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FUNCTIONAL MATERIALS

Design optimization of graphene laminates for maximum fundamental frequency

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Abstract. Design optimization of nanostructures is a new challenging research area. The modelling of multilayer graphene sheets has a similar character as the modelling of composite laminates. However, the traditional laminate plate theories are revised in order to incorporate nonlocal elasticity. The main aim of the current study is to point out the crotchet features arising in the design optimization of graphene laminates based on the theoretical analysis performed and numerical results obtained. The study is focused on the improvement of the mechanical performance of graphene and nanostructures, particularly vibration properties of multilayer graphene laminates.

Key words: graphene laminates, design optimization, genetic algorithms.

1. INTRODUCTION

During the last decade graphene nanostructures have attracted great attention in the literature. Most of the studies deal with their material characterization, structural analysis, chemistry, physics, etc. Design optimization of nanostructures is an emerging but not yet a well-covered research area. The main approaches used to describe the small-scale effect in the analysis of nanostructures include nonlocal continuum mechanics and the atomic theory of lattice dynamics [1].

The current study is based on the continuum mechanics approach. However, in the literature a number of continuum mechanics based plate models are available for describing nonlocal elasticity theory. Three most commonly used theories include Eringen's model ('strongly' nonlocal), strain gradient based model ('weakly' nonlocal), and hybrid model [1–3].

According to the nonlocal elasticity theory it is assumed that the stress at a point is a function of strains at all points in the continuum [3,4]. Nonlocal theory considers long-range inter-atomic interaction and yields results dependent on the size of a body. First the nonlocal plate theory was developed for Euler–Bernoulli beams and plates [1,4–10]. Later the effects of geometrical non-linearity, first and higher order shear deformation theory, etc. were incorporated in plate models [11–14]. New trends cover analysis of laminated nanostructures, functionally graded materials [15–17], and graphene structures [18–21].

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The numerical methods applied most commonly for vibration analysis of nanostructures include finite difference or differential quadrature methods [1,22–24], the Rayleigh–Ritz method [25], also the finite element method [26,27], etc. In [28] the Haar wavelet method was introduced for analysis of nanostructures. It was shown that the numerical order of convergence of the method is equal to two and the order of convergence of extrapolated results is equal to four. The latter results are in agreement with recently proved convergence theorems for the Haar wavelet method [29–30].

The main aim of the current study is to improve the vibration properties (fundamental frequency) of multilayer graphene sheets by determining the optimal configuration of design parameters such as orientation of the layers, material properties, etc. Proceeding from the principle of virtual work the governing equations of the graphene sheet are derived. Graphene laminate can be regarded as a sequence of sheets with orthotropic material symmetry. The global optimization methods and techniques developed for design optimization of composite structures and manufacturing processes were adapted by our research group for design optimization of graphene laminates [31–34].

2. NONLOCAL ELASTICITY APPROACH

According to the theory of nonlocal elasticity of Eringen, the stress at a reference point x is considered to be a functional of the strain field at every point in the body. The nonlocal stress tensor σ_{ij}^{NL} at point x is given as

$$\sigma_{ij}^{NL}(x) = \int \lambda(|x-x'|,\alpha) C_{ijkl}\varepsilon_{kl}(x')dV(x'), \qquad \forall x \in V, \tag{1}$$

where ε_{kl} and C_{ijkl} stand for strain tensor and fourth order elasticity tensor, respectively. The term $\lambda(|x-x'|,\alpha)$ is a kernel function representing nonlocal modulus, where $|x-x'|$ is a distance in Euclidean space and α is a material parameter depending on internal and external characteristics (lattice parameter, granular size, distance between C–C bonds, graphene sheet length, wave length, etc.). According to model (1), the stress at a given point x is determined by the spatial integral representing weighted averages of contributions of the strain at all points in the body. The given model is in accordance with the atomic theory of lattice dynamics and experimental observations on phonon dispersion [6]. It is shown in [3] that the nonlocal elasticity model (1) can be expressed in a differential form as

$$(1-\mu\nabla^2)\sigma_{ij}^{NL} = C_{ijkl}\varepsilon_{kl}. \tag{2}$$

In (2) ∇^2 is the Laplacian operator and μ is the nonlocal parameter defined as

$$\mu = e_0^2\alpha^2. \tag{3}$$

The value of the parameter e_0 is determined from the condition according to which the nonlocal elasticity model (2) provides satisfactory approximation of atomic dispersion curves of plane waves with those of atomic lattice dynamics [3]. The parameter α in formula (3) stands for the internal characteristic length (C–C bonds length, lattice parameter). Most commonly, the value of the $e_0\alpha$ in an interval of 0–2 nm is considered [4,6]. Obviously, the nonlocal elasticity model (2) reduces to generalized Hooke's law if the nonlocal parameter μ is equal to zero.

3. NONLOCAL CONSTITUTIVE RELATIONS IN TERMS OF DISPLACEMENTS

In the following the constitutive relations are derived proceeding from the orthotropic material model, nonlocal elasticity approach (2), linear strain–displacement relation, and classical laminated plate theory (CLPT).

The displacement field can be written as

$$\begin{aligned} u(x,y,z,t) &= u_0(x,y,t) - z\frac{\partial w}{\partial x}, \\ v(x,y,z,t) &= v_0(x,y,t) - z\frac{\partial w}{\partial y}, \\ w(x,y,z,t) &= w_0(x,y,t), \end{aligned} \tag{4}$$

where u, v, and w stand for the displacements along x, y, and z directions, respectively, and the midplane displacements are equipped with index 0.

The linear strain–displacement relationship is given as

$$\begin{Bmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{xy} \end{Bmatrix} = \begin{Bmatrix} \dfrac{\partial u_0}{\partial x} - z\dfrac{\partial^2 w}{\partial x^2} \\ \dfrac{\partial v_0}{\partial y} - z\dfrac{\partial^2 w}{\partial y^2} \\ \dfrac{1}{2}\left(\dfrac{\partial u_0}{\partial y} + \dfrac{\partial v_0}{\partial x} - 2z\dfrac{\partial^2 w}{\partial x \partial y}\right) \end{Bmatrix}, \quad \varepsilon_{zz} = 0, \quad \varepsilon_{xz} = 0, \quad \varepsilon_{yz} = 0. \tag{5}$$

The nonlocal elasticity model (2) can be expanded as

$$\begin{Bmatrix} \sigma_{xx}^{NL} \\ \sigma_{yy}^{NL} \\ \sigma_{xy}^{NL} \end{Bmatrix} - \mu\nabla^2 \begin{Bmatrix} \sigma_{xx}^{NL} \\ \sigma_{yy}^{NL} \\ \sigma_{xy}^{NL} \end{Bmatrix} = \begin{bmatrix} \overline{Q_{11}} & \overline{Q_{12}} & \overline{Q_{16}} \\ \overline{Q_{12}} & \overline{Q_{22}} & \overline{Q_{26}} \\ \overline{Q_{16}} & \overline{Q_{26}} & \overline{Q_{66}} \end{bmatrix} \begin{Bmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ 2\varepsilon_{xy} \end{Bmatrix}, \tag{6}$$

where $\overline{Q}$ is a reduced stiffness matrix obtained by the rotation of the original stiffness matrix Q:

$$\left[\overline{Q}\right] = [T][Q][T]^T. \tag{7}$$

In (7) the matrix T stands for the transformation matrix, describing the rotation about a transverse normal to the lamina. Due to the symmetry properties, the graphene sheet is modelled by orthotropic material, thus the matrix Q can be written in terms of engineering parameters as

$$\begin{bmatrix} Q_{11} & Q_{12} & Q_{16} \\ Q_{12} & Q_{22} & Q_{26} \\ Q_{16} & Q_{26} & Q_{66} \end{bmatrix} = \begin{bmatrix} \dfrac{E_1}{1-\nu_{12}\nu_{21}} & \dfrac{\nu_{12}E_2}{1-\nu_{12}\nu_{21}} & 0 \\ \dfrac{\nu_{12}E_2}{1-\nu_{12}\nu_{21}} & \dfrac{E_2}{1-\nu_{12}\nu_{21}} & 0 \\ 0 & 0 & G_{12} \end{bmatrix}. \tag{8}$$

The expressions for resultant forces and moments can be obtained by inserting the strain components (8) in the nonlocal elasticity model (6), multiplying Eqs (6) by 1 and z, respectively, and integrating over the thickness

$$\begin{Bmatrix} N_{xx} \\ N_{yy} \\ N_{xy} \end{Bmatrix} - \mu\nabla^2 \begin{Bmatrix} N_{xx} \\ N_{yy} \\ N_{xy} \end{Bmatrix} = \begin{vmatrix} A_{11} & A_{12} & A_{16} \\ A_{12} & A_{22} & A_{26} \\ A_{16} & A_{26} & A_{66} \end{vmatrix} \begin{Bmatrix} \dfrac{\partial u_0}{\partial x} \\ \dfrac{\partial v_0}{\partial y} \\ \left(\dfrac{\partial u_0}{\partial y} + \dfrac{\partial v_0}{\partial x}\right) \end{Bmatrix}, \tag{9}$$

$$\begin{Bmatrix} M_{xx} \\ M_{yy} \\ M_{xy} \end{Bmatrix} - \mu\nabla^2 \begin{Bmatrix} M_{xx} \\ M_{yy} \\ M_{xy} \end{Bmatrix} = \begin{bmatrix} D_{11} & D_{12} & D_{16} \\ D_{12} & D_{22} & D_{26} \\ D_{16} & D_{26} & D_{66} \end{bmatrix} \begin{Bmatrix} -\dfrac{\partial^2 w}{\partial x^2} \\ -\dfrac{\partial^2 w}{\partial y^2} \\ -2\dfrac{\partial^2 w}{\partial x \partial y} \end{Bmatrix}, \tag{10}$$

where the stretching and bending stiffness are given as

$$(A_{ij}, D_{ij}) = \int_{-\frac{h}{2}}^{\frac{h}{2}} \overline{Qij}(1, z^2)\, dz. \tag{11}$$

In the case of a symmetric graphene sheet the stretching–bending coupling stiffness matrix is zero ($B = 0$, see details in [35]).

4. NONLOCAL PLATE MODEL

Let us consider free vibrations of a single-layer graphene sheet and assume that the sheet is free from any inplane or transverse loading $(N_{xx} = N_{xy} = N_{yy} = 0)$. Using the principle of virtual work, applying the differential operator $L = 1 - \mu\nabla^2$ to classical equations of motion, and then substituting the stress resultants in equations of motion one obtains the governing equation of the nonlocal graphene sheet in terms of displacements as

$$\begin{aligned} &-D_{11}\frac{\partial^4 w}{\partial x^4} - 2(D_{12} + D_{66})\frac{\partial^4 w}{\partial y^4} - D_{22}\frac{\partial^4 w}{\partial y^4} - 4D_{16}\frac{\partial^4 w}{\partial x^3 \partial y} - 4D_{26}\frac{\partial^4 w}{\partial x \partial y^3} \\ &= 1(1 - \mu\nabla^2)\left[-q + m_0\frac{\partial^2 w}{\partial t^2} + m_2\left(\frac{\partial^4 w}{\partial x^2 \partial t^2} + \frac{\partial^4 w}{\partial y^2 \partial t^2}\right)\right], \end{aligned} \tag{12}$$

where m_0 and m_2 stand for mass moments of inertia.

Next let us consider multilayer graphene sheets embedded in a polymer matrix (Fig. 1). In that case the cover layers (first and last) interact with the polymer matrix and the adjacent layer. The remaining interlayers are interacting with two neighbouring layers (see Fig. 1). The transverse load applied to sheets can be expressed as shown by formula (13)[19].

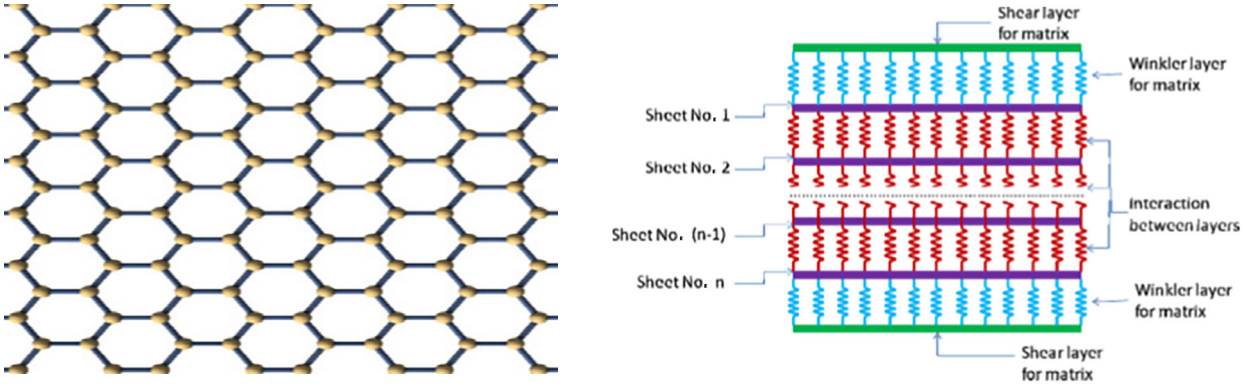

Fig. 1. (a) A single-layer graphene sheet; (b) continuum model of multilayered graphene laminate embedded in a polymer matrix [19].

$$
\begin{aligned}
q_1 &= -K_w w_1 + K_p\left(\frac{\partial^2 w_1}{\partial x^2} + \frac{\partial^2 w_1}{\partial y^2}\right) - c(w_1 - w_2),\\
q_k &= -c(w_k - w_{k-1}) - c(w_k - w_{k+1}), \qquad k = 2,\ldots n-1,\\
q_n &= -K_w w_n + K_p\left(\frac{\partial^2 w_n}{\partial x^2} + \frac{\partial^2 w_n}{\partial y^2}\right) - c(w_n - w_{n-1}),
\end{aligned}
\tag{13}
$$

where $w_k (k = 1,\ldots n)$ are axial deflections of the sheets; K_w and K_p stand for Winkler and shear modulus of the polymer matrix; respectively; and c is an interaction coefficient between two neighbouring sheets caused by Van der Waals forces. Taking in (13) q sequentially equal to $q_1,\ldots,q_n$ one obtains the governing differential equations of nonlocal multilayer graphene sheets. These detailed equations are omitted herein for conciseness sake.

5. FORMULATION OF THE OPTIMIZATION PROBLEM

The research done in the area of mechanics of nanostructures is most commonly related to material characterization and synthesis but also structural analysis. Herein an attempt is made to provide some results in the area of design optimization of mechanical characteristics in order to improve the mechanical performance of structures. In particular, the problem of free vibrations of multilayer graphene sheets is considered. The material properties of the graphene sheets can be described by orthotropic material symmetry. An analysis of graphene laminates is performed by incorporating the nonlocal elasticity approach in composite laminate theories.

The aim is to find an optimum configuration of the graphene laminate that has the maximum fundamental frequency value

$$
Maximum \;\; \Omega_1 = \Omega_1(\theta_1, \theta_2, \ldots, \theta_n), \tag{14}
$$

subjected to

$$
-90^\circ \le \theta_k \le 90^\circ, \qquad k = 1,\ldots,n. \tag{15}
$$

In (14) and (15) Ω_1 is the fundamental frequency and θ_k, $k = 1, \ldots, n$ stand for the material orientations angles in the layers 1, ..., n.

The fact that the design variables include the material orientations angles needs explanation because in the design optimization of traditional composite laminates most commonly also the thicknesses, materials,

and stacking sequences of the layers are considered as design parameters. However, in the case of graphene sheets the thicknesses and materials are most commonly fixed (selection limited). Including stacking sequences in design variables is justified only in the case where layers have different properties (material, thickness).

6. NUMERICAL SOLUTION

The simply supported boundary conditions considered are applied in all sides of the sheet, i.e. in all sides $u = v = w = M = 0$ holds good. The geometrical and material parameters used are the following: $E_1 = 1765$ GPa, $E_2 = 1588$ GPa, $v_{12} = 0.3$, $v_{21} = 0.27$, Winkler modulus $K_w = 1.13 \times 10^{18}$ Pa/m, polymer matrix shear modulus $K_p = 1.13$ Pa/m, interaction coefficient between layers $c = 4.5 \times 10^{19}$ Pa/m, thickness of each layer $h = 0.34$ nm, and length of breadth $L = 10.2$ nm.

6.1. Homogenized plate

The properties of graphene laminate material can be estimated by averaged values computed based on the properties of each layer. In the case of the posed problem, the bending stiffness matrix of the laminate can be computed as

$$D_{ij} = \frac{1}{3}\sum_{k=1}^{n} Q_{ij}^{k}(z_k^3 - z_{k-1}^3), \tag{16}$$

where Q_{ij}^{k} and z_k stand for the reduced stiffness matrix of the layer k and z coordinates between layers, respectively. By applying the Navier approach, the generalized displacements can be expressed as

$$w = \sum_{m=1}^{\infty}\sum_{n=1}^{\infty} W_{mn} X_m(x) Y_n(y) e^{i\omega_{mn} t}, \qquad X_m(x) = \sin\left(\frac{m\pi x}{a}\right), \qquad Y_n(x) = \sin\left(\frac{n\pi y}{b}\right). \tag{17}$$

Inserting (17) in the differential governing equation (12) yields the eigenvalue problem in the form

$$\begin{gathered}\left[D_{11}\alpha^4 + 2(D_{12} + D_{66})\alpha^2\beta^2 + D_{22}\beta^4 + 4D_{16}\alpha^3\beta + 4D_{26}\alpha\beta^3\right] W_{mn} = M_{mn}\lambda_{mn}\omega_{mn}^2 W_{mn}, \\ M_{mn} = m_0 + m_2(\alpha^2 + \beta^2), \qquad \lambda_{mn} = 1 + \mu(\alpha^2 + \beta^2), \qquad \alpha = \frac{m\pi}{\alpha}, \qquad \beta = \frac{n\pi}{b}.\end{gathered} \tag{18}$$

The necessary stationarity conditions for natural frequency ω_{mn}^{H} of the homogenized plate can be presented as

$$\frac{\partial \omega_{mn}^{H}}{\partial \theta_i} = \frac{\partial}{\partial \theta_i}\sqrt{\frac{D_{ef}^{H}}{M_{mn}\lambda_{mn}}} = 0, \tag{19}$$

where D_{ef}^{H} stands for the effective stiffness of the homogenized plate:

$$D_{ef}^{H} = D_{11}\alpha^4 + 2(D_{12} + D_{66})\alpha^2\beta^2 + D_{22}\beta^4 + 4D_{16}\alpha^3\beta + 4D_{26}\alpha\beta^3. \tag{20}$$

The posed optimization problem was solved by applying the genetic algorithm with integer values of variables (one-degree changes of orientation angles are available). Optimal material orientations corresponding to different values of the sheet length and width ratio a/b are given in Table 1.

Table 1. Optimal material orientations corresponding to maximal value of ω_{mn}^{H}

a/b	θ_1	θ_2	θ_3	θ_4	ω_{mn}^{H} increment (%)
2	27	27	27	27	0.6
1	45	45	45	45	1.9
0.5	63	63	63	63	3.8
0.2	79	79	79	79	5.1
0.1	84	84	84	84	5.3

In the case of an optimal solution, in each layer the values of the orientation parameter θ_i are the same (Table 1). The increase of the fundamental frequency parameter is relatively small (discussed in greater detail in Conclusion).

6.2. Layerwise laminate plate theory

Similarly to formula (17), the displacements can be expanded for each layer i as

$$w_i = \sum_{m=1}^{\infty}\sum_{n=1}^{\infty} W_{i,mn} X_m(x) Y_n(y) e^{i\omega_{mn} t}, \qquad i = 1,\ldots,n. \tag{21}$$

By inserting (21) in differential governing equations the eigenvalue problem can be derived in the form

$$\begin{aligned}
&D_{1,ef} W_{1,mn} + c\lambda_{mn}(W_{1,mn} - W_{2,mn}) = M_{mn}\lambda_{mn}\omega_{mn}^2 W_{1,mn},\\
&D_{2,ef} W_{1,mn} + c\lambda_{mn}(2W_{2,mn} - W_{1,mn} - W_{3,mn}) = M_{mn}\lambda_{mn}\omega_{mn}^2 W_{2,mn},\\
&\ldots\\
&D_{n,ef} W_{n,mn} + c\lambda_{mn}(W_{n,mn} - W_{n-1,mn}) = M_{mn}\lambda_{mn}\omega_{mn}^2 W_{n,mn}.
\end{aligned} \tag{22}$$

Based on layerwise theory, the natural frequency ω_{mn}^{LW} of the multilayer laminate can be presented as

$$\omega_{mn}^{LW} = \sqrt{\frac{D_{ef}^{H} + K_w\lambda_{mn} + K_p\lambda_{mn}(\alpha^2+\beta^2)}{M_{mn}\lambda_{mn}}} = 0. \tag{23}$$

The results of the application of the genetic algorithm for the maximization of ω_{mn}^{LW} seem somewhat surprising. Namely, the optimal solutions obtained by applying layerwise plate theory coincide with those corresponding to the homogenized plate given in Table 1. A detailed theoretical analysis of the necessary optimality conditions for both theories suggested that it implies from (19) that

$$\frac{\partial D_{ef}^{H}}{\partial \theta_i} = 0,$$

from which it implies that

$$D_{1,ef} = D_{2,ef} = \cdots D_{n,ef}, \text{ and } \frac{\partial D_{ef}^{LW}}{\partial \theta_i} = 0. \tag{24}$$

The main reason is that only the terms $D_{i,ef}\,(i = 1, \ldots, n)$ in (22) depend on design parameters (orientation angles of layers).

Thus, the behaviour of the numerical results has a theoretical foundation. However, these results hold good for the posed problem and cannot be extended without thoroughgoing analysis and validation.

7. CONCLUSION

Vibration analysis of multilayered graphene sheets was studied by applying Eringen's nonlocal elasticity theory. Design optimization of fundamental frequency parameters was performed. The necessary optimality conditions were derived for layerwise plate theory and homogenized plate. Optimal solutions were found.

Certain crotchet features were observed in the design optimization of graphene laminates:

- Orientational design: the situation is principally different from traditional material with one-directional or even multidirectional/variable angle fibres. The material properties of graphene sheets are determined by their hexagonal structure and the effect of rotation has significantly less impact on the performance of the material/structure;
- Thickness design: not applicable in the traditional sense because graphene sheets have a constant, predefined thickness in a limited range;
- Stacking sequence design: material selection is strictly limited.

In the case of the posed problem and data used, the optimal solution corresponding to layerwise plate theory and homogenized plate coincide.

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Grafeenlaminaatide optimeerimine maksimaalse esimese omavõnkesageduse määramiseks

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Nanostruktuuride optimeerimine on uus aktuaalne uurimisvaldkond. Mitmekihiliste grafeenlaminaatide modelleerimine on sarnane komposiitmaterjalide ja eriti laminaatide modelleerimisega. Traditsioonilist plaatide teooriat on kohandatud, arvestamaks mittelokaalset elastsusteooriat.

Antud töö eesmärgiks on välja selgitada peamised põhimõtted ja iseärasused, mis on omased grafeenlaminaatide optimeerimisele, lähtudes teoreetilisest analüüsist saadud tulemustest. Teiseks eesmärgiks on grafeeni struktuuri vibratsiooni omaduste parendamine esimese omavõnkesageduse maksimeerimise kaudu.