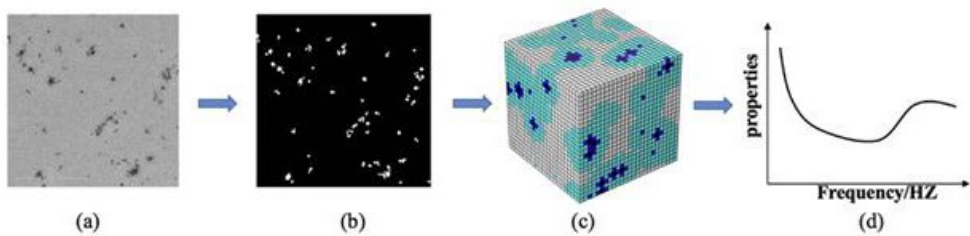


Figure 8: The configuration of the FEA model for dielectric simulations in COMSOL and viscoelastic simulations in ABAQUS is outlined as follows: a) The TEM image of the sample; b) A binary image depicting the matrix and filler phases; c) The reconstructed microstructure; d) The frequency-dependent dielectric properties or viscoelastic response predicted from the simulation (Wang *et al.* 2018).

These interphase FEA models have been utilized with a manual inverse approach to determine the interphase properties (Deng *et al.* 2012; Zhao *et al.* 2017). In these studies, the shift factors that link the interphase properties to the matrix properties are defined differently for each specific property case. In viscoelastic simulations, a broadening factor (B) and frequency-shifting factor (S) are used to describe the interphase behavior in relation to the matrix property. For the dielectric interphase, due to the multiple relaxations seen in

the pure matrix, the alpha and beta relaxations are modeled separately, and a five-dimensional shifting factor set is applied to the interphase model.

Adaptive optimization

The adaptive optimization accelerates the search for interphase properties in nanocomposite data arrays by solving the inverse problem using global optimization.

Wang *et al.* (2018) combined finite element analysis (FEA) with an adaptive global optimization method that integrates Gaussian Process (GP) modeling (Stein, 2012; Qian *et al.* 2006) and a sequential sampling strategy (Picheny *et al.* 2013) to optimize dielectric and mechanical properties, minimizing the discrepancy between the predicted bulk properties of a nanocomposite and the experimental data. Experimental samples were derived from 2 wt% Chloro-modified nanosilica in Polystyrene (PS) nanocomposites (Hassinger *et al.* 2016). The interphase properties were described by shifting factors based on the matrix's pure properties, represented by a Prony Series, which includes multiple relaxation times and strengths. Using experimental data from both pure matrix and bulk nanocomposite properties (dielectric or thermomechanical), the interphase properties were determined through an iterative trial-and-error process by matching the FEA simulations to the experimental results. The adaptive optimization approach was employed to identify the optimal shift factors that align the composite data. A Gaussian Process (GP) model was constructed as a surrogate for the objective function, with uncertainty quantification of the predictions. An adaptive sampling strategy was applied to navigate through the complex search space by iteratively selecting new sampling points based on an expected improvement function. The surrogate model and optimal solution continued to evolve until the desired objective was met. This approach was tested for simulations of both dielectric and viscoelastic properties in nanocomposites.

The adaptive optimization method is outlined in Figure 9, with the following components: (1) The empirical bounds of the shift factors are utilized to define the range for sampling initial training sets of the shift factors through the design of experiments (DOE) using the Optimal Latin Hypercube (OLHC) method. For each set of shifting factors, the FEA model is run to generate simulated results.

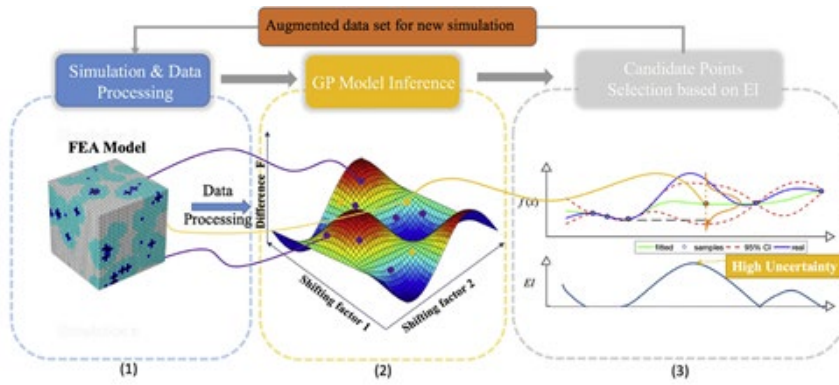


Figure 9: The automated adaptive optimization strategy for searching interphase properties involves the following steps: (1) FEA is performed on each point in the initial shift factor set derived from the DOE, and the results are processed to form the objective function by calculating the difference between the simulated outcomes and the experimental data using the mean square error (MSE); (2) A Gaussian Process (GP) model is used to create surrogates that predict the value of the objective function (Difference F) within the design space. The purple points represent the initial sampling points from the DOE, and the yellow points are generated sequentially through the Expected Improvement (EI) process in step (3); (3) EI identifies the best candidate points for additional simulations. These new candidate points expand the initial training shift factor set from the DOE, further refining the surrogate model and improving prediction accuracy (Wang *et al.* 2018).

The objective function is then formulated as the difference between the experimental data and the simulation, quantified using the mean square error (MSE); (2) A surrogate model, specifically a Gaussian Process (GP) model, is employed to analyze the training data, learning the relationship between the objective (Difference F) and the features (shifting factors), while accounting for uncertainties; (3) The adaptive optimization process (selector) identifies the most promising candidate points for new simulations and enhances the initial shift factor set from the DOE. New candidate points are selected based on feedback from the surrogate model in the previous step, with the Expected Improvement (EI) function guiding the selection. Steps (2) and (3) are often referred to as the adaptive optimizer, which refines the initial training shift factor set and drives the iterative enhancement of the surrogate model and its predictive accuracy.

Taguchi Method

The Taguchi Method is a robust design optimization technique developed by Dr. Genichi Taguchi to improve the quality of manufactured products and processes. It is a statistical approach that focuses on enhancing the product performance by minimizing the variability due to external factors (noise), leading to higher quality and reduced costs.

Principles of the Taguchi Method

➤ Quality Loss Function

Taguchi introduced the Quality Loss Function (QLF), which quantifies the loss in quality as deviation from the target value increases. Unlike traditional quality control, which focuses on meeting specifications, QLF emphasizes reducing variation around the desired value.

The loss function is given as:

$$L=k(y-T)^2 \quad (3)$$

where L is the quality loss; k is the constant based on cost; y is the actual performance value; T is the target value.

This function penalizes deviations from the target, even if they are within specifications.

➤ Robust Design and Signal-to-Noise (S/N) Ratio

Taguchi's approach focuses on designing robust products and processes that perform consistently under varying conditions (noise factors). He introduced the *Signal-to-Noise (S/N) Ratio*, which quantifies the performance stability.

There are three common types of *S/N ratios*:

1. *Smaller-the-Better*: used for minimizing defects, wear, or noise (e.g., pollution, errors).

$$S/N=-10\log(1/n\sum u^2) \quad (4)$$

2. *Larger-the-Better*: used for maximizing outputs like efficiency or strength.

$$S/N = -10 \log(1/n \sum 1/u^2) \quad (5)$$

3. *Nominal-the-Best*: used for achieving a precise target value (e.g., dimensions, voltage).

$$S/N = -10 \log(\bar{u}^2/s^2) \quad (6)$$

where u is the observed response, n is the number of experiments, $\bar{u}$ is the mean response, and s is the standard deviation.

➤ Orthogonal Arrays (OAs) and Design of Experiments (DOE)

Instead of testing all possible combinations (which is impractical), Taguchi introduced Orthogonal Arrays (OAs) to efficiently design experiments.

- OAs help in reducing the number of experimental runs while still capturing the effects of multiple parameters.
- The selection of an OA depends on the number of factors and levels.
- Example: An L9 orthogonal array allows testing 4 factors at 3 levels each in just 9 experiments instead of 81.

➤ Analysis of Variance (ANOVA)

Taguchi integrates ANOVA to determine which factors significantly affect the performance.

- ANOVA quantifies the contribution of each parameter to the response variable.
- It helps in identifying the most influential control factors for optimization.

ANOVA results typically include:

- Sum of squares (SS) – Measures variability due to a factor.
- Degrees of freedom (DF) – Number of independent values that can vary.
- Mean square (MS) – SS divided by DF.
- F-ratio (F-test) – Determines statistical significance.

A high F-ratio suggests that a factor has a strong impact on the response variable.

Advantages of the Taguchi Method

- Reduces experimental costs – Uses fewer runs than full factorial designs.
- Improves quality & reliability – Minimizes variability in products/processes.
- Identifies key process factors – ANOVA and S/N ratio help to find optimal settings.
- Applies to various industries – Used in manufacturing, automotive, electronics, and healthcare.

Applications of the Taguchi Method

- Automotive Industry: Optimizing engine performance, fuel efficiency, and durability.
- Manufacturing: Reducing defects in machining, welding, and casting.
- Aerospace: Improving material strength and aerodynamics.
- Electronics: Enhancing PCB design, semiconductor fabrication, and signal processing.
- Healthcare & Pharmaceuticals: Optimizing drug formulations and medical device manufacturing.

Challenges & Limitations of the Taguchi Method

➤ Assumption of Independence

The method assumes that factor interactions are minimal or negligible, which may not always be true in complex real-world processes. Ignoring interactions can lead to suboptimal results.

➤ Limited Handling of Nonlinear Relationships

The Taguchi method may not effectively capture nonlinear relationships between factors and responses, making it less effective for highly complex systems.

➤ Fixed Orthogonal Arrays (OA)

The method relies on predefined OAs, which may not always fit specific experimental requirements. The customization of OAs can be complex and may require additional statistical expertise.

➤ Lack of Comprehensive Statistical Analysis

Compared to other experimental design techniques (e.g., full factorial or response surface methodology), Taguchi's approach provides limited statistical insights, such as p-values and confidence intervals.

➤ Large Number of Experiments for High Factors

As the number of control factors increases, the number of experiments required can grow significantly, making it resource-intensive.

➤ Inability to Optimize Multiple Responses Simultaneously

The method focuses on optimizing a single response variable. Handling multiple quality characteristics requires additional techniques like Grey Relational Analysis (GRA).

➤ Subjectivity in Selection of Signal-to-Noise (S/N) Ratios

Choosing the correct S/N ratio for a given problem can be subjective, and an incorrect choice may lead to misleading conclusions.

➤ Not Suitable for Dynamic Systems

The Taguchi method is better suited for static problems. When dealing with dynamic processes where parameters change over time, other optimization methods may be more effective.

➤ Neglects Certain Experimental Errors

Unlike some other statistical design methods, Taguchi does not emphasize measuring and quantifying experimental errors in detail.

➤ Limited Software Support

While statistical software like Minitab and MATLAB support the Taguchi method, it is not as widely integrated as other experimental design approaches like Design of Experiments (DOE).

The Taguchi method, based on analysis of variance (ANOVA), is used to study the effect of individual parameters on stress and weight.

Beygi *et al.* (2012) utilized a design of experiments approach based on the Taguchi method to synthesize $\text{FeNiAl}_2\text{O}_3$ nanocomposite powders through the mechanical alloying of Fe_2O_3 , Al, and Ni powder mixtures. They explored the influence of various parameters, such as Al_2O_3 weight percentage, uniaxial cold pressure, sintering temperature, and sintering time, on the fabrication process (including densification and consolidation) and the

mechanical properties (hardness, compression strength, and specific wear rate) of the resulting nanocomposites.

Stan *et al.* (2014) applied metamodeling techniques, including the Taguchi method, to optimize injection molding parameters (melt temperature, injection pressure, and strain rate) in the context of mechanical properties (Young's modulus, yield strength/strain, stress/strain at break) for polypropylene filled with different amounts of multi-walled carbon nanotubes (MWNTs). The study revealed that the reinforcing effect of MWNTs was more significant at higher injection pressures, and both yield strength, stress at break, and Young's modulus increased with higher MWNT content and strain rate.

Topological Optimization (TOP)

Topology Optimization (TO) is an advanced computational technique used to design lightweight, high-performance structures by optimizing stiffness, strength, or other performance criteria while minimizing material usage in nanocomposite structures. It integrates finite element analysis (FEA), optimization algorithms, and additive manufacturing to push the boundaries of design. Despite computational challenges, TO is widely adopted in aerospace, automotive, biomedical, and architectural engineering.

Unlike traditional design methods, which refine existing geometries, TO starts from an initial design space and removes inefficient material to achieve an optimal shape.

Principles of Topology Optimization

➤ Design Space and Constraints

- The design starts with a fully defined geometric space (e.g., a rectangular block for a bracket).
- Loads, boundary conditions, and constraints are applied to define how the structure should perform.

➤ Finite Element Analysis (FEA) Integration

- The design space is discretized into finite elements (mesh).
- FEA is used to calculate stresses, strains, and deformations for each element.

➤ **Optimization Algorithm**

- Objective Function: Defines what to maximize or minimize (e.g., stiffness, weight, natural frequency).
- Material Density Variable: Each element is assigned a variable (0 = no material, 1 = full material).
- Iterative Process: The algorithm removes inefficient material while ensuring structural integrity.

➤ **Filtering and Post-Processing**

- Filtering techniques prevent checkerboarding (unrealistic pixelated structures).
- The final shape is smoothed and transformed into a manufacturable design.

Types of Topology Optimization Methods

➤ **Density-Based Method (SIMP – Solid Isotropic Material with Penalization)**

- Most common approach, assigns a density value to each element.
- Uses a penalty factor to force elements to be either solid (1) or void (0).
- Example: Used in aircraft wing spars and automotive components.

➤ **Level Set Method**

- Represents the boundary of the structure as an evolving surface.
- Works well for problems involving moving boundaries and multi-material designs.

➤ **Evolutionary Structural Optimization (ESO/BESO)**

- Iteratively removes inefficient elements based on stress distribution.
- The Bi-directional Evolutionary Structural Optimization (BESO) approach also adds material back if needed.

➤ **Topology Gradient-Based Methods**

- Uses gradient-based optimization techniques to adjust material distribution.
- Suitable for problems requiring precise control of stress and compliance.

Applications of Topology Optimization

➤ **Aerospace Engineering**

- Aircraft and spacecraft structural components are optimized to reduce weight while maintaining strength.
- Example: Airbus and NASA use TO for lightweight satellite structures.

➤ **Automotive Industry**

- Used for chassis design, suspension systems, engine components to improve fuel efficiency and crash safety.
- Example: Bugatti 3D-printed titanium brake caliper optimized using TO.

➤ **Civil and Architectural Engineering**

- Applied in bridge structures, skyscrapers, and lightweight roofs to maximize load-bearing efficiency.
- Example: Eiffel Tower-inspired designs for modern architectural elements.

➤ **Biomedical Engineering**

- Used to create lightweight, patient-specific implants (e.g., bone scaffolds, orthopedic implants).
- Example: Porous titanium hip implants designed for improved osseointegration.

➤ **Consumer Products & Sports Equipment**

- Applied in bicycle frames, drone structures, and athletic shoes for lightweight, durable performance.
- Example: Adidas 3D-printed midsoles optimized for weight and cushioning.

Advantages of Topology Optimization

- **Reduces Material Usage:** Significant weight savings lead to lower costs and environmental impact.
- **Improves Structural Efficiency:** Designs are optimized for stiffness, strength, and durability.

- Enables Innovative Geometries: Produces organic, nature-inspired shapes not so likely to be involved with traditional CAD.
- Enhances Performance in Multiple Fields: Used across automotive, aerospace, biomedical, and consumer industries.
- Can be combined with Additive Manufacturing (3D Printing): Creates complex, optimized parts that are easy to manufacture via metal and polymer 3D printing.

Challenges & Limitations of Topology Optimization

- Manufacturability Issues: Complex organic shapes may be difficult to fabricate using traditional machining.
- Computational Cost: Requires significant computational power for large models.
- Post-Processing Required: Often, smoothing and redesigning are needed to make the part manufacturable.
- Limited Material Considerations: Some TO methods do not account for composite materials or anisotropic behaviors.

Future of Topology Optimization

- AI & Machine Learning Integration – Automating TO with AI-driven design for faster iteration.
- Multi-Material & Composite Optimization – Designing heterogeneous materials for improved performance.
- Real-Time TO for Adaptive Structures – Future designs may adjust topology dynamically based on loads.
- Sustainability & Eco-Design – TO will play a key role in minimizing material waste and reducing CO₂ footprint.

Seifert *et al.* (2015) performed an analysis and optimization to determine the maximum resistance change and minimum strain energy in a carbon nanotube-epoxy composite. The analysis employed the finite element method and incorporated coupled mechanics, electrostatics, and piezoelectricity. The optimization process was carried out in steps, starting with minimizing strain energy, followed by solving two resistance maximization problems. After addressing each individual problem, a weighted sum approach was used for multi-objective optimization, balancing both strain energy minimization and resistance change maximization. The

study also discussed the impact of topology optimization as a design tool for the shape of the optimized cross-sections and explored potential extensions of using the coupled physics topology optimization algorithm.

Arhore *et al.* (2021) investigated how the outer adherend geometry influences the strength of an adhesively bonded joint, utilizing a genetic algorithm (GA) alongside high-fidelity explicit finite element analysis (FEA) and topology optimization (TOP). Both methods were applied to a simplified pseudo-2D model as well as a full-scale 3D model. The study found that the outer adherend geometry had a significant impact on the strength of joints under tensile load, but minimal effect on joints subjected to bending load. The GA optimization process resulted in identical geometry for both the 2D and 3D models, whereas the TOP process yielded different optimal geometries. The joints optimized by TOP demonstrated the highest overall strength, while the GA-optimized joints provided the best strength-to-weight ratio.

3. Examples of Optimization of Nanocomposite Materials

- **Improved Adhesion Strength:** By adding nanoparticles such as graphene, carbon nanotubes, or fullerene to the adhesive, the tensile strength and four-point bending strength of a composite joint can be significantly enhanced. For example, adding 1 wt% graphene to a structural adhesive (DP270/T) increases the composite joint's failure strength by 28% (Akpınar *et al.* 2017).
- **Optimization of Hysteresis Damping:** By adjusting material parameters such as elastic mismatch and interfacial shear strength, optimal damping can be achieved in CNT-polymer nanocomposites. For example, the two-parameter optimization of the interfacial shear strength and CNT volume results in a nanocomposite with a 950% increase in average damping (Formica *et al.* 2018).
- **Optimization of Shear Strength and Shear Resistance:** Using artificial intelligence (AI) algorithms, the shear strength and shear resistance of nanocomposites can be improved (Yu *et al.* 2019).

4. Challenges and Future Directions

- **Dispersion of Nanoparticles:** Achieving a uniform dispersion of nanoparticles within the matrix is a key challenge that affects the properties of the composite (Champa-Bujaico *et al.* 2022).
- **Scaling:** Developing cost-effective methods for large-scale production of nanocomposites with optimized properties.
- **Modeling:** Developing models that accurately predict the behavior of nanocomposites under different loading conditions and environmental factors (Wang *et al.* 2018).
- **Multifunctionality:** Designing nanocomposites with multiple functionalities, such as damping, conductivity, and strength (Formica *et al.* 2018; Champa-Bujaico *et al.* 2022).
- **Integration of AI:** Using machine learning and artificial intelligence techniques to accelerate the design and optimization process of nanocomposites (Yu *et al.* 2019; Champa-Bujaico *et al.* 2022).

5. Conclusions

The optimization of nanocomposites is a complex but crucial field that has the potential to bring significant improvements in various engineering applications. By combining experimental research, computer simulations, and optimization techniques, it is possible to create nanocomposites with enhanced properties and functionality. Further research and development in this area are essential for expanding the application of nanocomposites across various industries.

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Notations list

Notation	Meaning
Y	output vector in ANN model
A	activation function (sigmoid, tanh, softmax, softplus etc.) in ANN model
x	input vector in ANN model
W	matrix that contains the synaptic weights in ANN model

B_i	column vector of biases from the input layer to the hidden layer in ANN model
B_0	column vector of biases from the hidden layer to the output layer in ANN model
F	scaling factor in DE algorithm
x_{r1}, x_{r2} and x_{r3}	randomly selected individuals in DE algorithm
v_i	differential mutation operator in DE algorithm
L	quality loss in Taguchi method (eq. 3)
k	constant based on cost in Taguchi method (eq. 3)
y	actual performance value in Taguchi method (eq. 3)
T	target value in Taguchi method (eq. 3)
S/N	Signal-to-Noise (S/N) Ratio in Taguchi method (eqs. 4, 5, 6)
u	observed response in Taguchi method (eqs. 4, 5, 6)
n	number of experiments in Taguchi method (eqs. 4, 5, 6)
$\bar{u}$	mean response in Taguchi method (eqs. 4, 5, 6)
s	standard deviation in Taguchi method (eqs. 4, 5, 6)

Chapter 6. Optimal safety intervals for geometry and loads in polymer nanocomposites by multi-parameter optimization

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Annotation

In this chapter, the optimization problem for finding the optimal design (geometrical dimensions) and the optimal loading (mechanical and thermo-mechanical) for layered nanocomposite structures without delamination in them, is defined and solved. The optimization problem is multi-parametric (MOP) with single objective function; the nanocomposite geometry (length and layers' thicknesses) and the magnitude of static loading (mechanical or/and thermal difference) are considered as parameters and through MOP they vary in preliminary fixed technological limits. All material properties in the nanocomposite remain fixed constants. As an objective function (OF) in the MOP the analytical model criterion for "no delamination" in the nanocomposite is used (for definition of criteria see Chapter 1 and 2 of this book). The OF is a function of the nanocomposite materials' properties and of the abovementioned parameters. The implementation of MOP is done by authors' developed programs, using metaheuristic Genetic Algorithm in Mathcad and in some cases, by alternative deterministic algorithm in Mathematica. The developed MOPs are applied successfully on distinct nanocomposites structures, studied in Chapters 1 and 2: graphene/SU-8/PMMA, graphene/MoS₂/PET, WS₂/SU-8/PMMA, Mxene/PMMA, and hBN/PMMA. The applied optimal values (or intervals of values) for the parameters are obtained for all considered case studies. It is checked that at these optimal values, the model interfacial shear stress (ISS) maximal value does not exceed the ultimate shear stress (USS) in the interfacial layer. The obtained results were also compared (where it is possible) with the available literature data for the optimal values for some of the parameters in the considered case studies.

1. Introduction

Generally, the optimal design of polymer nanocomposites involves the even distribution of the individual nanoparticles within a polymer matrix. Achieving a uniform dispersion of the nanoparticles is a critical factor in unlocking the full potential for property enhancement (Müller *et al.*, 2017; Bitinis *et al.*, 2011). A well-dispersed nanofiller leads to a larger interface between the nanomaterial and the polymer chains, which can result in better properties compared to traditional polymer composites containing macro- or micro-fillers. The reinforcing effect of the nanofiller depends on various factors, such as the type of nanofiller, its concentration, the aspect ratio, geometry, size, orientation, and distribution (Luceño-Sánchez *et al.*, 2021; Díez-Pascual, 2019). The interphase region (between the nanofiller and the polymer matrix) also plays a crucial role in determining the overall properties of the nanocomposite, as it influences the interaction between the filler material and the surrounding polymer matrix. Its characteristics, including its composition, thickness, and structure, are critical to enhancing the performance of nanocomposites. In the polymer nanocomposites, the selection of the appropriate polymer matrix/substrate material is also important - its geometry and properties are decisive, especially in the case of influence of external temperature, humidity or external loadings (static or cyclic) on the nanocomposite structure.

In other words, the optimization of nanocomposite structures involves several key parameters (as the above-mentioned ones) that must be carefully considered to achieve the desired mechanical, thermal, and chemical properties of NCs. These parameters influence the overall performance, durability and applicability of the NC structures in the industry. The key parameters for the optimization of nanocomposite structures could be classified as: 1) *Nanocomposite geometry and its structural characteristics* (Size and type of the nanofiller, Aspect ratio, Shape and Morphology, Surface energy and roughness, Functional groups, Crystallinity and Structure, Dispersion and Distribution, etc.); 2) *Loading and environmental conditions for the NC* (type, magnitude, and direction of applied forces to NC, environmental factors such as temperature, humidity, and exposure to chemicals). There are many studies concerned with optimization in composites and old type NC as carbon nano-tubes reinforcement, but rare ones for nanocomposites, which consist of 2D nano flakes (see reviewed literature in Chapters 1, 2 and 5). There are published data from single (parametric) optimizations as 1 or 2 parameters for NC structures – for example, for optimal NC length (Xu *et al.* 2016; Wang, 2017; Wang, 2021;

Gong, 2012), for the optimal thickness of nanomaterial or that of the interfacial layer (Wang *et al.* 2020; Lui *et al.* (2022), Becker *et al.* 2023) and how this affects the important NC characteristics and behaviour. In our previous works the parametric analyses have been performed for various 2D NC structures: graphene-polymer and heterostructures NCs (Apostolov *et al.* 2022 and 2024); WS₂-polymer NC (Kirilova *et al.* 2023); few-layers graphene-polymer and MoS₂-polymer NC at thermo-mechanical load (Vladova *et al.* 2022 and 2025). They show the influence of the layers' thicknesses and that of the applied loads on the delamination in the considered NCs.

So far, apart from our recent works (Petrova *et al.* (2024); Boyadjiev *et al.* (2024) and Kirilova *et al.* (2025)), no optimization problem has been considered for **simultaneously** varying all parameters and finding their optimal values according to a given criterion (objective function) for NC structures. This is the main originality and contribution of the studies presented here below to the optimization in NC structures.

2. Model and model criteria used in optimization

The formulation and derivation of analytical model solutions for stresses (and strains) in a 3-layer nanocomposite structure (Fig. 1) by 2D stress-function variational method were already described in detail in our previous works (Kirilova *et al.* (2019) and Petrova *et al.* (2022)). Here only the most important formulas will be given, in relation with the model criteria, used in MOP.

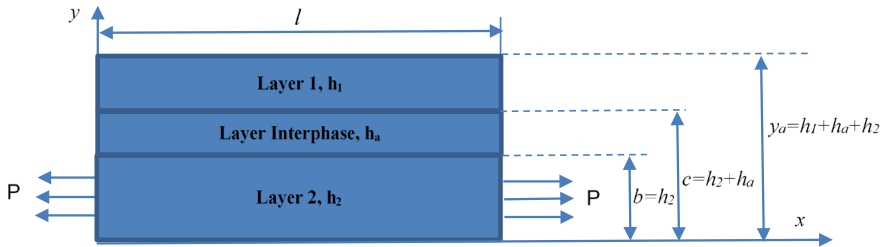


Figure 1: Representative volume element (RVE) for three-layer nanocomposite structure, where: h_1 , m – nanomaterial layer; h_a , m – interfacial layer or adhesive layer; h_2 , m – substrate layer, P , N/m – static tension force ($\sigma_0 = P/h_2$).

As was described in Chapter 1, the 2D stress-function variational method allows to obtain analytical solutions of a fourth-order ordinary differential inhomogeneous equation with constant coefficients, concerning the unknown axial stress function σ_1 in the first layer. Two types of analytical solutions (eqs. (1) and (2)) for the axial stress σ_1 in the first layer were derived, wherein the coefficients depend on the geometry of the three-layer nanocomposite, its material properties, and external loading.

$$\sigma_1(x) = C_1 \cdot \exp(\lambda_1 \cdot x) + C_2 \cdot \exp(\lambda_2 \cdot x) + C_3 \cdot \exp(\lambda_3 \cdot x) + C_4 \cdot \exp(\lambda_4 \cdot x) - A \quad (1)$$

$$\sigma_1(x) = \exp(-\alpha x)[M_1 \cos(\beta x) + M_2 \sin(\beta x)] + \exp(\alpha x)[(M_3 \cos(\beta x) + M_4 \sin(\beta x)) - A] \quad (2)$$

In Eq. (1) and (2), the constant A ($A = D_5/2D_1$) represents the solution for the inhomogeneous ordinary differential equation and is dependent on the external static load, while C_i, M_i are the integration constants in the model solutions, determined by the corresponding boundary conditions. All other stresses, including the interfacial shear stress, are expressed by Eqs. (1) or (2) and their derivatives. Eq. (2) represents the solution for the case of four complex roots $\pm (\alpha \pm i\beta)$, whereas Eq. (1) corresponds to the scenario of four real roots λ_i . The nature of the roots depends on the chosen layers' thicknesses and length of the nanocomposite structure, see Petrova (2023). The model criterion for no interfacial delamination in the nanostructure, at known value for the ultimate shear stress (USS) of the interfacial layer, is as follows:

$$ISS = \sigma_{xy}^{(a)}(x) = h_1 \sigma_1' \leq \sigma_{USS}^{(a)} \quad (3)$$

If the ultimate shear stress is exceeded, graphically the delamination initiates at both ends of the structure, representing the intersection of the ISS model curve with the straight horizontal line corresponding to the USS.

3. Multi-parameter optimization problems formulation

To find the optimal safety intervals for the geometry of the nanocomposite structure and the applied load without delamination, multi-parameter optimization problems are formulated and solved for both types of ISS model solutions, featuring real and complex roots. These formulations define the relevant decision variables, constraints, and objective functions.

Decision variables

All geometric characteristics of the considered nanostructure, including layer (h_1, h_a, h_2) thicknesses and the length of the structure (l), as well as the external load ($\sigma_0, \Delta T$), affect a potential delamination. That's why all these factors are chosen as decision variables.

Constraints

The MOP includes constraints on the bounds of variation of the decision variables, as well as a constraint that tracks whether the ISS reaches the ultimate shear stress (Eq. 3).

Objective function

The objective of the optimization for both types of model solutions for ISS, with real and complex roots, is to find the optimal values of all 5 (6 for the case of thermo-mechanical loading) decision variables at which the minimal difference between ISS and USS is obtained. With the latter in mind, the objective function represents the minimization of the difference between ISS and USS (eq. (3)).

4. Optimization methods

For solution of formulated multi-parameter optimization problems (MOPs) with both types of analytical solutions for ISS with real and complex roots, two approaches have been applied. The first one is called BASIC genetic algorithm (GA) (see Shopova and Vaklieva-Bancheva (2006)) and was implemented in Mathcad Prime v.6.0 (mainly for Eq. (2)). The second one represents a deterministic optimization procedure developed by “Wolfram Mathematica 13.0.1” software (for Eq.(1)). BASIC GA operates on foundational principles common to all genetic algorithms. It includes various types of schemes for the genetic operators for selection, crossover, and mutation, providing users with the flexibility to choose among them to address a specific optimization problem. Additionally, it can be adjusted for the concrete problem by tuning its global and local parameters. The first ones are: the number of generations (iterations); the number of samples selected for the process of recombination (crossover), the probabilities for crossover and mutation. The local parameters are related with the different schemes of the genetic operators.

For the nanocomposite structures, the objective of GA MOP is to simultaneously determine the optimal values of the decision variables (length l , layer thicknesses h_1, h_a, h_2 , and of the external loads as $\sigma_0, \Delta T$), at which the objective function has a minimum value (Fig.2a). The decision variables vary within predefined technological boundaries (see *Table 2*).

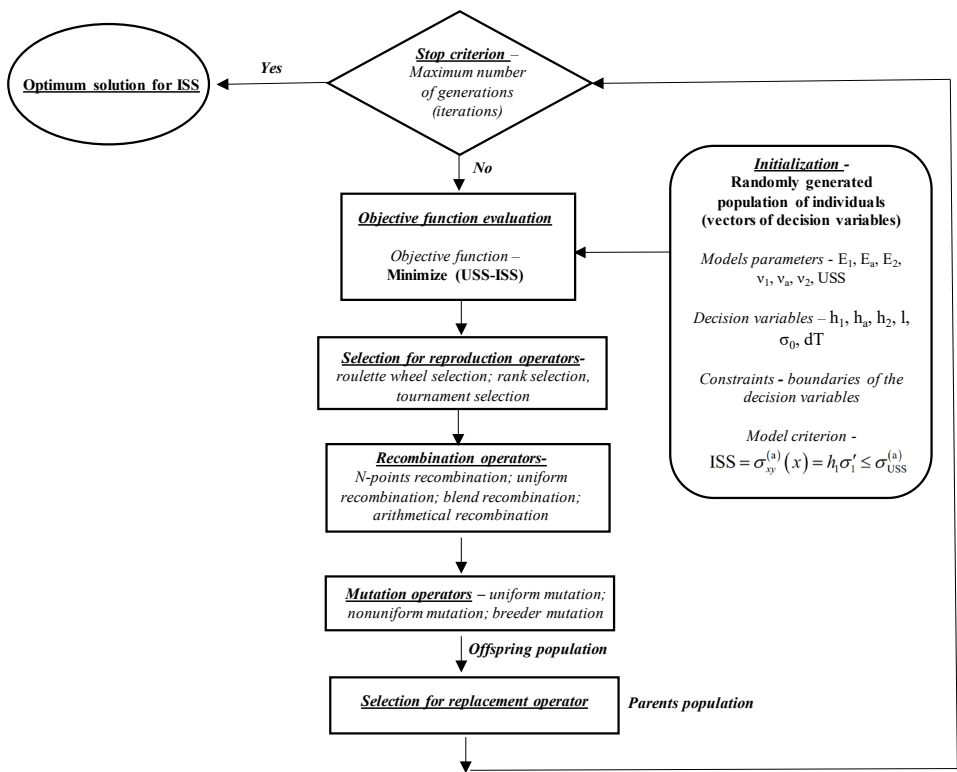


Figure 2a: Scheme of GA optimization MOP in the case of thermo-mechanical loading.

The other optimization method represents a procedure developed using the software package “Mathematica” (Figs 2b and 2c). In this procedure, different sets of geometry (and the temperature difference for the case of thermo-mechanical loading) are included in the optimization loop for the interval of values for external load, checking whether the objective function (Eq. (3)) is satisfied or not at the solutions obtained, e.g., to ensure, that delamination does not occur. In Figure 2b the scheme of this algorithm is shown, and the

other algorithm for checking the model assumption for the interfacial layer can be seen in Figure 2c.

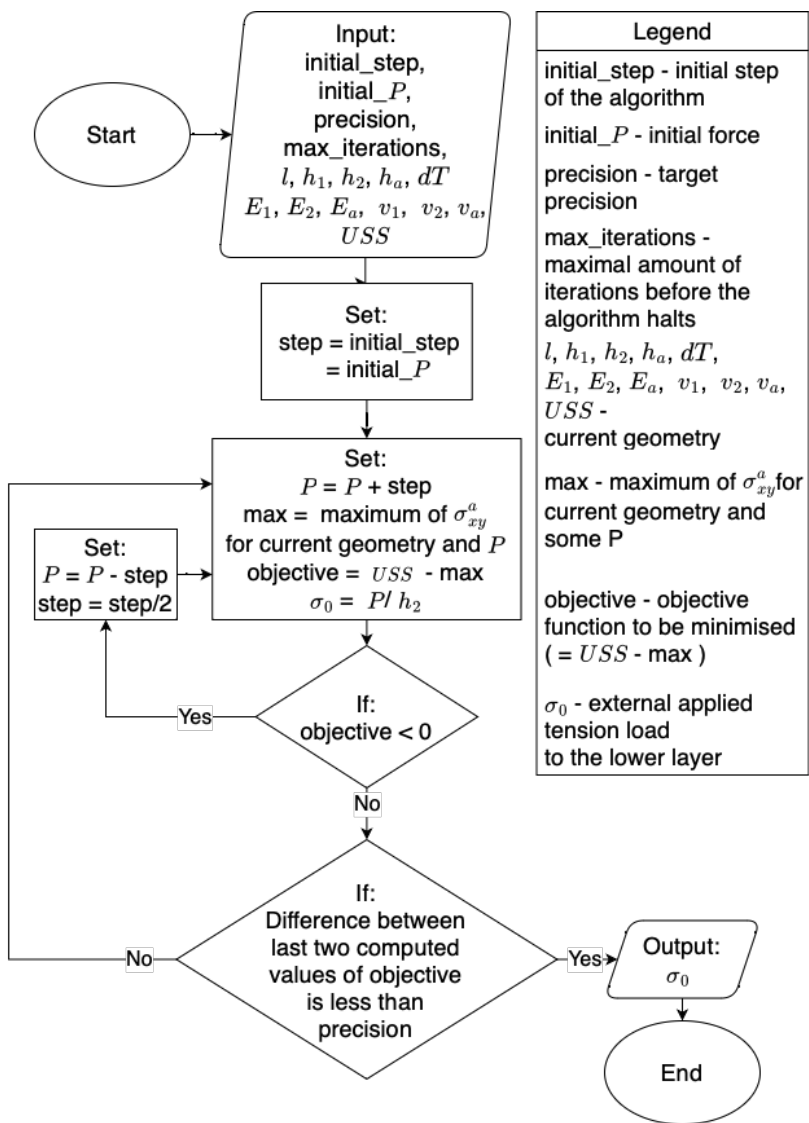


Figure 2b: Scheme of optimization algorithm to find maximum possible σ_0 for a particular geometry /and ΔT in the case of thermo-mechanical loading.

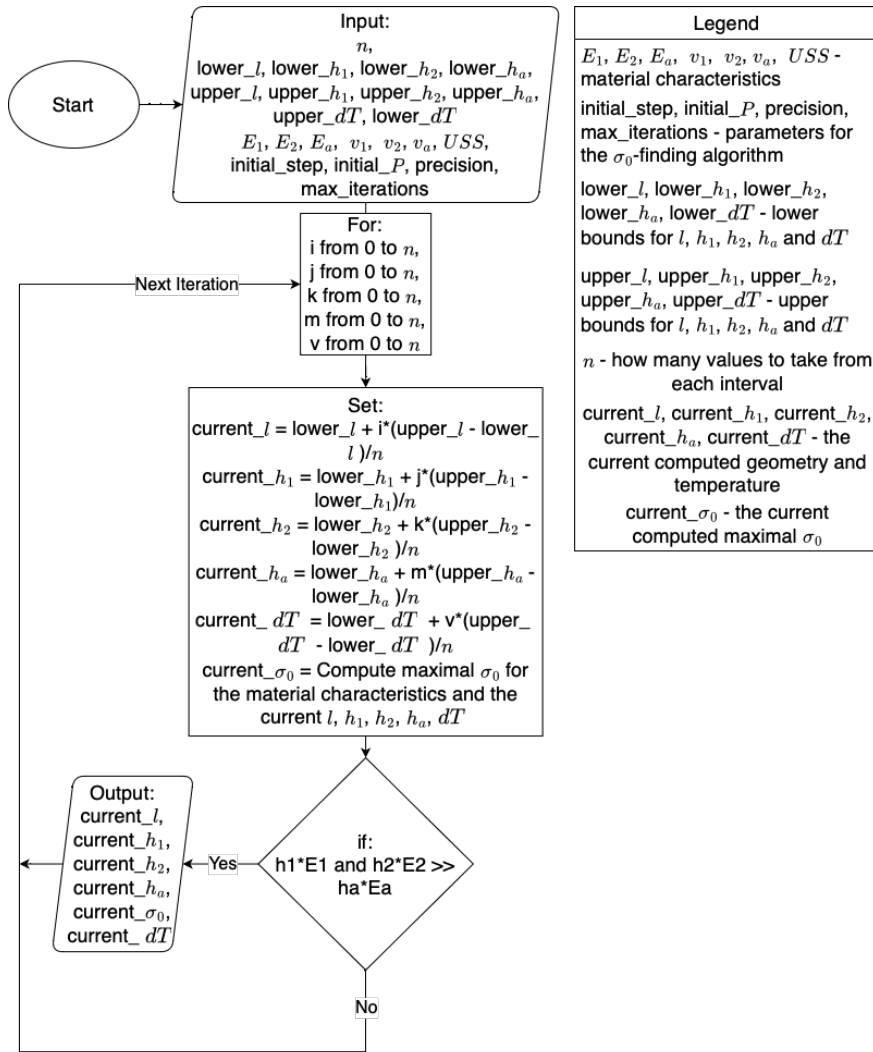


Figure 2c: Scheme of optimization algorithm to find maximum possible σ_0 for a particular geometry /and ΔT in the case of thermo-mechanical loading.

5. Results and discussion

Five nanocomposite structures are considered for testing the proposed MOP procedures: hBN/Interfacial layer/PMMA, WS₂/SU-8/PMMA, graphene/MoS₂/PET, graphene/SU-8/PMMA and Ti₃C₂ Mxene/Interfacial

layer/PMMA. For the first four NCs, MOPs are tested to find the optimal geometry and optimal mechanical load (5 decision variables), for the last two nanostructures – for 6 decision variables taking into account the temperature difference, too. The material properties of the considered nanocomposite structures as Young’s modulus E , (Pa) and Poisson’s ratio, ν , (-) are taken from the literature (Gong, 2012; Wang, 2021; Wang *et al.* 2020; Du *et al.* 2022; Lui *et al.* 2022) and are shown in *Table 1*.

Table 1: Input data for MOPs

Material	Young’s modulus, GPa	Poisson’s ratio, -
Graphene	1000	0.13
MoS ₂	270	0.25
PET	2.3	0.43
hBN	600	0.21
Interfacial layer for hBN/PMMA	3.5	0.25
PMMA	3.5	0.35
WS ₂	270	0.22
SU-8	2	0.22
Ti ₃ C ₂ Mxene	300	0.23
Interfacial layer for Mxene/PMMA	3.5	0.29

In addition, the lower and upper boundaries, between which all decision variables have been defined to vary during the MOP implementation, are shown in *Table 2*.

Table 2: Lower and upper boundaries for varying the decision variables for mechanical loading.

Model solution	σ_0 , (Pa)	l , (m)	h_1 , (m)	h_a , (m)	h_2 , (m)
Eq. (1)	$1.10^5 \div 1.10^7$	$1.10^{-5} \div 1.10^{-4}$	$0.3.10^{-9} \div 8.10^{-9}$	$1.10^{-9} \div 1.10^{-7}$	$1.10^{-7} \div 1.10^{-3}$
Eq. (2)	$1.10^5 \div 1.10^{10}$	$1.10^{-5} \div 1.10^{-4}$	$0.3.10^{-9} \div 5.10^{-9}$	$1.10^{-9} \div 1.10^{-7}$	$1.10^{-7} \div 1.10^{-3}$

For two of the case NCs structures the adhesive layer is a SU-8 glue, which plays the role of the interfacial layer with $U_{SS} = 30$ MPa. It should be borne in mind that the adhesive properties, especially the critical value of its

interfacial shear stress (USS), play an important role in the delamination of nanostructures. For the NC structures hBN/Interfacial layer/PMMA and Ti_3C_2 Mxene /Interfacial layer/PMMA, the USS and the properties of the interfacial layer are determined according to the approach used in Becker *et al.* (2023) for nano-clay NCs and proposed first by Zhu and Narh (2004) (see Chapter 1). For the interfacial layer in hBN/PMMA and in graphene/MoS₂/PET the value of USS is taken as 0.26 MPa and for the interfacial layer in Mxene/PMMA it is fixed as 55 MPa.

Results from MOPs for hBN/Interfacial layer/PMMA

In *Table 3* the obtained results from the performed GA MOP (OF is ISS for complex roots) can be seen for hBN/Interfacial layer/PMMA. For the case of real roots for the ISS the alternative Mathematica optimization procedure was developed and solved with the same optimization criterion Eq. (3). The results from Mathematica for hBN/Interfacial layer/PMMA (OF is ISS for real roots) are presented in *Table 4*. For convenience, the following abbreviations will be used in the text below: complex roots (CR) and real roots (RR). The graphical representation of the obtained optimal values for the involved parameters is shown in Figure 3.

Table 3: Optimal values of control variables from GA for hBN/Interfacial layer/PMMA (complex roots)

Sol. No.	Optimal load σ_0 , (Pa)	Optimal length l , (m)	Optimal h_1 , (m)	Optimal h_a , (m)	Optimal h_2 , (m)	Methods and schemes used in GA*
1	5.52e+09	2.42e-05	2.83e-09	3.31e-08	6.61e-04	TS, AC, NM
2	4.92e+09	2.73e-05	1.95e-09	9.15e-09	7.17e-04	TS, AC, NM
3	4.55e+09	2.13e-05	4.10e-09	1.51e-09	5.44e-04	TS, AC, NM
4	1.73e+09	2.55e-05	1.69e-09	3.17e-08	4.71e-04	RS, AC, NM
5	1.73e+09	2.55e-05	1.69e-09	3.17e-08	4.71e-04	RS, AC, UM
6	3.20e+08	8.31e-05	2.80e-09	4.40e-09	8.62e-04	RWS, TPC, NM

7	3.30e+08	8.31e-05	1.46e-09	3.51e-09	8.62e-04	RWS, UC, BMD
8	3.25e+08	8.31e-05	1.46e-09	4.16e-09	8.57e-04	RWS, BC, PBMD
9	5.57e+09	2.25e-05	5.00e-09	1.00e-09	6.14e-04	RWS, OPC, NM
10	3.29e+08	8.31e-05	1.46e-09	4.27e-09	8.61e-04	RWS, UC, PBMD
11	2.07e+09	3.18e-05	5.57e-10	9.66e-08	7.87e-04	RWS, UC, PBMD
12	1.60e+09	2.04e-05	3.03e-09	3.18e-08	4.22e-04	RWS, UC, PBMD
13	1.71e+09	2.13e-05	1.54e-09	3.21e-08	4.32e-04	TS, AC, NM

* Tournament selection, Arithmetical crossover, Nonuniform mutation (TS, AC, NM);

Rank selection, Arithmetical crossover, Nonuniform mutation (RS, AC, NM);

Rank selection, Arithmetical crossover, Uniform mutation (RS, AC, UM);

Roulette wheel selection, Two-points crossover, Nonuniform mutation (RWS, TPC, NM);

Roulette wheel selection, Uniform crossover, Parameter based mutation Deb (RWS, UC, PBMD);

Roulette wheel selection, Blend crossover, Parameter based mutation Deb (RWS, BC, PBMD);

Roulette wheel selection, One-point crossover, Nonuniform (RWS, OPC, NM);

Roulette wheel selection, Uniform crossover, Parameter based mutation Deb (RWS, UC, PBMD).

Table 4: Optimal values of the parameters from Mathematica optimization procedure, for hBN/Interfacial layer/PMMA (real roots)

Solution** No.	M2	M6	M10	M14
Optimal load σ_0 , MPa	209	113	209	113
Optimal l , m	1e-05	1e-05	2e-05	2e-05
Optimal h_1 , m	3.5e-10	1e-09	3.5e-10	1e-09
Optimal h_a , m	1e-08	1e-08	1e-08	1e-08
Optimal h_2 , m	1e-06	1e-06	1e-06	1e-06

** to differentiate the solutions in the graphic results, these from Mathematica are noted with M

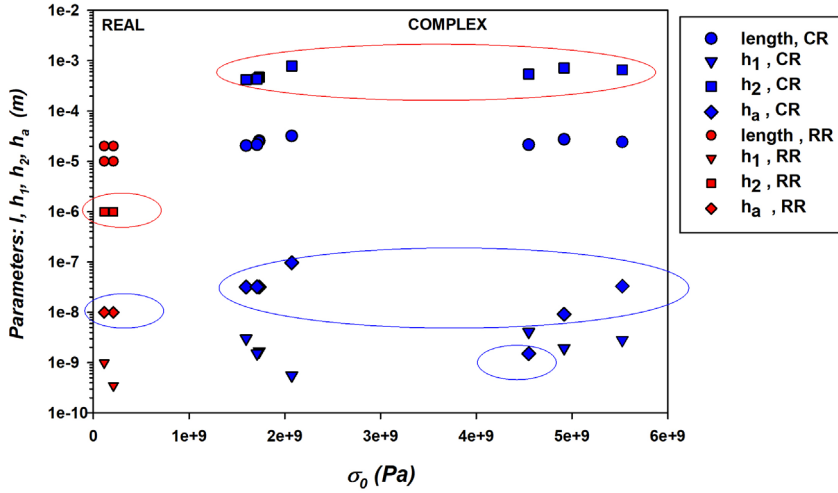


Figure 3: Optimal solutions for 5 decision variables from Mathcad and Mathematica optimization algorithms: CR (incrementing) and RR (cubic root), for hBN/Interfacial layer/PMMA.

It can be seen from Figure 3 that along the ordinate, each decision variable changes within certain boundaries (intervals) for each of the two types of solutions Eqs.(1) and (2) for the ISS included in the OF Eq. (3). The boundaries of the changes in the optimal thicknesses of PMMA h_2 and of the interfacial layer h_a for the cases of RR and CR roots are particularly well distinguished. The intervals of variation for h_1 and l are almost similar for both possible solutions (Eq. (1)) and (Eq. (2)). Along the abscissa, each different set of geometry data corresponds to a particular optimal mechanical load. Thus, for each combination of the five decision variables, the objective function is satisfied, or the predicted ISS model at those load values and geometry is equal to or below the USS value.

Validation of obtained optimal values of parameters for hBN/Interfacial layer/PMMA by ISS

In order to verify the obtained results for hBN/Interfacial layer/PMMA nanocomposite structure, in the following Figures 4 and Figures 5 the distributions of the model ISS $\sigma_{xy}^{(a)}(x) = h_1 \sigma_1'$ along the length x of the nanocomposite are presented, calculated for the optimal values of the parameters.

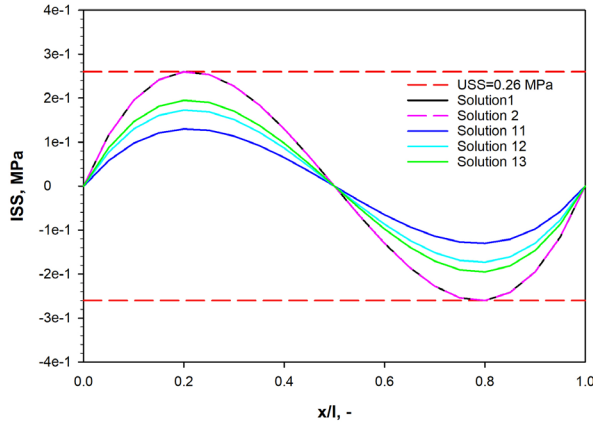


Figure 4: Model interfacial shear stress distribution calculated at the optimal values of parameters (complex roots) for hBN/Interfacial layer/PMMA.

As can be seen, for each type of solution, the maximal value of the model ISS actually meets the criterion Eq. (3) and does not exceed the USS value, i.e., there are no delaminations in hBN/Interfacial layer/PMMA. For the case of model ISS, calculated by Mathematica for RR (Figure 5), it is worth noting that these optimal values of parameters assure that $ISS \ll USS$, i.e., this optimal geometry and load assure more safety design in comparison with the case of ISS for CR (Figure 4).

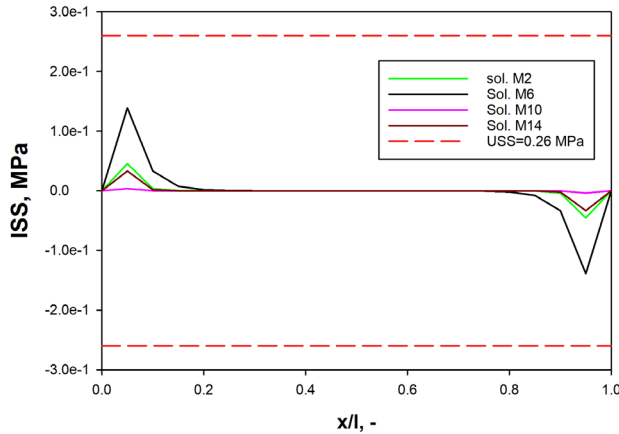


Figure 5: Model interfacial shear stress distribution calculated at the optimal values of parameters (real roots) for hBN/Interfacial layer/PMMA.

Up to now, no experimental ISS data for hBN/Interfacial layer/PMMA are found in the available literature in order to compare with our validation results

for ISS at optimal values of parameters (Figs. 4 and 5). The only data predictions for ISS in (50-layer hBN)/PMMA are available in Wang (2021): for applied external strains $0.1 \div 0.3 \%$, the prediction from shear-lag model ISS is $3.8 \div 9.4$ MPa. Our results for the maximal values of model ISSs calculated at the optimal parameters for both solutions are far from this range; one can be sure that at these optimal values of parameters no delamination will happens in the structure.

Other similar data found for the model ISS in the literature for other boron nitride forms and distinct substrates give even higher values. For example, for boron nitride nanotubes (BNNT)/PMMA interfacial layer it is found by Gou and Ke (2019) that the maximum interfacial shear strength (IFSS) predicted using the strain-hardening model and pull-out force is 71 ± 2 MPa; the prediction of the elastic model for the same is 236 ± 11 MPa. In the paper of Yi *et al.* (2019) on hBN/Si, the maximum IFSS is 1.25 GPa, unlike much lower values of IFSS for BNNT/epoxy – 323 MPa. Another important fact obtained by Yi *et al.* (2019) is that the thickness of the interfacial layer between hBN/Si is 8.1 nm, which is very close to the value in Gou and Ke (8.05 nm) for BNNT/PMMA. Yi *et al.* (2019) for an interfacial layer thickness between hBN/epoxy of 0.06 nm an IFSS of 9.5 MPa have obtained also for the interfacial layer thickness between hBN/epoxy to be $0.6 \text{ \AA}$ (0.06 nm) and IFSS 9.5 MPa. As is seen, the interfacial layer thickness and interfacial shear stress/strength depend on both layer materials and their properties, constituting the nanocomposite. Our common interval of obtained optimal values for the thickness of the interfacial layer h_a , for both cases of model ISS (real and complex), is $(1e-09 \div 9.6e-08 \text{ m})$; the respective values for h_a of Gou and Ke (2019) is in this interval.

Results from MOPs for graphene/MoS₂/PET

In the same way as in the previous case, the results for graphene/MoS₂/PET from the performed MOPs are obtained (*Table 5* (complex) and *Table 6* (real roots)). The graphical representation of the optimal values of the five parameters from both MOPs are shown in Figure 6. Again, the intervals for h_2 and h_a are well distinguished for both types of solutions (CR and RR). For this NC structure, the real roots optimal solutions for the parameters appeared for lower loading in respect to those for hBN/PMMA.

Table 5: Obtained results from GA (complex roots) for graphene/MoS₂/PET.

Sol. No.	σ_0	l	h_1	h_a	h_2	GA methods*
1	2.84e+09	1.76e-05	2.14e-09	1.00e-09	3.85e-04	TS, AC, NM
2	3.60e+09	1.75e-05	3.05e-09	2.48e-09	4.15e-04	RWS, AC, NM
3	3.74e+09	1.73e-05	5.00e-09	1.00e-09	4.15e-04	RWS, TPC, NM
4	5.61e+09	3.17e-05	3.82e-09	3.09e-09	8.70e-04	TS, BC, NM
5	1.53e+09	1.87e-05	1.06e-09	3.61e-09	3.32e-04	RS, BC, NM
6	5.78e+09	3.18e-05	4.49e-09	1.42e-09	8.81e-04	TS, OPC, NM
8	2.77e+08	7.49e-05	5.00e-09	6.83e-10	9.45e-04	TS, AC, NM
9	5.86e+09	1.46e-05	4.81e-09	6.51e-10	4.64e-04	TS, AC, NM
10	4.70e+08	4.48e-05	5.00e-09	6.65e-10	5.89e-04	TS, AC, NM

* Tournament selection, Arithmetical crossover, Non-uniform mutation (TS, AC, NM);
Roulette wheel selection, Arithmetical crossover, Non-uniform mutation (RWS, AC, NM);
Roulette wheel selection, Two-points crossover, Non-uniform mutation (RWS, TPC, NM);
Tournament selection, Blend crossover, Non-uniform mutation (TS, BC, NM);
Rank selection, Blend crossover, Non-uniform mutation (RS, BC, NM);
Tournament selection, One-point crossover, Non-uniform mutation (TS, AC, NM).

Table 6: Optimal values of parameters from Mathematica optimization procedure for graphene/MoS₂/PET (real roots)

Solution* * No.	M2	M11	M12	M29	MLimit
Optimal load σ_0 , MPa	1	1	0.182	1	0.95
Optimal l , m	1e-05	1e-05	1e-05	1.5e-05	1e-05
Optimal h_1 , m	0.35e-09	0.675e-09	0.675e-09	0.35e-09	1e-09
Optimal h_a , m	1e-10	1e-10	1e-10	1e-10	1e-10
Optimal h_2 , m	1e-06	1e-06	5.5e-06	1e-06	1e-06

** to differentiate the solutions in graphic results, these from Mathematica are noted with M

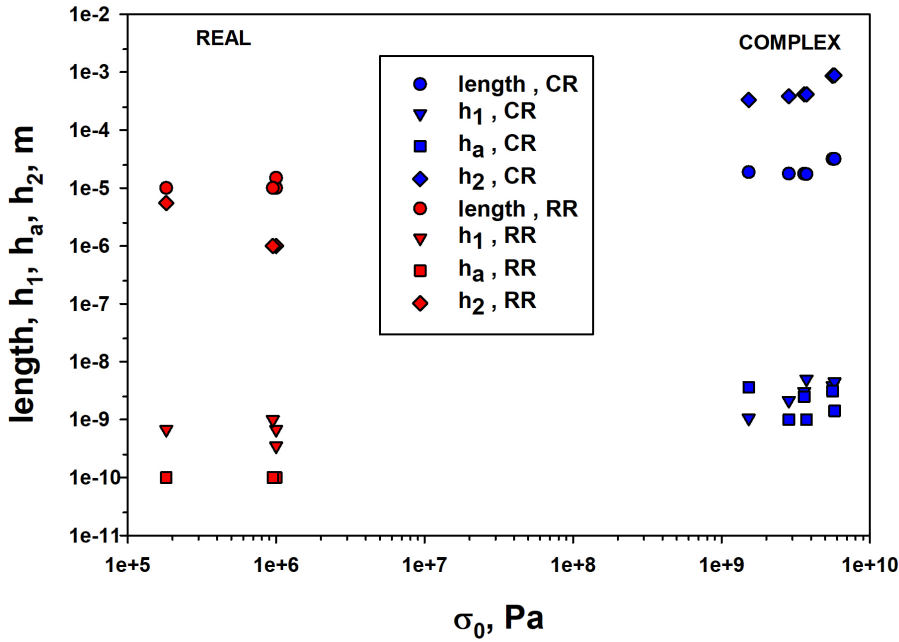


Figure 6: Optimal solutions for the 5 parameters from Mathcad and Mathematica MOPs for graphene/MoS₂/PET: complex (blue) and real roots (red).

Validation of obtained optimal values of parameters for graphene/MoS₂/PET by ISS

Similarly, to verify the obtained results for a graphene/MoS₂/PET nanocomposite structure, the Figure 7 and Figure 8 have been generated, in which the model ISS distributions along the length of the nanocomposite, obtained at the optimal parameter values, are calculated. Again, the ISS maximal value along its distribution on x does not exceed the USS. According to Du *et al.* (2022) the reported maximal value of interfacial shear stress (known as an interfacial shear strength) for graphene/MoS₂ interfacial layer is 0.19 MPa and that between MoS₂/PET is 0.34 MPa; both these values are predicted by their model. Also, Dong *et al.* (2023) fixed interfacial shear strength between MoS₂/PMMA as 0.26 MPa for applied external strains $0.4 \pm 0.7\%$.

The ISS result of Dong *et al.* (2023) is for a different substrate and is between the respective values obtained by Du *et al.* (2022). In Du *et al.* (2022) the ISS of two specimens are modeled: the first is MoS₂/PET and the second

is a heterostructure graphene/MoS₂/PET; the respective interfacial shear strengths are 0.34 and 0.48 MPa. All these data are larger than the maximal values of ISS obtained here, i.e., no delamination is observed. In Du *et al.* (2022) the debonding stages in both specimens are reached after 2% and 1.75% external deformation applied.

From the available literature, the value obtained by Yu *et al.* (2014) - (0.8e-09 m) for graphene/MoS₂/Si, is in the interval of the results for h_a obtained here, despite the different substrate used. Our interval of obtained optimal values for h_a is (1e-10 ÷ 3.6e-09 m) for the investigated nanostructure graphene/MoS₂/PET.

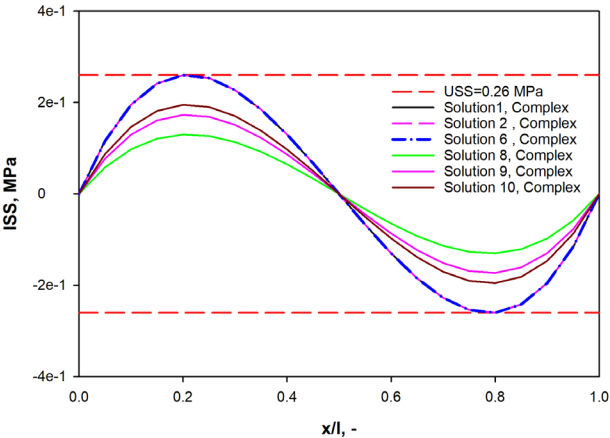


Figure 7: Model interfacial shear stress distribution calculated by the optimal values of parameters (complex roots) for a graphene/MoS₂/PET.

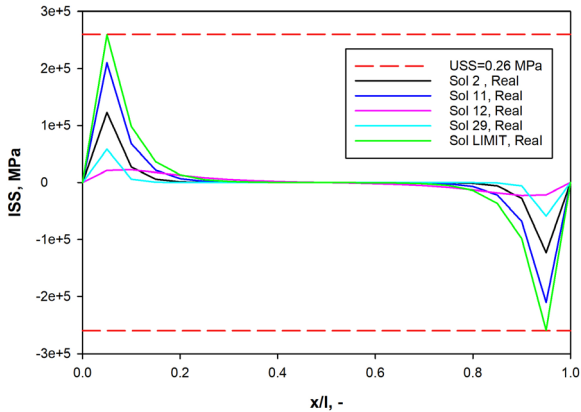


Figure 8: Model interfacial shear stress distribution calculated at the optimal values of parameters (real roots) for a graphene/MoS₂/PET.

Results from MOPs for WS₂/SU-8/PMMA

Following the previous sections, in Figure 9 for the cases of complex and real roots for ISS in Eq. (3), the obtained optimal values of the decision variables (external load, layer thicknesses, and the length of the overlap zone) are plotted (symbolically) for NC WS₂/SU-8/PMMA. In Table 7 the obtained solutions by both MOPs are presented. As it is well seen, two types of possible equations for the axial stress (CR and RR) for calculating the ISS in OF gave two separated groups of optimal values of parameters. This is a clear visible tendency in the graphical representation of the optimal solutions for all NC, investigated up to now and later. Also, it is revealed, that the obtained optimal loads σ_0 for RR OF are lower than those for CR OF. Practically, it means that the thinner design of the NC layers remains intact at lower loads; the opposite is true for the thicker design of NC layers – it withstands to delaminate for larger values of external loads (see for example, Solution C1 and Solution R1 in Table 7). This is a physically correct and expected result and shows the relationship between the optimal NC design, the optimal load which it can withstand without delamination and the type of ISS model solution (CR or RR). Later, this connection between load and geometry is better visible in the validation of the obtained optimal values of parameters by ISS distribution, calculated at these values.

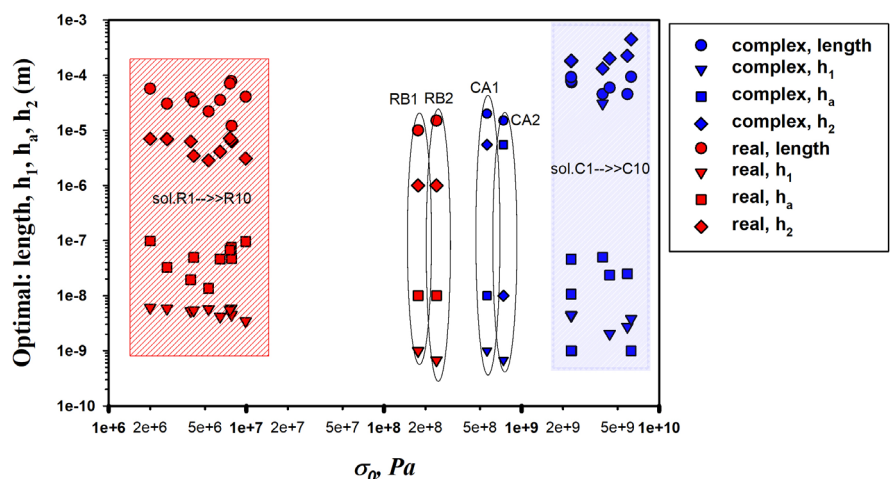


Figure 9: Optimal solutions for 5 decision variables from BASIC GA and Mathematica optimization algorithms: complex (blue) and real roots (red) of WS₂/SU-8/PMMA NC

Table 7: Obtained results for parameters from GA and deterministic* MOPs (complex and real roots) for WS₂/SU-8/PET.

Solution No., CR, Eq. (2)	Optimal length l, (m)	Optimal h_1, (m)	Optimal h_a, (m)	Optimal h_2, (m)	Optimal load σ_0, (Pa)
Solution C1	8.94e-05	4.45e-09	1.00e-09	1.84e-04	2.29e+09
Solution C2	9.23e-05	4.48e-09	1.00e-09	1.84e-04	2.29e+09
Solution C3	9.27e-05	4.49e-09	1.06e-08	1.84e-04	2.29e+09
Solution C4	7.43e-05	4.40e-09	1.00e-09	1.84e-04	2.31e+09
Solution C5	7.86e-05	4.32e-09	4.61e-08	1.80e-04	2.29e+09
Solution C6	4.54e-05	2.73e-09	2.50e-08	2.26e-04	5.88e+09
Solution C7	4.54e-05	3.06e-05	4.98e-08	1.33e-04	3.89e+09
Solution C8	5.94e-05	2.03e-09	2.36e-08	2.01e-04	4.37e+09
Solution C9	9.23e-05	4.48e-09	1.00e-09	1.84e-04	2.29e+09
Solution C10	9.35e-05	3.80e-09	1.00e-09	4.49e-04	6.25e+09
Solution CA1*	2.00e-5	1.00e-9	1.00e-8	5.50e-6	5.61e+8
Solution CA2*	1.50e-5	6.75e-10	1.00e-8	5.50e-6	7.39e+8
Solution No., RR, Eq. (1)	Optimal length l, (m)	Optimal h_1, (m)	Optimal h_a, (m)	Optimal h_2, (m)	Optimal load σ_0, (Pa)
Solution R1	5.70e-5	6.03e-9	9.77e-8	7.05e-6	1.99e+6
Solution R2	3.94e-5	5.25e-9	1.93e-8	6.30e-6	3.94e+6
Solution R3	3.04e-5	5.81e-9	3.26e-8	6.92e-6	2.64e+6
Solution R4	1.20e-5	4.52e-9	4.73e-8	6.34e-6	7.80e+6
Solution R5	3.32e-5	5.43e-9	4.92e-8	3.45e-6	4.13e+6
Solution R6	3.54e-5	4.18e-9	4.62e-8	4.11e-6	6.44e+6
Solution R7	4.05e-5	3.46e-9	9.61e-8	3.09e-6	9.88e+6
Solution R8	7.80e-5	5.89e-9	7.51e-8	6.67e-6	7.76e+6
Solution R9	7.10e-5	5.50e-9	6.67e-8	7.14e-6	7.59e+6
Solution R10	2.20e-5	5.70e-9	1.35e-8	2.86e-6	5.30e+6
Solution RB1*	1.00e-5	1.00e-9	1.00e-8	1.00e-6	1.77e+8
Solution RB2*	1.50e-5	6.75e-10	1.00e-8	1.00e-6	2.41e+8

*Notation for solutions, obtained by deterministic approach

During the optimization procedures, the decision variables varied in the following preliminary defined intervals. The lower and upper boundaries of all 5 decision variables are shown in *Table 8*.

Table 8: Lower and upper boundaries for varying the decision variables for WS₂/SU-8/PET.

Model solution	σ_0 , (Pa)	l , (m)	h_1 , (m)	h_a , (m)	h_2 , (m)
Eq. (1)	$1.10^5 \div 1.10^7$	$1.10^{-5} \div 1.10^{-4}$	$0.6.10^{-9} \div 8.10^{-9}$	$1.10^{-9} \div 1.10^{-7}$	$1.10^{-7} \div 1.10^{-3}$
Eq. (2)	$1.10^5 \div 1.10^{10}$	$1.10^{-5} \div 1.10^{-4}$	$0.6.10^{-9} \div 5.10^{-9}$	$1.10^{-9} \div 1.10^{-7}$	$1.10^{-7} \div 1.10^{-3}$

Validation of obtained optimal values of parameters for WS₂/SU-8/PMMA by ISS

Figure 10 and Figure 11 present a part of the ISS distributions along the length of the nanocomposite WS₂/SU-8/PMMA, obtained at the optimal values of the decision variables. It can be seen that for each type of solution, the optimal values of the decision variables satisfy the objective function in the considered nanocomposite structure. In the case of ISS calculated for real roots (Eq. (1)) (Fig. 10), it is notable that the solutions obtained with the BASIC GA (marked with numbers R7, R8, R9, and R10) for the geometry of the considered nanostructure and loads ensure an absolutely safe operation of the structure (far from USS=30 MPa). These solutions provide a significant difference between ISS and USS, with no observed delamination of the structure.

Conversely, solutions obtained with the other optimization procedure (marked as Sol RB1 and Sol RB2) provide a geometry and a mechanical loading where the ISS is closer to the USS, but still does not reach it. Fig. 11 shows solutions for the ISS calculated with complex roots (Eq. (2)). The majority of these solutions are obtained using BASIC GA (marked with numbers C1 to C10), while the remaining solutions are derived from the deterministic optimization procedure (marked as Sol CA1 and Sol CA2). It can be seen from Figure 11 that for most of solutions, a minimum difference between ISS and USS is reached. For sol. CA1 this difference is larger, but still fulfills the criterion eq. (3).

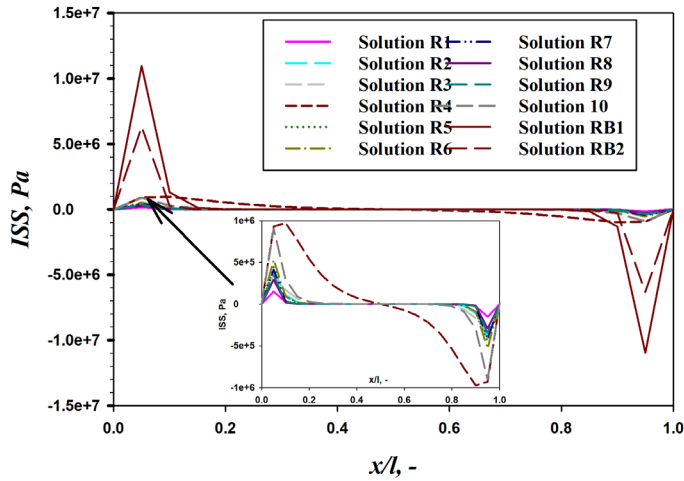


Figure 10: Model interfacial shear stress solutions obtained at the optimal values of decision variables. Case of model solution with real roots for NC WS₂/SU-8/PMMA.

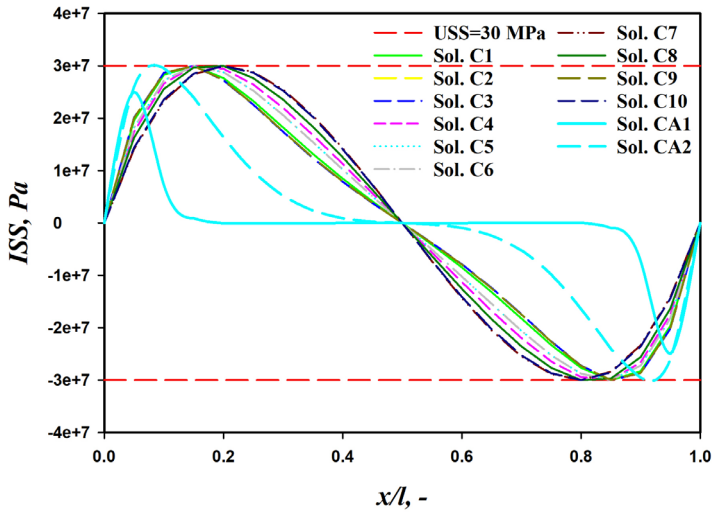


Figure 11: Model interfacial shear stress solutions obtained at the optimal values of decision variables. Case of model solution with complex roots for NC WS₂/SU-8/PMMA.

The only data to compare our results with respective ones in the literature, are Kim *et al.* (2014) for h_a and in Wang (2017) for l . In Kim *et al.*'s paper a fixed value of 0.5 nm for the interfacial layer thickness is used for a WS₂/PVA

nanocomposite to simulate its tensile modulus; at this value, their model described better the experimental data and this value is very close to the lowest boundary ($1\text{e-}09\text{ m}$) of the h_a 's optimal interval. Wang (2017) reported that “no reinforcement is expected for WS_2 flakes < 4 microns in diameter, some reinforcement is expected at > 4 microns and large WS_2 flakes ($\sim 40\text{ }\mu\text{m}$) are required for full reinforcement to take place” for $\text{WS}_2/\text{SU-8}/\text{PMMA}$. Our optimal intervals for both CR and RR cases for length l in $\text{WS}_2/\text{SU-8}/\text{PMMA}$, include Wang’s best value $40\text{ }\mu\text{m}$ (see *Table 7*).

Results for Mxene/Interfacial layer/PMMA and graphene/SU-8/PMMA (mechanical load)

The last two NC structures, optimized by MOPs for 5 parameters - mechanical load and geometry of NC, are Ti_3C_2 Mxene/Interfacial layer/PMMA and graphene/SU-8/PMMA. Here, $\text{USS}=55\text{ MPa}$ for the first and 30 MPa for the second one. The obtained optimal values of parameters from both MOPs for Mxene/Interfacial layer/PMMA and graphene/SU-8/PMMA, are presented in *Table 9* and *Table 10*, respectively.

The graphical representation of the optimal geometrical values distribution in respect to the optimal load for Mxene/Interfacial layer/PMMA is given in Fig. 12. Here, because of the limited number of geometry combinations tested in the deterministic MOP, the observed “separation” for the intervals of optimal values of h_a , h_2 obtained for CR and for RR is not seen, as for the previous NC structures.

Table 9: Obtained results for parameters from deterministic MOPs (complex and real roots) for Mxene/Interfacial layer/PMMA NC, deterministic MOP.

Solution	l , (m)	h_1 , (m)	h_a , (m)	h_2 , (m)	σ_0 , (Pa)
sol.38, RR	1.67e-05	5.67e-10	1.00e-09	1.00e-06	4.17e+08
sol.14, RR	1.00e-05	1.00e-09	1.00e-09	1.00e-06	2.89e+08
sol.30, RR	1.33e-05	1.00e-09	1.00e-09	1.00e-06	2.89e+08
sol.46, RR	1.67e-05	1.00e-09	1.00e-09	1.00e-06	2.89e+08
sol.54, RR	2.00e-05	5.67e-10	1.00e-09	1.00e-06	4.17e+08
sol.6, RR	1.00e-05	5.67e-10	1.00e-09	1.00e-06	4.17e+08
sol.10, RR	1.00e-05	7.83e-10	1.00e-09	1.00e-06	3.37e+08
sol.65, RR	1.33e-05	5.67e-10	1.00e-09	1.00e-06	3.85e+08
sol.43, RR	1.00e-05	1.00e-09	1.40e-08	6.67e-07	1.94e+08

sol.180 , RR	2.00e-05	7.83e-10	2.70e-08	8.33e-07	3.08e+08
sol. 2, CR	1.00e-05	3.50e-10	1.00e-09	1.00e-06	5.77e+08
sol. 18, CR	1.33e-05	3.50e-10	1.00e-09	1.00e-06	5.77e+08
sol.34, CR	1.67e-05	3.50e-10	1.00e-09	1.00e-06	5.13e+08
LIMIT, CR	2.00e-05	7.83e-10	1.00e-09	2.00e-05	2.70e+09
sol.39, CR	1.67e-05	5.67e-10	3.40e-08	1.00e-06	4.23e+09
sol.51, CR	1.33e-05	3.50e-10	1.00e-09	6.67e-07	3.86e+08
sol.156, CR	2.00e-05	3.50e-10	2.70e-08	8.33e-07	4.62e+08
sol.121, CR	1.67e-05	5.67e-10	2.70e-08	1.00e-06	3.85e+08
sol.3, CR	1.00e-05	3.50e-10	1.00e-09	6.67e-07	3.86e+08
sol.3m, CR	1.00e-05	3.50e-10	1.00e-09	6.67e-07	5.80e+08

Table 10: Obtained results for parameters from deterministic MOPs (complex and real roots) for graphene/SU-8/PMMA NC, by both MOPs.

Solution No., type	l , (m)	h_1 , (m)	h_a ,(m)	h_2 ,(m)	σ_0 , (Pa)
Sol. 57, CR	1.00e-05	1.00e-09	4.00e-08	1.00e-04	1.48e+08
Sol. 165, CR	1.67e-05	7.83e-10	1.00e-08	1.00e-04	2.5e+06
Sol. 129, CR	1.33e-05	1.00e-09	1.00e-07	1.00e-04	1.41e+10
Sol. 3, CR	1.00e-05	3.50e-10	1.00e-08	3.46e-05	2.88e+05
Sol. 4, CR	1.00e-05	3.50e-10	1.00e-08	6.73e-05	1.48e+05
Sol. 5, CR	1.00e-05	3.50e-10	1.00e-08	1.00e-04	1.00e+05
Sol. 7, CR	1.00e-05	3.50e-10	4.00e-08	3.46e-05	4.74e+08
Sol. 8, CR	1.00e-05	3.50e-10	4.00e-08	6.73e-05	2.46e+08
Sol. 1-GA, CR	9.50e-05	1.97e-09	1.34e-08	3.81e-04	3.60e+09
Sol. 2-GA, CR	9.21e-05	4.00e-09	7.86e-08	5.43e-04	7.46e+09
Sol. 3- GA, CR	9.46e-05	2.24e-09	1.00e-09	5.30e-04	7.04e+09
Sol. 4- GA, CR	9.76e-05	3.20e-09	2.69e-09	6.19e-04	9.28e+09
Sol. 5- GA, CR	8.84e-05	1.11e-09	3.30e-08	3.45e-04	4.27e+09
Sol. 6- GA, CR	6.88e-05	1.89e-09	2.80e-09	3.86e-04	6.92e+09
Sol. 7- GA, CR	7.77e-05	4.61e-09	4.61e-08	4.26e-04	6.00e+09
Sol. 2, RR	1.00e-05	3.50e-10	1.00e-08	2.00e-06	5.00e+06
Sol. 50, RR	1.00e-05	1.00e-09	1.00e-08	2.00e-06	5.00e+06
Sol. 66, RR	1.33e-05	3.50e-10	1.00e-08	2.00e-06	1.89e+08
Sol. 130, RR	1.67e-05	3.50e-10	1.00e-08	2.00e-06	1.89e+08
Sol. 194, RR	2.00e-05	3.50e-10	1.00e-08	2.00e-06	1.89e+08
Sol. 242, RR	2.00e-05	1.00e-09	1.00e-08	2.00e-06	1.01e+08

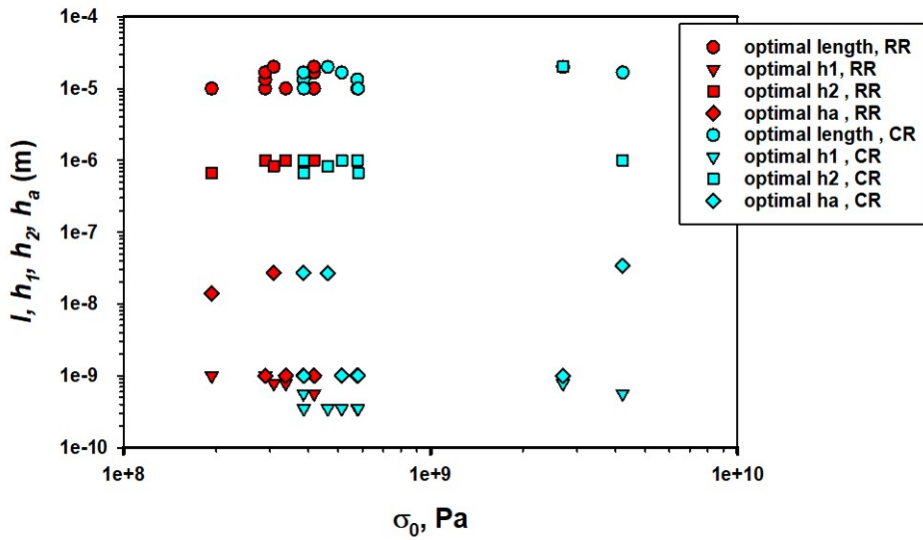


Figure 12: Optimal solutions for both complex and real roots complex (blue) and real roots (red) for a Ti_3C_2 Mxene/PMMA nanocomposite structure.

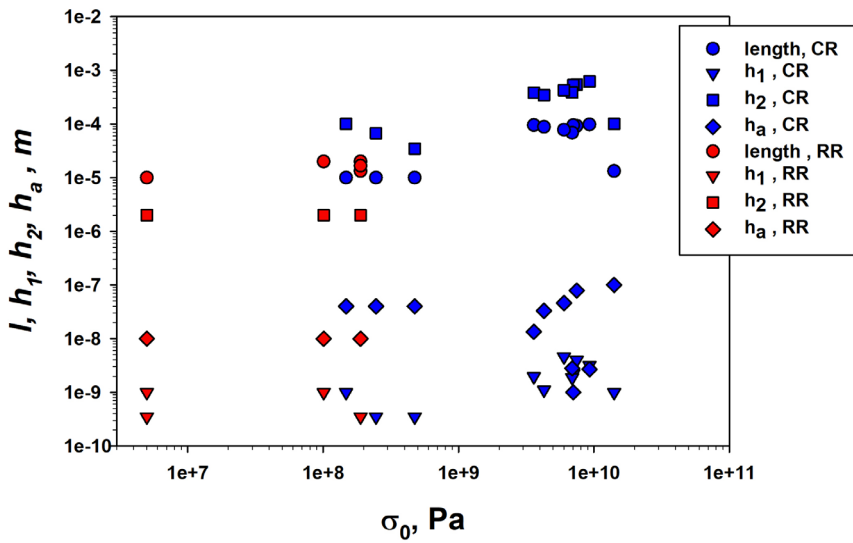


Figure 13: Optimal solutions for both complex and real roots complex (blue) and real roots (red) for a graphene/SU-8/PMMA nanocomposite structure.

The graphical visualization for the obtained optimal parameters for graphene/SU-8/PMMA NC is presented in Fig.13, where the well distinguished intervals for h_a , h_2 obtained for CR and for RR are visible.

Validation of the obtained optimal values of parameters for Ti_3C_2 Mxene/Interfacial layer/PMMA and graphene/SU-8/PMMA by ISS (mechanical load)

As in the previous cases, it is checked that the distribution over x of the model ISS solutions for CR and RR, calculated for optimal values of the parameters for both NC structures, does not exceed their USSs (Figs. 14-17). For brevity, only parts of the results from *Tables 9* and *10* are visualized here, but all data for ISSs were checked and found to fulfill Eq. (3). In our results, the USS value is set equal to the UTS of PMMA for Mxene/Interfacial layer/PMMA, because in the literature other values for the USS of the interfacial layer between Mxene and PMMA were not found.

The only available literature results for ISS in Mxene/PMMA NC are found in Liu *et al.* (2022); the maximal ISS values predicted by shear-lag analysis at 0.2 and 0.4% external strain are 2.0 and 4.0 MPa, respectively, for Mxene flake 8 μm in length and 1 nm thick. It has to be noted, that shear-lag analysis considers the interface as a material line, not like a layer. According to the shear-lag prediction of ISS, its value (likewise the quality of stress transfer) depends on the shear-lag parameter ns , in which the aspect ratio ($s=\text{length}/\text{thickness}$) reflects the geometrical dimensions of the nanoflake.

The shear-lag parameter $n = \sqrt{\frac{G_m}{E_{nano}} \left(\frac{t}{T} \right)}$ (see Chapter 1) depends on the shear

modulus and the thickness of the substrate and on the effective modulus and thickness of the MXene flake. Liu *et al.* (2022) reported that an effective aspect ratio of the order of >500 is expected to facilitate good interfacial stress transfer and therefore gives the highest effective modulus when used to reinforce polymers. This aspect ratio is currently achievable in $1\div 10$ layer MXene flakes; the aspect ratio for the above mentioned Mxene flake is $2666 \gg 500$. If someone calculates the aspect ratio according to our optimal results for l and h_1 , it is easy to see, that our aspect ratios are much larger than 500, i.e., they will assure good interfacial stress transfer.

About the comparison of the obtained optimal values for the parameters, the available data in the literature are used to compare and discuss our results. For the first NC structure, Mxene/Interfacial layer/PMMA, Liu *et*

al. (2022) reported, that: "...Ti₃C₂ MXene is able to offer an efficient mechanical reinforcement to a polymer matrix with a flake length of >10 μm and a thickness of 10s of nanometers." Our obtained interval for the optimal values of l in Table 9 are in the range ($1\text{e-}05 \div 2\text{e-}05$ m), which is in coincidence with Liu *et al.* (2022). The optimal values from MOPs for h_1 varied from 0.35 nm to 1 nm (Table 9), which is less than the values of the flake thicknesses, obtained in Liu *et al.* (2022); they are in the range about from 3 to 40 nm. On the other hand, in Zhang *et al.* (2018) the value obtained by density functional theory calculations for the layer thickness of 2D pristine Ti₃C₂ Mxene is 0.464 nm, which is in our interval of h_1 optimal values.

MXenes with a larger monolayer thickness have a better structural stability, according to Zhang *et al.* (2018). Firestein *et al.* (2020) have performed tensile tests for Mxene nanosheets and have analyzed the fracture character during them. For thicker nanosheets (80-90 nm) they observed a layer-by-layer fracture and a large number of incomplete layers, bending of layers and their partial delamination. By contrast, for the thinner nanosheets (35-45 nm) the crack was initiated at the edge, i.e., the failure begins in the edge areas which have microcracks and/or defects, with the latter acting as stress concentrators. It has to be noted, that in Firestein *et al.*'s results during test experiments they have never observed plastic deformation of Ti₃C₂ nanosheets; all stress displacement curves had an elastic character. As the boundaries of our preliminary intervals for varying the Mxene thickness h_1 in MOPs ($0.35 \text{ nm} \div 5 \text{ nm}$), are far away from the values, tested in Firestein's work; one can be sure, that the delamination/elastic brittle fracture in this NC structure will not arise for these thicknesses of Mxene.

Kilikevičius *et al.* (2021) reported that a stronger interfacial layer between Mxene and epoxy is able to improve both the maximum stress and the maximum strain, while the volume fraction of MXene is able to improve the maximum stress, but the maximum strain is then reduced as the composite becomes more brittle. The same authors set the thickness of the interfacial layer in the simulation and analysis of effective interfacial layers in Mxene/epoxy NC to 1 nm, which is in the interval of the optimal values for h_a in Table 9 obtained by us – ($1\text{e-}09 \div 3.40\text{e-}08$ m), despite the different substrate used. Their conclusion is that the MXene/epoxy interfacial layer did not have a significant influence on the effective Young's modulus of this composite; however, higher properties of the interfacial layer resulted in significantly higher values of the NC tensile strength.

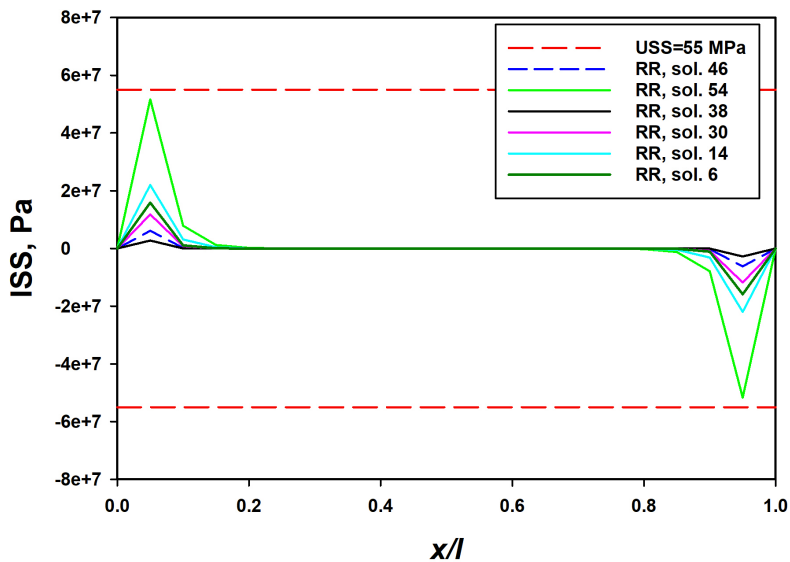


Figure 14: Model interfacial shear stress solutions for RR roots, calculated at the optimal values of decision variables, for Ti_3C_2 Mxene/PMMA

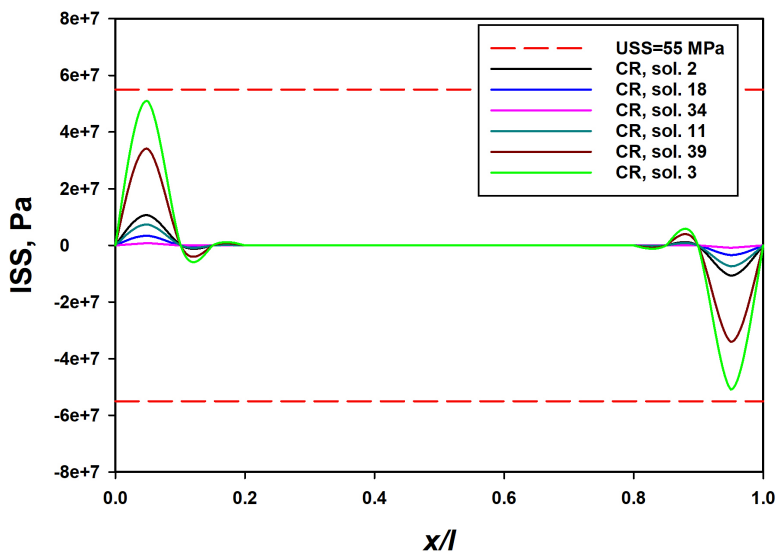


Figure 15: Model interfacial shear stress solutions for CR roots, calculated at the optimal values of decision variables, for Ti_3C_2 Mxene/PMMA.

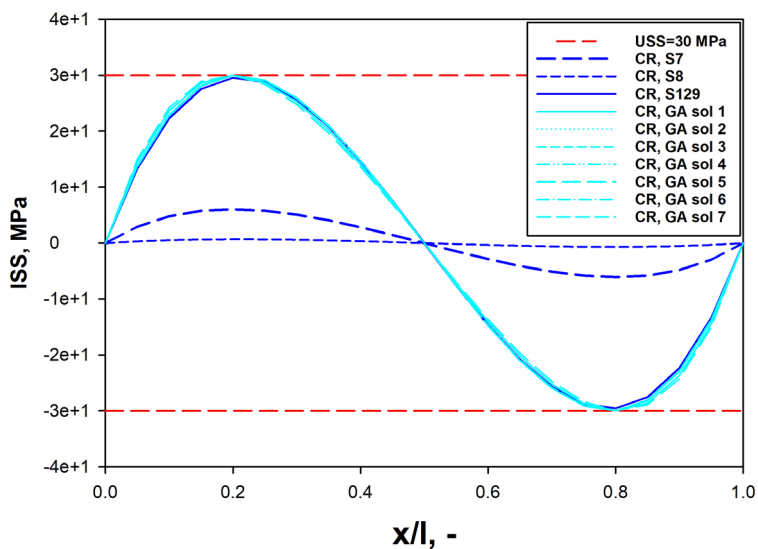


Figure 16: Model interfacial shear stress solutions for CR roots, calculated at the optimal values of decision variables, for graphene/SU-8/PMMA.

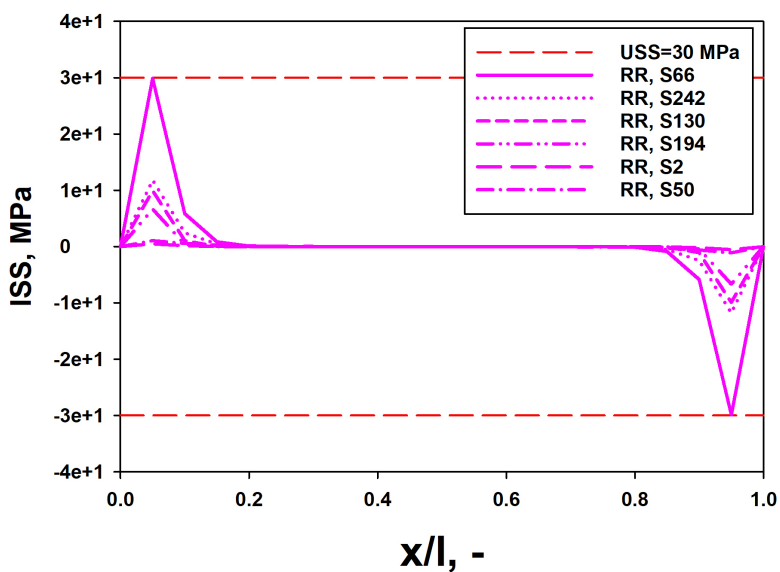


Figure 17: Model interfacial shear stress solutions for RR roots, calculated at the optimal values of decision variables, for graphene/SU-8/PMMA.

As the graphene is the first 2D nanomaterial discovered and studied from 2004 (see Chapter 1), the available data for the factors, affecting stress transfer in the graphene-polymer NCs are well known and circumstantially investigated. The detailed review on these factors' influence is presented in Chapter 2 of this book. Briefly, the main factors, affecting stress transfer in graphene-polymer NCs (and their ISS in particular) are: the graphene flake length, its thickness, the properties and thickness of the interfacial layer between the flake and polymer, the magnitude of applied load and the temperature influence. Also, in Chapter 2, *Tables 1* and *2*, the reported literature data for the interfacial layer thickness h_a in the graphene-polymer NCs are summarized: they varied between 0.03 nm (Kooloor *et al.* 2019) in graphene/epoxy NC to 90 nm (Mehdipour *et al.* 2024) for graphene nanoplatelets/epoxy. The rest of the data between are from few nm (Lu *et al.* 2021) to 10s of nm (Liu *et al.* 2016, Manta, 2018). Our results (*Table 10*) for the optimal h_a are in an interval ($1\text{e-}09 \div 1\text{e-}07$ m) for graphene/SU-8/PMMA, which are in consistence with the abovementioned data found in the literature. Gong (2012) advised for graphene/SU-8/PMMA to use large flakes $l > 30\mu\text{m}$ for an efficient reinforcement in this NC. Similar results in graphene/PET for the length influence on ISS and NC properties in the range $l \in (20 \div 10000\mu\text{m})$ are reported in Xu *et al.* (2016). If l increases in this interval, the interfacial tension decreases until complete exfoliation occurs, which is confirmed by Liu *et al.* (2022a) for graphene/formvar/PDMS. According to Xu *et al.* (2016), beyond $l > 1000\mu\text{m} = 1\text{mm}$ the mechanical properties of graphene/PET NC do not depend on the graphene flake length yet. Chae *et al.* (2022) have found optimal values of $l \in (1 \div 2\mu\text{m})$ for an efficient strain transfer from the substrate in graphene/PMMA NC. Our previous findings (Apostolov *et al.* 2022, 2024) on the flake length influence on the stress transfer and ISS value in graphene/SU-8/PMMA confirmed the results of Gong (2012), Xu *et al.* (2016) and Chae *et al.* (2022). The obtained results (*Table 10*) for the optimal lengths l in graphene/SU-8/PMMA without delamination are $l \in (10 \div 97.6\mu\text{m})$ which is in accordance with the literature results.

Apostolov *et al.*'s results by parametric analysis show, that the magnitude of external load mainly influences the value of ISS in graphene/SU-8/PMMA; for loads over 350 MPa (RR) delamination takes place for RR and fixed geometry. As it is seen in *Table 10* and Fig. 17 for RR, the optimal values for σ_0 are below this value. For CR, at fixed geometry in Apostolov *et al.* (2022) it is obtained that over 750 MPa delamination takes

place. There are optimal values for σ_0 in *Table 10* over $7.5\text{e}+08$ Pa, but they correspond to the other values for NC geometry (sol. 129 and GA 1-7). It is shown in Fig. 16, that the corresponding ISSs does not exceed USS.

Results for graphene/SU-8/PMMA and Ti_3C_2 Mxene/Interfacial layer/PMMA (thermo-mechanical loading)

The obtained values for safety intervals for 6 parameters in the MOPs procedures, performed for 2 structures - Ti_3C_2 Mxene/Interfacial layer/PMMA and graphene/SU-8/PMMA, subjected to thermomechanical loading, are presented below in *Tables 11* and *12*.

The optimal values of 6 parameters are presented in Figures 18 and 19 below in the form of 3D and top view plots, in order to show a detailed distribution for all parameters.

Table 11: Obtained results for parameters (complex and real roots) for Mxene/Interfacial layer /PMMA NC, 6 parameters (with temperature).

Solution No., type	l , (m)	h_1 , (m)	h_a , (m)	h_2 , (m)	σ_0 , (Pa)	ΔT , (K)
sol. 11, CR	1.00e-05	0.35e-09	1.00e-09	1.00e-06	6.04e+08	-200
sol.55, CR	2.00e-05	0.35e-09	1.00e-09	1.00e-06	5.58e+08	200
sol.16, CR	1.00e-05	0.35e-09	1.00e-09	1.00e-06	5.75e+08	50
sol.50, CR	2.00e-05	0.35e-09	1.00e-09	1.00e-06	5.87e+08	-50
sol.12, CR	1.00e-05	0.35e-09	1.00e-09	6.67e-07	4.65e+08	-150
sol. 31, CR	1.00e-05	0.35e-09	1.00e-09	1.00e-06	5.92e+08	-100
sol.62, CR	1.00e-05	0.35e-09	1.40e-08	8.33e-07	5.22e+08	100
sol.1512, CR	2.00e-05	0.57e-09	2.70e-08	1.00e-06	4.32e+08	150
sol.65m, CR	1.00e-05	0.35e-09	1.40e-08	3.00e-06	1.20e+09	150
sol.498m, CR	1.33e-05	0.35e-09	1.40e-08	4.00e-06	1.80e+09	-150
sol. 12, CR	1.00e-05	0.35e-09	1.00e-09	1.00e-06	5.98e+08	-150
sol. 47, CR	2.00e-05	0.35e-09	1.00e-09	1.00e-06	6.04e+08	-200
sol. 443, CR	1.33e-05	0.35e-09	1.00e-09	6.67e-07	4.71e+08	-200
sol. 914, CR	1.67e-05	0.35e-09	1.40e-08	6.67e-07	4.71e+08	-50
sol. 31, RR	1.00e-05	1.00e-09	1.00e-09	1.00e-06	3.12e+08	-100
sol. 5, RR	1.00e-05	0.35e-09	1.00e-09	5.00e-07	3.80e+08	-50
sol. 63, RR	2.00e-05	1.00e-09	1.00e-09	5.00e-07	1.86e+08	150
sol. 25, RR	1.00e-05	1.00e-09	1.00e-09	5.00e-07	1.96e+08	50

sol.2, RR	1.00e-05	0.35e-09	1.00e-09	5.00e-07	3.96e+08	-200
sol. 73, RR	2.00e-05	1.00e-09	1.00e-09	1.00e-06	2.77e+08	200
sol.62, RR	2.00e-05	1.00e-09	1.00e-09	5.00e-07	1.92e+08	100
sol.22, RR	1.00e-05	1.00e-09	1.00e-09	5.00e-07	2.14e+08	-100
sol.43, RR	2.00e-05	0.35e-09	1.00e-09	5.00e-07	3.68e+08	50
sol.32, RR	1.00e-05	1.00e-09	1.00e-09	1.00e-06	3.06e+08	-50
sol.32m, RR	1.00e-05	1.00e-09	1.00e-09	1.00e-06	5.00e+08	-50
SM, RR	1.00e-05	1.00e-09	1.00e-09	1.00e-06	5.00e+08	50

Table 12: Obtained results for parameters (complex and real roots) for graphene/SU-8/PMMA NC, 6 parameters (with temperature).

Solution No., type	l , (m)	h_1 , (m)	h_a , (m)	h_2 , (m)	σ_0 , (Pa)	ΔT , (K)
Sol.1, CR	9.44e-05	2.37e-09	2.29e-08	2.88e-04	2.20e+09	-68.62
Sol.2, CR	6.93e-05	4.66e-09	3.52e-08	3.02e-04	3.31e+09	-38.09
Sol. 3, CR	8.92e-05	4.83e-09	5.65e-09	3.74e-04	3.12e+09	71.33
Sol. 4, CR	6.82e-05	4.02e-09	3.05e-08	2.94e-04	3.30e+09	-78.85
Sol. 5, CR	7.09e-05	3.92e-09	1.00e-09	3.12e-04	3.50e+09	-80.56
Sol. 6, CR	7.63e-05	2.47e-09	7.15e-08	3.22e-04	3.50e+09	-30.73
Sol. 7, CR	7.98e-05	2.69e-09	1.01e-09	2.93e-04	2.60e+09	77.69
Sol. 8, CR	8.85e-05	3.30e-09	5.56e-08	3.68e-04	3.28e+09	69.7
Sol. 9, CR	2.32e-05	4.88e-09	1.00e-09	3.37e-04	3.23e+09	-18.76
Sol. 10, CR	4.53e-05	2.69e-09	9.12e-08	4.05e-04	3.14e+09	70.86
Sol. 11, CR	4.77e-05	3.05e-09	2.45e-08	3.03e-04	2.98e+09	-43.94
Sol. 12, CR	7.43e-05	1.64e-09	3.53e-08	3.37e-04	2.99e+09	37.24
Sol. 1, RR	8.47e-05	3.62e-09	1.00e-09	1.43e-05	2.50e+08	11.12
Sol. 2, RR	5.95e-05	2.55e-09	1.00e-09	1.11e-05	2.37e+08	96.11
Sol. 3, RR	6.65e-05	9.22e-09	8.90e-09	9.16e-06	1.12e+08	-19.25
Sol. 4, RR	2.86e-05	3.68e-09	1.77e-09	1.16e-05	1.66e+08	46.32
Sol. 5, RR	4.35e-05	4.44e-09	4.55e-08	1.60e-05	1.74e+08	75.89
Sol. 6, RR	5.95e-05	2.58e-09	1.00e-09	1.05e-05	2.37e+08	81.17
Sol. 7, RR	1.31e-05	2.82e-08	5.11e-08	1.15e-04	7.29e+08	1.85
Sol. 8, RR	2.35e-05	2.37e-08	3.28e-08	9.47e-05	3.05e+08	93.5
Sol. 9, RR	6.12e-05	8.02e-09	2.27e-08	3.28e-05	5.47e+07	87.06
Sol. 10, RR	1.15e-05	2.00e-08	1.02e-09	5.26e-05	2.22e+09	99.99

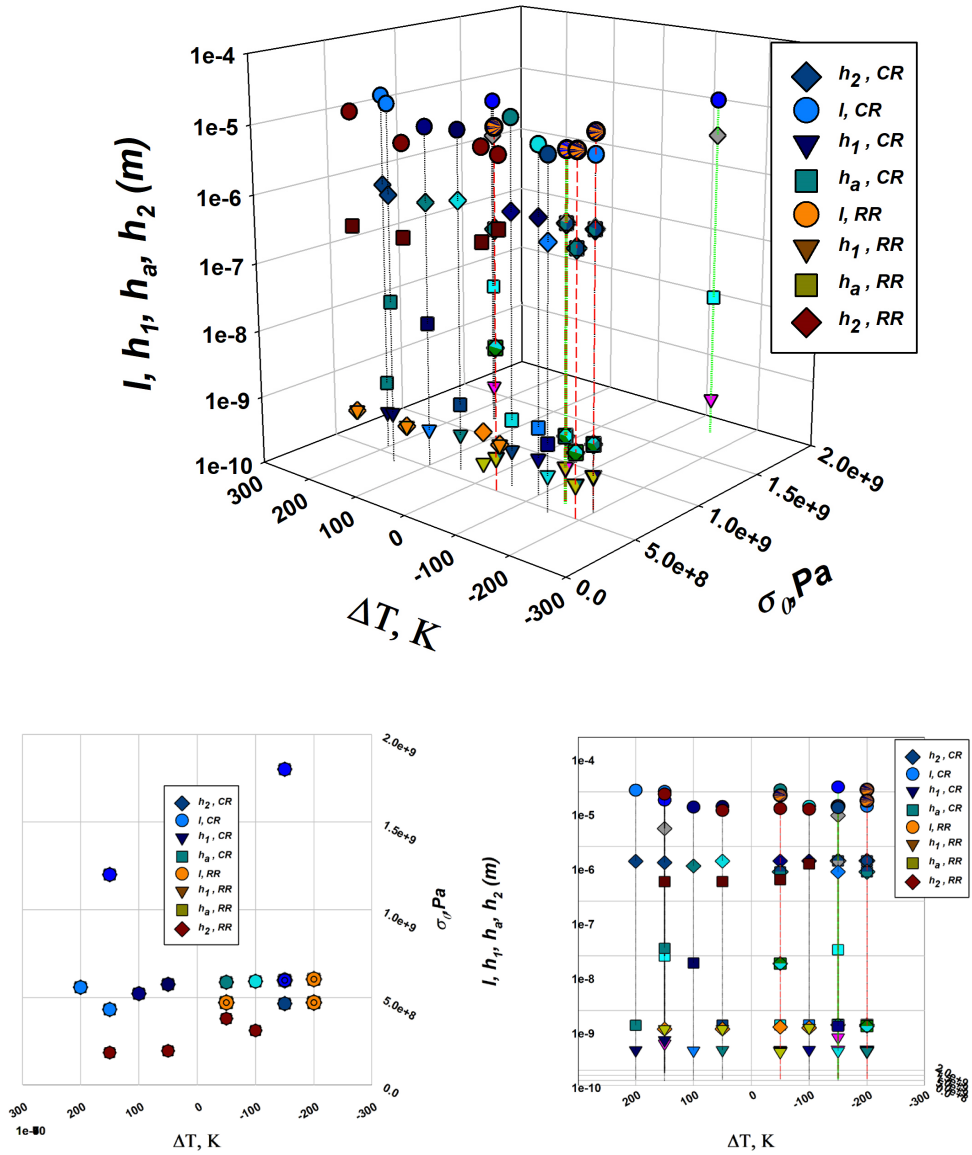


Figure 18: Optimal solutions for 6 decision variables from two optimization algorithms: CR (ocean colors) and RR (earth colors) for Mxene/Interfacial layer /PMMA; top - 3D view, bottom, left and right – top and front view.

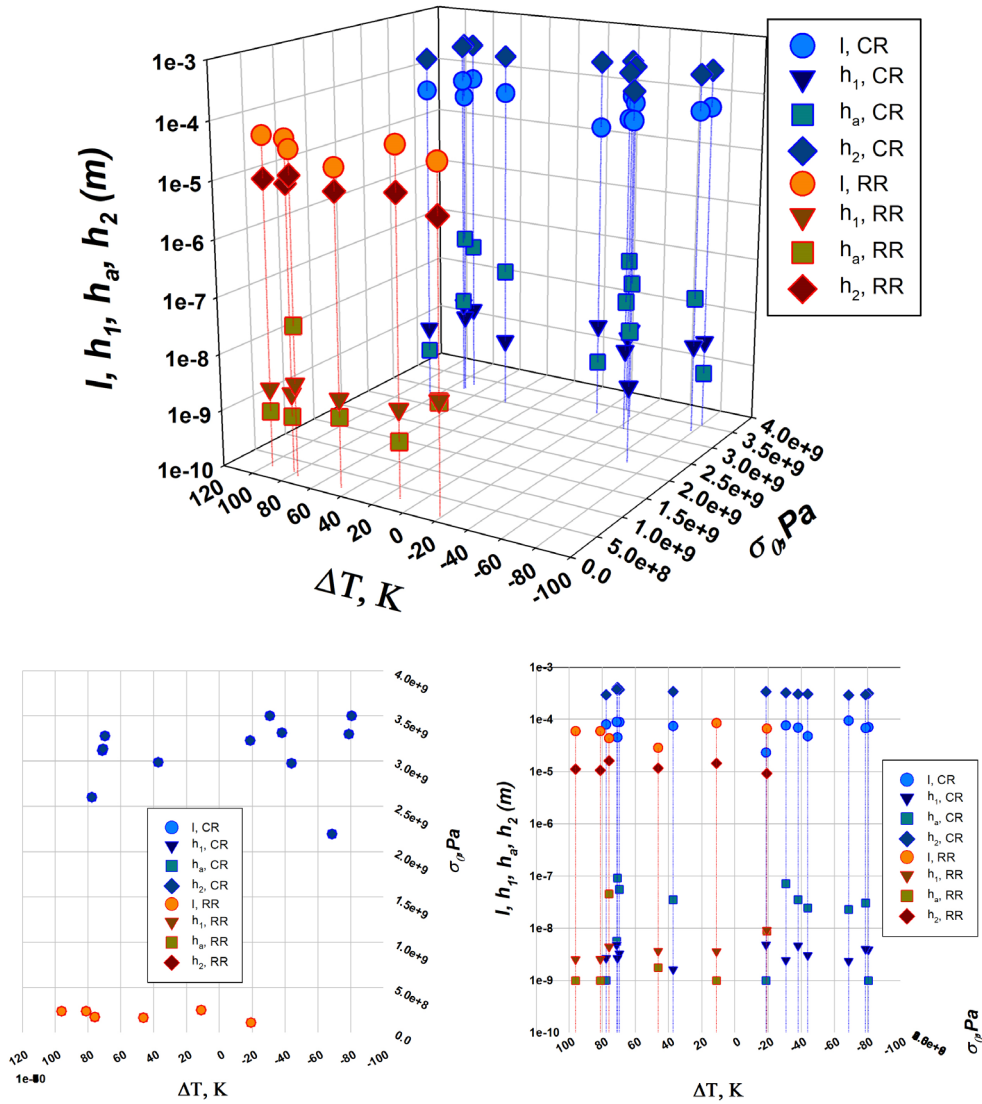


Figure 19: Optimal solutions for 6 decision variables from two optimization algorithms: CR (ocean colors) and RR (earth colors) for graphene/SU-8/PMMA: top - 3D view; bottom, left and right – top and front view.

It is seen, that the optimal intervals of all geometrical parameter found for graphene/SU-8/PMMA are well distinguished not only in respect to the mechanical loading (Fig. 19, top view). Different intervals are obtained for the geometrical parameters h_a, h_2 in CR and RR cases (Fig.19, front view).

The respective results for Mxene/Interfacial layer/PMMA do not follow this tendency (Fig.18); the explanation is because different MOPs (GA and deterministic) were used for each of the NCs.

Again, as in the previous NCs, the model ISSs values, calculated at optimal values of the parameters in Tables 11 and 12 are visualized in Figs. 20-21 in order to check their correctness for the considered NC structures, subjected to thermo-mechanical loading.

If Tables 9 and 11 are compared for the Mxene/Interfacial layer /PMMA, and Tables 10 and 12 for graphene/SU-8/PMMA, without and with temperature difference applied to NCs, one can see that adding of the temperature will influence mainly the upper boundary of the optimal interval for h_2 in case CR for Mxene/Interfacial layer /PMMA – it decreases by one order of magnitude. The temperature has a much weaker effect on the upper limit of the optimal interval for σ_0 - its value decreases by half for CR, in respect to the same value for mechanical load only.

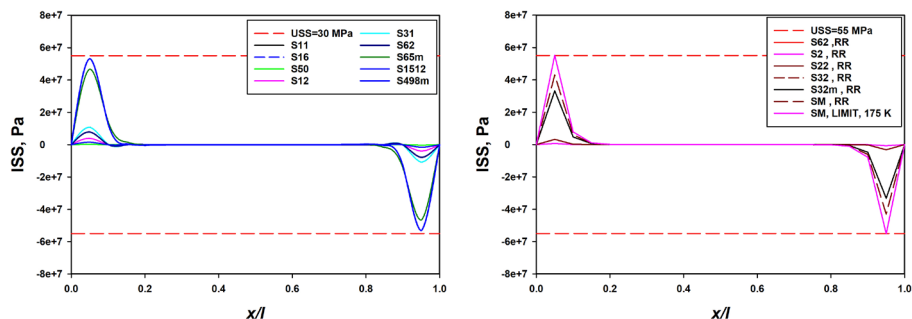


Figure 20: Model interfacial shear stress solutions for CR (left) and RR (right) roots, calculated at the optimal values of 6 decision variables, for Mxene/Interfacial layer/PMMA.

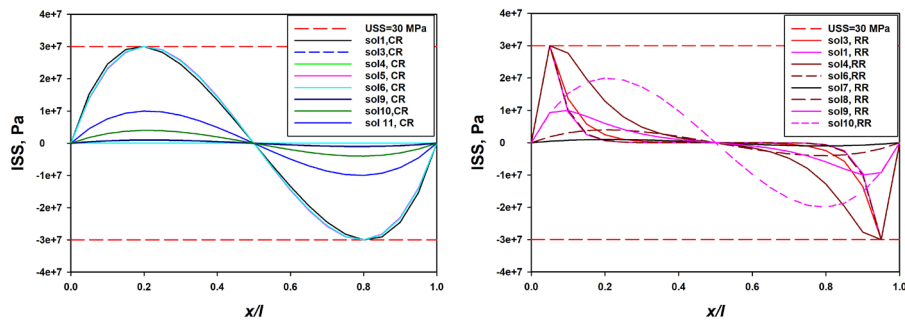


Figure 21: Model interfacial shear stress solutions for CR and RR, calculated at the optimal values of 6 decision variables, for graphene/SU-8/PMMA.

For graphene/SU-8/PMMA, the changes in the values of the lower and upper boundaries for optimal parameters when adding a temperature, are most pronounced again for h_2 (up to 2 orders of magnitude), but also are visible for σ_0 especially for CR, too.

About comparison of our results from MOPs with literature data, unfortunately, there are not found similar results up to now for the considered here Mxene/Interfacial layer /PMMA and graphene/SU-8/PMMA according to the authors knowledge. In Chapter 1 and 2 the effect of temperature is commented mainly for strains, and it was found, that the length and temperature difference have less influence on the ISS, but in combination with specific values of the mechanical load can significantly affect its value. Because the ISS is included in the MOPs objective function and is part of the optimization criteria, it is important to check the effect of this influence. Strictly speaking, in our 2D model the influence of temperature has to be taken into account in the Young moduli of the layers in the NC structures, but it will be a subject of future work.

6. Conclusions

This chapter proposes an optimization framework aimed at determining the optimal geometric parameters and applied load magnitude and temperature, necessary to ensure the safe operation of a three-layer adhesively bonded nanocomposite structures under axial mechanical or thermo-mechanical loading. The optimization framework incorporates a non-linear criterion for delamination in the NC as objective function; it is based on the solutions for the ISS from two-dimensional stress function model. As decision variables, the external load, layers' thicknesses, structure length and temperature difference are considered, varying within predefined technological boundaries. The objective function aims to minimize the difference between ISS and USS in the model criterion. Two optimization approaches were applied for both types of ISS model solutions (with real and complex roots) – BASIC GA and an optimization procedure developed with software “Mathematica”. The obtained results for the intervals of optimal values for each of the parameters are obtained and validated by ISS model distributions calculated at all optimal values found. Some of the results are verified and are in coincidence with available literature data for optimal values of the NC length, interfacial layer thickness and loads.

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Notations list

Notation	Meaning
σ	Stress, Pa
τ	Interfacial shear stress (ISS), Pa
ν	Poisson ratio, -
A	Constant, solution of non-homogeneous ODE , Pa
E	Young's modulus, Pa
G _m	Interfacial layer shear modulus, Pa
l	Length of the structure/flake, m
h _i	Thickness of the layers in NC, m
M _i , C _i	Integration constants in the model solutions
n	Parameter in shear-lag model, -

P	Axial tension force P , N/m
$s=L/a$	Thread size ratio (aspect ratio), length to diameter, -
t, T	Thicknesses of the layers in NC, m
$T, \Delta T$	Temperature and temperature difference, K
x, y	Cartesian coordinate system, m

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