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Free Vibration of Heterostructures of Graphene and Boron Nitride in Thermal Environment via Aifantis Theory with Velocity Gradients and Ritz Method

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ABSTRACT: This article aims to investigate the free vibration of mono-/ multi-layered hererostructures of graphene and boron nitride in thermal environment. To this end, at first, the nonlinear model of inter-layered interaction between different layers are estimated based on Lenard-Jones 6-12 potential, then two variable refined plate theory is used to model the vibrational behavior of in-plane heterostructures of graphnme/boron nitride or vertically stacked graphene/ boron nitride hybrid structures. To incorporate the size effect into two-variable refined plate hypothesis, Aifantis's theory is used to derive potential energy. To formulate the kinetic energy, an additional length scale which adds gradient velocity to kinetic energy is also used. The eigen-frequency equations are obtained based on Hamilton principle and Ritz method. The results show that the layout of graphene and boron nitride layers only affect out-of-phase natural frequency of multilayered nano-plates. Also, the significant impact of number of boron nitride layers used in heterostructures on the reduction of natural frequency of hybrid structure is demostrated. By controlling the area occupied by boron nitride in mono-layered hybrid structures, one can enhance the natural frequency of nano-sheets. The effects of the value of length scale parameter and temperature change on natural frequencies are studied as well.

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1- Introduction

To complement the properties of pure graphene and h-Boron Nitride (BN) sheet, researchers have proposed hybrid graphene–BN sheets [1]. Yuan and Liew's study [2] showed that graphene in BN/G/BN may be employed as a new sensing element in micro/nano force sensors due to high-sensitivity of the natural frequency of mid-layer graphene in BN/G/BN to external pressure loads. Liu et al. [1] showed that the two-dimensional devices, such as a split closed-loop resonator which works as a bandpass filter can be made of the in-plane heterostructures of graphene and h-BN. Then, the study of mechanical behavior of heterostructures of graphene and h-BN can be important due to the applicability of different configurations of heterostructures in micro-/nano-devices.

Based on the author's knowledge, there is not a notable study on vibrational behavior of heterostructures of graphene and h-BN. Thus, the main objective of this paper is to investigate the effect of different multi-layered and in-plane architectures of graphene/h-BN heterostructures on natural frequencies in thermal environment. To this end, hypothesis of two variable refined plate theory in conjunction with Aifantis' gradient elasticity theory and velocity gradients are used to obtain strain energy and kinetic energy of nano-structures. Hamilton's principle is combined with Ritz method to obtain the system of ordinary differential equations governing eigen frequency equations. The linear approximation of van der waals interaction between different layers in multi-layered architectures is obtained as well.

2- Methodology

Based on Hamilton's principle, one can write

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$$\int_0^{t_1}\left(\sum_{k=1}^{N}\left(\delta T^{(k)}-\delta U^{(k)}\right)+\delta W\right)dt=0 \tag{1}$$

in which N is the total number of layers; T, U and W are kinetic energy, potential energy and external work, respectively. According to the form II simplified Mindlin's theory, one can state the variation of kinetic energy as follows [3]:

$$\delta T=\int_V\left(\rho\dot{u}\delta\dot{u}+\rho\dot{v}\delta\dot{v}+\rho\dot{w}\delta\dot{w}\right)dV+\int_V\left(\rho l_1^2\left(\dot{u}_{,i}\delta\dot{u}_{,i}+\dot{v}_{,i}\delta\dot{v}_{,i}+\dot{w}_{,i}\delta\dot{w}_{,i}+\right)\right)dV \tag{2}$$

where (u,v,w) are defined based on two variable refined plate theory hypothesis as follows [4]:

$$u(x,y,z)=u_0-z\frac{\partial w_b}{\partial x}+z\left(\frac{1}{4}-\frac{5}{3}\left(\frac{z}{h}\right)^2\right)\frac{\partial w_s}{\partial x} \tag{3}$$

$$v(x,y,z)=v_0-z\frac{\partial w_b}{\partial y}+z\left(\frac{1}{4}-\frac{5}{3}\left(\frac{z}{h}\right)^2\right)\frac{\partial w_s}{\partial y} \tag{4}$$

$$w(x,y,z)=w_b(x,y,0)+w_s(x,y,0) \tag{5}$$

in which (u_0,v_0,w) are displacement components of mid-plane; w_b and w_s are bending component and shear component of lateral displacement of mid-plane, respectively. l_1 is length scale.

On the basis of Aifantis' gradient elasticity theory, one can express the variation of potential energy as follows [3]:

$$\delta U = \int_V \left(C_{ijkl} \left(\varepsilon_{kl} - l^2 \varepsilon_{kl,mm} \right) \right) \delta \varepsilon_{ij} dV \tag{6}$$

where ε_{kl} and $\varepsilon_{kl,mm}$ are the component of strain tensor and component of laplacian of strain tensor, respectively. l is length scale. C_{ijkl} is the component of stiffness matrix.

The external work of van der waals interactions between different layers can be expressed as:

$$\delta W = \int_A \sum_{i=1}^{N} \sum_{j=1}^{N} \bar{C}_{ij} \left(w_i - w_j \right) \left(\delta w_i - \delta w_j \right) dA, \; \bar{C}_{ii} = 0 \tag{7}$$

where $(-\bar{C}_{ij})$ is the coefficient of the spring stiffness used to simulate the van der waals interaction between layers.

Estimating the components of displacement of mid-plane (u_0, v_0, w) by shape functions satisfied geometrical boundary conditions and substituting Eqs. (2) to (7) as well as estimated shape functions into Eq. (1), one can obtain the system of ordinary differential equations governing eigen frequency equations.

3- Results and Discussion

After verifying the ability and the accuracy of present model to estimate natural frequencies of graphene and graphene like structures (see Table 1), the effects of temperature rise, length scale parameter, and layers arrangement on natural frequencies of in-plane strip heterostructures and multi-layered heterostructures are investigated.

Table 1: Comparison of first natural frequencies (GHz) of bilayer simply supported graphene sheets

ΔT, K	Length scale $l = l_1$, nm	Present study	MD [5]
0	0.115	50.42	50.42
100	0.35	39.63	39.62

The effect of layers arrangement on in-phase (ω_{11}) and out-of-phase ($\bar{\omega}_{11}$) natural frequencies of multi-layered simply supported heterostructures are listed in Table 2. Results clearly shows the influence of layers arrangement on out-of-phase natural frequency. It maybe because of the interlayer interactions which change with varying the layers arrangement. In-phase natural frequencies do not vary with changing layers arrangement because interlayer interactions are inactive in in-phase modes of vibration.

The effects of temperature rise and length scale parameter are shown in Fig.1. As it is seen, with an increase in the temperature, the natural frequencies decrease because of the softening effect of biaxial compressive thermal load. As expected, the natural frequencies decrease as the length scale increases. The similar behaviors can be seen in Tables 3 and 4, respectively.

Table 2: The effect of layers arrangement on in-phase and out-of-phase frequencies (ΔT=K, l=l_1=0 nm)

layers arrangement	$\bar{\omega}_{11}$, THz	ω_{11}, THz
BN/BN/G/BN/BN	1.9991	0.2465
G/BN/BN/BN/BN	1.9256	0.2465
BN/BN/BN/G/BN	1.9702	0.2465

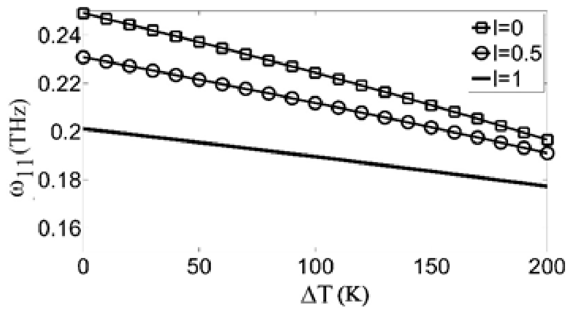

Fig.1: The effect of temperature rise and length scale on the in-phase natural frequency of BN/BN/G/BN/BN/G/BN/BN/G/BN/BN (l=$l_1$nm)

Table 3: The effect of small scale on fundamental natural frequency (THz) of the in-plane strip heterostructure (l=l_1=0.5nm)

No. of BN strips	ΔT = 0 K	ΔT = 100 K	ΔT = 200 K
1	0.1417	0.1410	0.1375
2	0.1401	0.1395	0.1361
3	0.1390	0.1385	0.1352

Table 4: The effect of small scale on fundamental natural frequency (THz) of the in-plane strip heterostructure (ΔT=0K, l=$l_1$nm)

No. of BN strips	l = 0 nm	l = 0.5 nm	l = 1 nm
1	0.1626	0.1417	0.1342
2	0.1605	0.1401	0.1332
3	0.1590	0.1390	0.1324

Tables 3 and 4 clearly reveal that if the number of BN strips used to construction of G/BN nano-sheet increase, the natural frequency decreases. It is worth mentioning that the data listed in Tables 3 and 4 are based on the assumption that the area occupied by BN-to-area occupied by graphene is constant.

4- Conclusions

The findings of this article can be summarized as follows:

1- The stiffness coefficient corresponding to van der waals interaction will change if the arrangement of layers changes; 2- In a multi-layered heterostructure, the variation of layers arrangement do not affect in-phase natural frequency of heterostructure significantly; 3- In a multi-layered heterostructure, the out-of-phase natural frequency can be maximized (minimized) by selecting proper layers arrangement; 4-With an increase in the temperature and/or length scale, the first in-phase natural frequency of the multi-layered heterostructure and natural frequency of in-plane strip heterostructure decrease; 5- In in-plane strip heterostructures in which the area occupied by BN-to-area occupied by graphene is constant, if the number of BN strips increase, the natural frequency decreases.

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