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# Size-dependent dynamic characteristics of graphene based multi-layer nano hetero-structures

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# Size-dependent dynamic characteristics of graphene based multi-layer nano hetero-structures

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## Abstract

Carbon-based nano hetero-structures are receiving increasing attention due their ability in multi-synchronous modulation of a range of mechanical and other critically desirable properties. In this paper, the vibration characteristics of two different graphene based heterostructures, graphene-hexagonal boron nitride (hBN) and graphene-molybdenum disulfide (MoS<sub>2</sub>), are explored based on atomistic finite element approach. Such vibrational characteristics of nanostructures are of utmost importance in order to access their suitability as structural members for adoption in various nano-scale devices and systems. In the current analysis, the developed atomistic finite element model for nano-heterostructures is extensively validated first with the results available in literature considering elastic responses and natural frequencies. Thereafter a range of insightful new results are presented for the dynamic behaviour of various configurations of graphene-hBN and graphene-MoS<sub>2</sub> heterostructures including their size, chirality and boundary dependence. The investigation of tunable vibrational properties along with simultaneous modulation of other mechanical, electronic, optical, thermal and chemical attributes of such nano-heterostructures would accelerate their application as prospective candidates for manufacturing nanosensors, electromechanical resonators, and a wide range of other devices and systems across the length-scales.

**Keywords:** 2D materials, dynamics of heterostructures, hexagonal nano-structures, atomistic finite element, graphene, hexagonal boron nitride, molybdenum disulfide

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## 1. Introduction

Since the discovery of superlative monolayers and thin films of graphite [1, 2], research interest in the engineering and scientific applications of carbon nanostructures has been growing exponentially due to their prospective unprecedented multi-functional applications in a range of nanoelectromechanical systems and devices. The superlatives identified in graphene has also lead to an increased interest in other possible two-dimensional (2D) materials that could offer exceptional electronic, optical, thermal, chemical and mechanical characteristics [3, 4, 5, 6]. Since the last decade curiosity in quasi-two-dimensional family of nano materials has grown from hexagonal boron nitride (hBN), boron-carbon-nitride (B-C-N), graphene oxides, chalcogenides such as molybdenum disulfide ( $\text{MoS}_2$ ), molybdenum diselenide ( $\text{MoSe}_2$ ) to stanene, silicene, sermanene, phosphorene, borophene etc [7, 8, 9, 10]. It is essential to investigate these materials at nanoscale since the superlative properties appear in atomic scale and in single or few layer forms [11]. 2D nano materials investigated in the literature are of various geometrical patterns and among these, hexagonally shaped (interesting to note that hexagonal shapes exist in various natural structures across different length scales [12, 13, 14, 15]) nano-structures are found in abundance [4, 10]. Such single layer nano materials have been extensively investigated using *ab initio* calculations [16, 17, 18], molecular dynamics (MD) [19, 20, 21] and molecular mechanics (MM) [22, 23, 24, 25, 26, 27] based approaches.

Though single layers of different 2D materials have shown exceptionally promising properties covering the electronic, optical, thermal, chemical and mechanical characteristics, they can not show multiple desirable properties in a single nanostructure. For example,  $\text{MoS}_2$  is rich in electronic and piezoelectric properties, but this is mechanically so weak that it can not be used in the nanoelectromechanical devices. On the other hand graphene is mechanically very strong. Thus it is possible to combine these two nanostructures to form a single heterostructure, where the electronic and piezoelectric properties as well as mechanical strength can be achieved. Considering the emergence of so many single layer 2D nanostructures with their diverse properties and possibility of combining them in different stacking sequences open up a whole new domain of research for developing nanostructures with tunable multi-synchronous properties (analogous to metamaterials [28, 29] at nanoscale). Besides the electronic, optical, thermal and chemical properties of heterostructures, recent studies can be found in literature

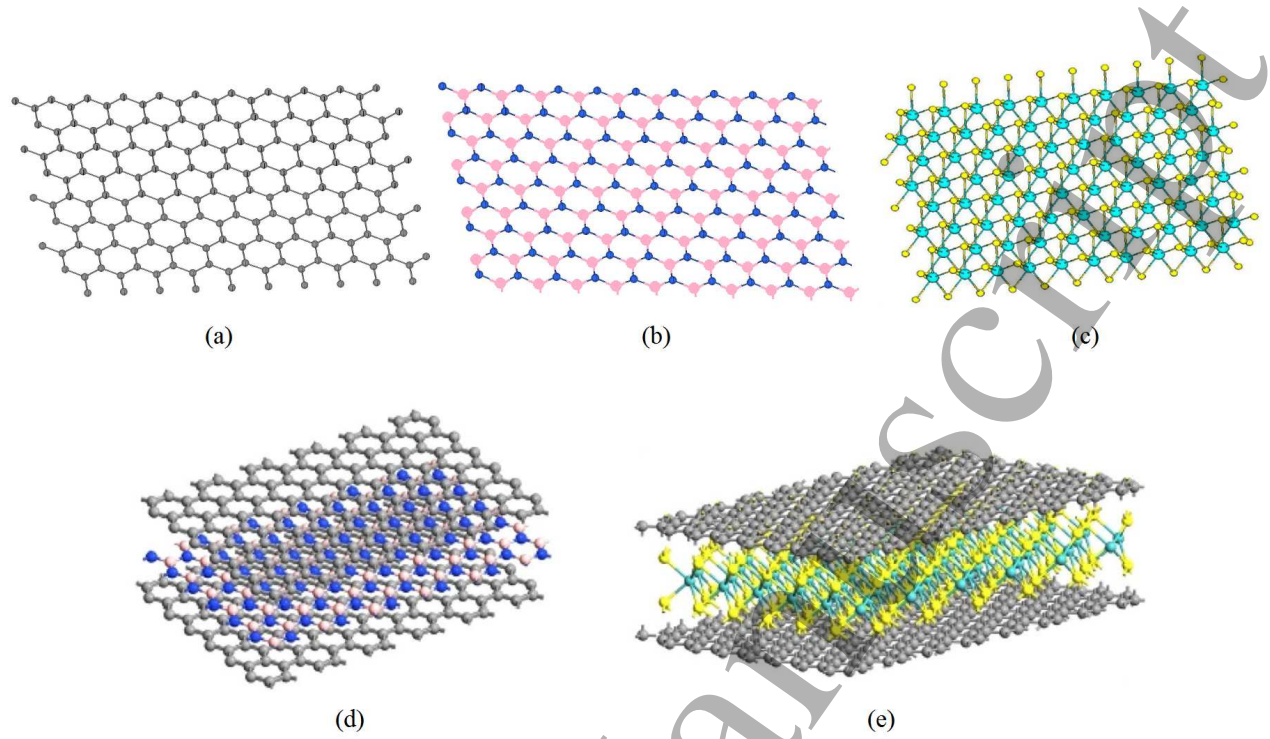


Figure 1: Isometric views of nanostructures and heterostructures. (a) Graphene (monoplanar nanostructure) (b) hBN (monoplanar nanostructure) (c) MoS<sub>2</sub> (multiplanar nanostructure, refer to figure 2(a) for further structural details) (d) Graphene-hBN heterostructure (hBN layer sandwiched between two graphene layers) (e) Graphene-MoS<sub>2</sub> heterostructure (MoS<sub>2</sub> layer sandwiched between two graphene layers). Black dots: carbon atoms, pink dots: boron atoms, blue dots: nitrogen atoms, aqua dots: molybdenum atoms and yellow dots: sulphur atoms.

focusing on their effective mechanical properties [30, 31, 32, 33, 7, 34, 35, 36].

Vibrational characteristics of nanostructures are of utmost importance in order to access their performance as structural members for adoption in nano-scale devices and systems. However, barring a single investigation [37], the dynamics and vibration of nano-heterostructures have not received any attention yet. Thus here we aim to investigate the size-dependent dynamic behavior of nano hetero-structures in terms of natural frequencies and mode shapes by developing a generic atomistic finite element (FE) model. In this context, it can be noted that 2D material monolayers could have either all the atoms situated in a single plane (such as graphene, hBN), or the atoms may be situated in different planes (such as MoS<sub>2</sub>), referred as monoplanar and multiplanar nanostructures respectively [10]. In this article, we would focus on two different forms of graphene based heterostructures by stacking graphene with both monoplanar (graphene-hBN) and multiplanar (graphene-MoS<sub>2</sub>) structures (refer to figure 1).

Hereafter this paper is organised as follows. In the second section, the derivation for mechanical equivalence of atomic bonds is shown. This is followed by an overview of the

atomistic simulation methodology utilized to model nano hetero-structures (third section). Here we describe the finite element based atomistic modelling of individual sheets of graphene, hBN, MoS<sub>2</sub> and the weak van der Waals interactions between them. The results and discussion are presented in the fourth section. The atomistic finite element model of the heterostructure is first validated against available results from literature considering two different mechanical properties, Young's modulus and natural frequency. After gaining adequate confidence on the atomistic finite element model through extensive validation, we have presented new results for detailed dynamic analysis of graphene-hBN and graphene-MoS<sub>2</sub> nano hetero-structures. The results investigate the influence size parameters (length, aspect ratio), boundary conditions and chirality on the natural frequencies and mode shapes of nano hetero-structures. In the final section, concluding remarks are given along with a perspective of the current analysis.

## 2. Mechanical equivalence of atomic bonds

In case of the atomic scale behaviour of materials, total inter-atomic potential energy can be expressed as a summation of various individual energy components relevant to bonding and non-bonding atomic interactions [22, 10]. Total strain energy ( $E_E$ ) can be represented as summation of the energy components from bond bending ( $E_b$ ), stretching of bonds ( $E_s$ ), bond torsion ( $E_t$ ) and energies contributed by non-bonded terms ( $E_{nb}$ ) like van der Waals attraction, core repulsions and coulombic energy.

$$E_E = E_s + E_b + E_t + E_{nb} \quad (1)$$

The influence of stretching and bending is significant in case of small deformations as compared to all other energy components [24, 38]. For the case of hexagonal multiplanar structures (like MoS<sub>2</sub>), the strain energy due to bending is contributed by two different components, in-plane ( $E_{bI}$ ) and out-of-plane ( $E_{bO}$ ) [10]. The deformation mechanisms for the multiplanar nanostructure (like MoS<sub>2</sub>) are shown in figure 2 – 3. The out-of-plane angular component reduces to zero for monoplanar structures (like graphene and hBN). The total inter-atomic potential energy ( $E_E$ ) can be expressed as

$$\begin{aligned} E_E &= E_s + E_{bI} + E_{bO} \\ &= \frac{1}{2}k_r(\Delta l)^2 + \left( \frac{1}{2}k_\theta(\Delta\theta)^2 + \frac{1}{2}k_\theta(\Delta\alpha)^2 \right) \end{aligned} \quad (2)$$

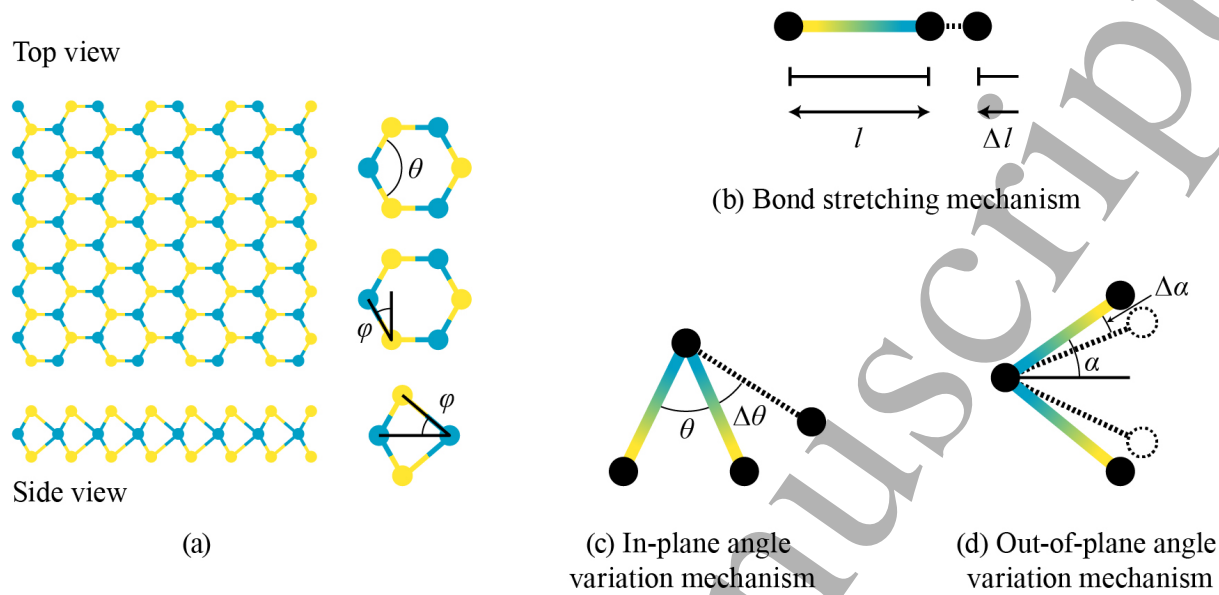


Figure 2: (a) Top and side views of a multiplanar hexagonal nanostructure such as MoS<sub>2</sub> (b) Bond stretching induced strain energy (c) In-plane angle variation induced strain energy (d) Out-of-plane angle variation induced strain energy.

where  $\Delta l$ ,  $\Delta\theta$  and  $\Delta\alpha$  are the variation in bond length, variation in in-plane angle and variation in out-of-plane angle respectively (refer to figure 2). The parameters  $k_r$  and  $k_\theta$  are the force constants associated with bond stretching and bending respectively. The first term in Equation 2 represents strain energy relevant to stretching ( $E_s$ ), while the other terms represent the strain energies contributed by in-plane ( $E_{bI}$ ) and out-of-plane ( $E_{bO}$ ) angle deformation, respectively.

The force constants of atomic bonds ( $k_r$  and  $k_\theta$ ), as described above, can be expressed in the form of structural mechanics equivalence [39]. As per classical structural mechanics theory (refer to figure 3), strain energy of a uniform circular beam with length  $l$ , cross-sectional area  $A$ , second moment of area  $I$  and Young's modulus  $E$  under pure axial force  $N$  (refer to figure 3(b)) can be expressed as

$$U_a = \frac{1}{2} \int_0^L \frac{N^2}{EA} dl = \frac{1}{2} \frac{N^2 l}{EA} = \frac{1}{2} \frac{EA}{l} (\Delta l)^2 \quad (3)$$

The strain energies due to pure bending moment  $M$  (refer to figure 3(c)) can be written as

$$U_b = \frac{1}{2} \int_0^L \frac{M^2}{EI} dl = \frac{1}{2} \frac{EI}{l} (2\Delta\phi)^2 \quad (4)$$

Comparing Equation 3 with Equation 2 for the expression of strain energy due to stretching



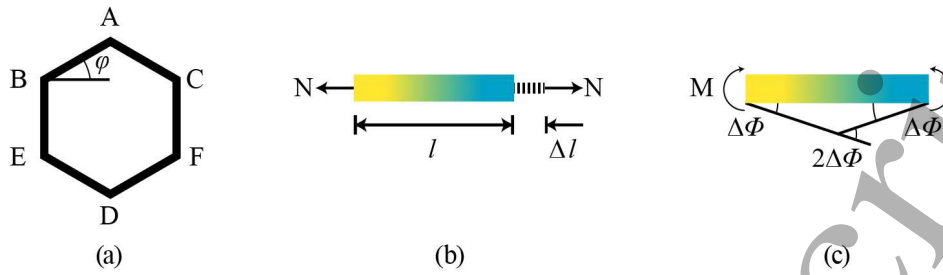


Figure 3: (a) A hexagonal unit cell involving of 6 idealized beam elements (refer to figure 2(a)) (b) A beam element under the influence of pure tension (c) A beam element under the influence pure bending.

( $E_s$ ), it can be concluded that  $K_r = \frac{EA}{l}$ . As per figure 3(c), it is reasonable to assume for bending that  $2\Delta\phi$  is equivalent to  $\Delta\theta$  and  $\Delta\alpha$  for in-plane and out-of-plane angle deformations respectively. Thus comparing Equation 4 with the expressions for the strain energies due to in-plane ( $E_{bI}$ ) and out-of-plane ( $E_{bO}$ ) angle deformations (refer Equation 2), the following equivalence can be obtained:  $k_\theta = \frac{EI}{l}$ . Such mechanical equivalence between molecular mechanics parameters ( $k_r$  and  $k_\theta$ ) and structural mechanics parameters ( $EA$  and  $EI$ ) can be used to derive beam (covalent bond) properties used in the atomistic simulations. In the current work, the effective elastic moduli and natural frequencies of nano hetero-structures are computed by using these beams representing covalent bonds.

### 3. Atomistic finite element model of nano heterostructures

The concept of idealizing atomic bonds as equivalent beam elements, as presented in the preceding section, is utilized to model the nano-heterostructures in a finite element based framework [40, 41, 42, 43]. It is the first ever attempt to develop any such atomistic finite element model for heterostructures, which could be a generic computationally efficient framework for characterizing the vibrational properties. In this research work, the finite element analysis tool OPTISTRUC [44] has been used to model the dynamic behaviour of nano hetero-structures. The covalent bonds are represented by 3D Timoshenko finite element beams and the atoms are represented by finite element nodes. Within the finite element analysis tool OPTISTRUC, the element type CBEAM has been used to represent beams. The cross sectional diameter and the Young's modulus ( $E$ ) of the beam elements are computed by using the equations of force-field constants  $K_r$ (stretching) and  $K_\theta$ (bending), as described in section 2.



Table 1: Bond angles and sheet thickness for nano materials[10]. Refer figure 2 for angle representations.

Nanomaterial	$\alpha$ (in $^\circ$ )	$\theta$ (in $^\circ$ )	Sheet thickness (nm)
Graphene	0	120	0.34
hBN	0	120	0.098
MoS <sub>2</sub>	48.15	120	0.603

Table 2: Bond properties for each individual nano material[10].

Nanomaterial	$K_r$ in N nm <sup>-1</sup>	$K_\theta$ in N-nm-rad <sup>-2</sup>	$L$ in nm	$d$ in nm	$E$ in GPa
Graphene	$6.52e-7$	$8.76e-10$	0.142	0.146	1370.91
hBN	$4.86e-7$	$6.95e-10$	0.145	0.151	1047.1
MoS <sub>2</sub>	$1.64e-7$	$1.67e-9$	0.242	0.403	882.1

The numerical values of force constants  $K_r$  and  $K_\theta$  along with the necessary geometric attributes (bond lengths and bond angles) are shown in the Table 1 - 2 [10]. By substituting these values in the equations  $K_r = \frac{EA}{l}$  and  $k_\theta = \frac{EI}{l}$ , essential parameters to model covalent bonds such as beam diameter  $d$  and beam Young's modulus  $E$  can be calculated. The calculated values of beam diameter and beam Young's modulus are shown in Table 2, wherein it is evident that MoS<sub>2</sub> has the highest interatomic bond length, while graphene has the lowest bond length among the three materials considered in this work. The C-C bond length within graphene sheets is very close to that of B-N bond length in hBN sheets. Atomic masses of carbon, boron, nitrogen, molybdenum and sulphur have been considered by modeling mass elements on the nodes. The atomic masses considered here are  $1.9943 \times 10^{-26}$  kg,  $1.7952086 \times 10^{-26}$  kg,  $2.3258671 \times 10^{-26}$  kg,  $1.593121 \times 10^{-25}$  kg and  $1.593121 \times 10^{-23}$  kg for carbon, boron, nitrogen, molybdenum and sulphur, respectively. Within the finite element analysis tool OPTISTRUCT [44], the element type CONM2 has been used to represent masses.

Interlayer interaction between two adjacent layers of a heterostructure can be modelled using Lennard-Jones (L-J) potential. The equivalent axial force for an L-J potential between pair of atoms (i, j) belonging to different nano layers is defined as [45]

$$F_{ij} = \frac{\partial V_{ij}}{\partial r} \quad (5)$$

where  $r$  denotes the atomic displacement along  $ij$  (layer-layer length). The force between two

Table 3: Constants of L-J potentials.

Nanomaterial	$\epsilon$ in meV	$\sigma$ in Å	Source
C-Mo	3.325	2.82	[32]
C-S	7.355	3.22	[32]
Mo-Mo	2.43	2.72	[33]
S-S	1.19	3.59	[33]
Mo-S	2.49	3.16	[33]
C-B	3.6	2.2132	[46]
C-N	9	3.2222	[46]
B-B	4.16	3.453	[47]
N-N	6.281	3.365	[47]

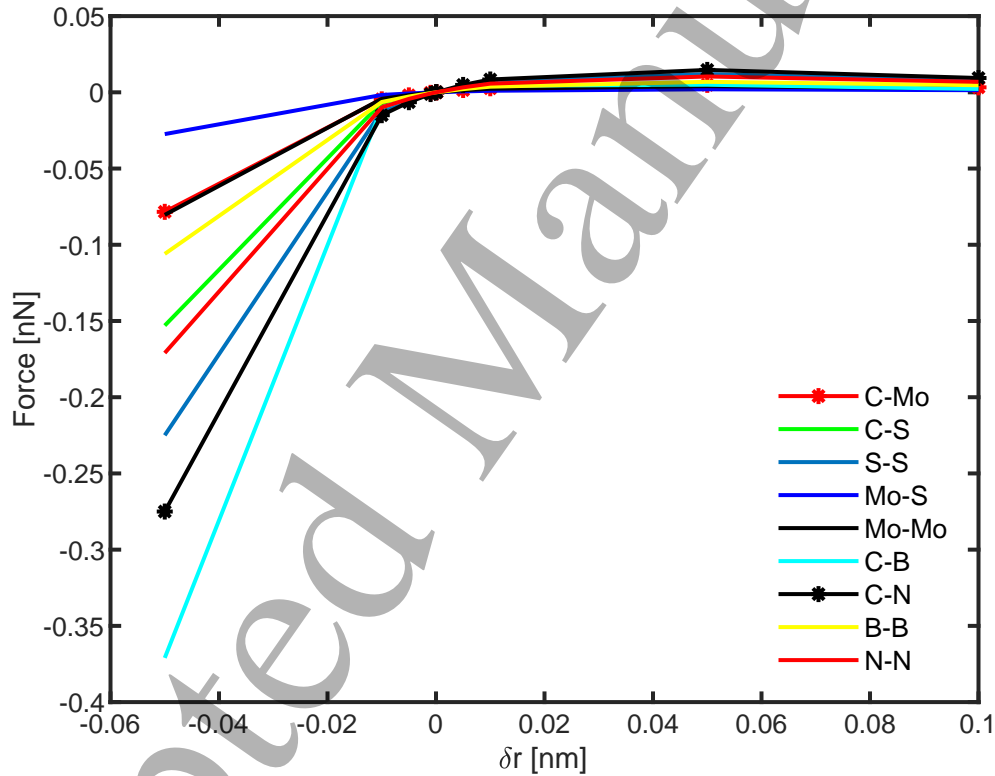


Figure 4: Curves of L-J potential forces obtained by Equation 6.

atoms ( $ij$ ) can also be expressed as [48]

$$F_{ij} = -12\epsilon \left[ \left( \frac{r_{min}}{y} \right)^{13} - \left( \frac{r_{min}}{y} \right)^7 \right] \quad (6)$$

where,  $y = r_{min} + \delta r$ , and  $\delta r$  represents the atomic displacement along the length of  $\mathbf{ij}$ . The quantity  $r_{min}$  (in Å) is given by  $2^{\frac{1}{6}} \sigma$ , where  $\sigma = (A/B)^{1/6}$ . The parameters  $B$  and  $A$  denote attractive and repulsive constants, respectively. In the current research work, three different nano sheets are considered namely graphene, hBN and MoS<sub>2</sub>. Thereafter heterostructures

of graphene-hBN and graphene-MoS<sub>2</sub> are studied under dynamic conditions. These heterostructures lead to C-B, C-N, B-B, N-N, C-Mo, C-S, Mo-Mo, Mo-S and S-S atomic interactions, where C, B, N, Mo and S are carbon, boron, nitrogen, molybdenum and sulphide atoms, respectively. The values of  $\sigma$  and  $\epsilon$  for each individual van der Waals atomic interactions are given in Table 3. These values have been obtained from various references [32, 33, 46, 47]. In the atomistic FE simulations, we have modelled spring elements to obtain a nonlinear connection between two adjacent layers of a heterostructure representing the L-J interactions. The force-deflection curve for such L-J springs are calculated by using Equation 6, as shown in figure 4. Within the finite element analysis tool OPTISTRUCT [44], the L-J springs of interlayer interactions are modeled by element type CBUSH incorporating the curves of figure 4 as input properties.

In the atomistic FE approach, coupled nano sheets of heterogenous nature are modeled like space-frame structures. Overall stiffness and mass matrices of the atomistic FE models are obtained by assembling the equivalent matrices of the beams representing C-C, C-S, Mo-Mo, S-S, Mo-S, C-B, C-N, B-B and N-N bonds and the concentrated masses situated at each node. Here the lumped mass matrix in case of a single beam element can be expressed as:

$$[\mathbf{M}]_e = \text{diag} \left[ \frac{m_a}{n} \quad \frac{m_a}{n} \quad \frac{m_a}{n} \quad 0 \quad 0 \quad 0 \right] \quad (7)$$

where  $m_a$  (in kg) is the mass of atoms and  $n$  is the number of bonds attached to an atom in the nanosheet. To obtain the natural frequencies and mode shapes of nano-heterostructures, the general equation of motion of an undamped system ( $[\mathbf{K}]\mathbf{x} + [\mathbf{M}]\ddot{\mathbf{x}} = \mathbf{0}$ ) leading to the standard eigenvalue problem ( $([\mathbf{K}] - \omega^2 [\mathbf{M}]) \{\mathbf{x}\} = \{\mathbf{0}\}$ ) can be solved using Block Lanczos algorithm [49] within the atomistic finite element analysis code [44].

#### 4. Results and discussion

Here we start by validating the developed atomistic finite element model of heterostructures using two different mechanical properties, Young's modulus and natural frequency. After gaining adequate confidence on the proposed model, insightful new results are presented for the dynamic behaviour of graphene based heterostructures including the effect of size, boundary condition and chirality.

#### 4.1. Validation of Young's modulus ( $E$ ) of graphene, hBN and MoS<sub>2</sub>

In this subsection, the Young's modulus of graphene, hBN and MoS<sub>2</sub> has been obtained using the atomistic finite element method and compared with the corresponding values available in literature. For each nano material, the elastic analysis has been performed in zigzag and armchair directions. With respect to armchair and zigzag directions, one end of the nano sheet has been constrained and an unit load has been applied to the other end. The unit load has been introduced through a rigid element (multi point constraint) connected to the group of nodes at the end of nanosheet. The resulting strain due to the applied unit load has been numerically calculated using the atomistic FE simulations. Based on this strain and applied stresses due to the unit load, the Young's modulus of the 2D materials has then been obtained. Here the Young's modulus with respect to armchair direction is referred as  $E_1$  and that with respect to zigzag direction is referred as  $E_2$ . The Young's moduli  $E_1$  and  $E_2$  have been converted to tensile rigidities  $E_{1T}$  and  $E_{2T}$  by multiplying the corresponding modulus with the sheet thickness shown in the Table 1.

For the case of graphene and hBN sheets, four separate finite element models have been constructed with sheet sizes  $1.775 \text{ nm} \times 3.074 \text{ nm}$ ,  $1.775 \text{ nm} \times 3.813 \text{ nm}$ ,  $1.775 \text{ nm} \times 4.55 \text{ nm}$  and  $1.775 \text{ nm} \times 5.534 \text{ nm}$ . The largest among these four finite element models has resulted in upto 654 beam elements and 513 nodes. The aspect ratio of these four finite element models are 1.73, 2.14, 2.56 and 3.11. Also, for the case of MoS<sub>2</sub> sheets, 4 separate finite element models have been constructed with sheet sizes  $1.483 \text{ nm} \times 2.625 \text{ nm}$ ,  $1.483 \text{ nm} \times 2.94 \text{ nm}$ ,  $1.483 \text{ nm} \times 3.359 \text{ nm}$  and  $1.483 \text{ nm} \times 4.199 \text{ nm}$ . The largest among these four finite element models has resulted in upto 958 beam elements and 587 nodes. The aspect ratio of these four finite element models are 1.77, 1.98, 2.26 and 2.83. The variation of  $E_{1T}$  and  $E_{2T}$  against aspect ratio (AR) for all three nano materials are shown in figure 5. Within these plots, are also presented the  $E_{1T}$  and  $E_{2T}$  obtained from literature [10]. The authors [10] considered an analytical closed-form formula to determine unique values of  $E_{1T}$  and  $E_{2T}$  of graphene, hBN and MoS<sub>2</sub> by considering a single hexagonal unit cell of each nano material. Due to this fact, the curves from the literature [10] remain flat in the plots of figure 5. As per these plots, the numerically predicted values are quite close to that of the analytical prediction of literature. However, the current values are found to be slightly lower as compared

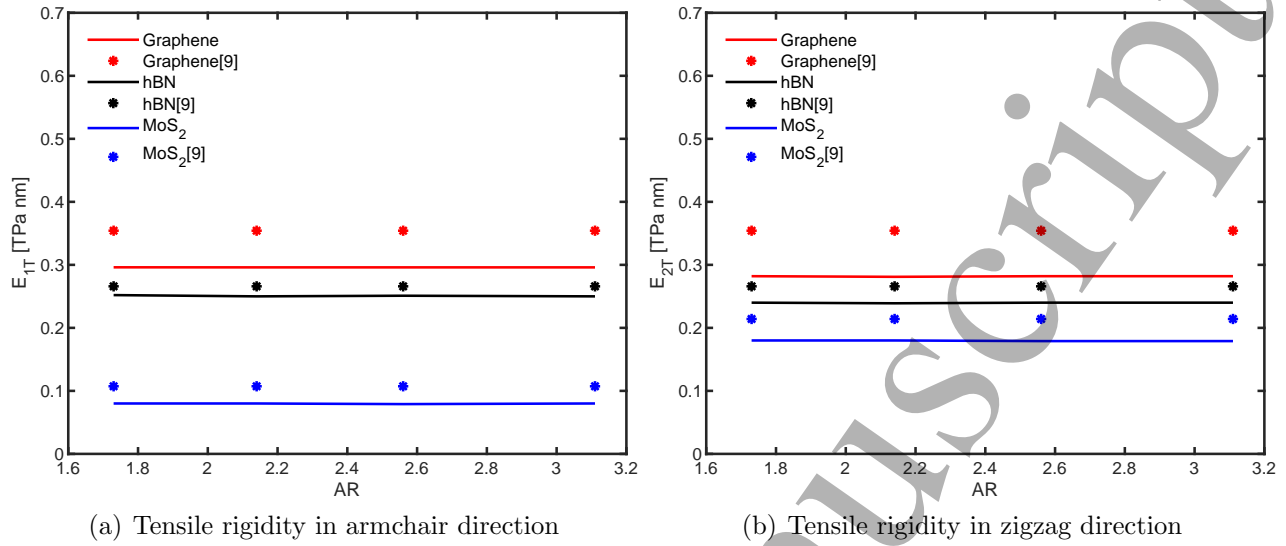


Figure 5: Variation of tensile rigidity against aspect ratio (AR). The results obtained using the current atomistic FE simulations are validated against literature [10].

to the analytical predictions of literature. This can be attributed to the fact that the analytical predictions are based on a single unit cell, where the shear deformations were neglected. In the current numerical analysis shear based deformation is allowed in the lattice system considering Timoshenko finite element beams, leading to more flexibility in the nanosheets. Moreover, within the atomistic finite element simulations multiple number of unit cells in each sheet are considered, resulting in a high number of beam elements. As the number of beam elements increases, more flexibility is added to the model. The cumulative effect of such flexibility can underpredict the elastic modulus of the nano structures. The variation of tensile rigidities with respect to aspect ratio is found to be negligible in figure 5. At larger aspect ratios ( $> 10$ ), the values of tensile rigidities increase slightly ( $< 1\%$ ). Furthermore, the numerically obtained single layer tensile rigidities have also been compared against the results from various other publications covering *ab initio* calculations, molecular dynamic simulations and experimental investigations (refer to Table 4). From the results presented in this subsection, it can be concluded that the tensile rigidities calculated using the atomistic FE model are in good agreement with the numerical values available in literature, corroborating the validity of the developed computational model. In the Table 4, for the case of graphene, the current approach predicted tensile rigidity ( $E_{1T}=0.296$  TPa nm) close to that of experimental work [51] (0.306 TPa nm). For the case of hBN and MoS<sub>2</sub>, the current predicted tensile rigidity values are

Table 4: Results for Young's moduli in the form of tensile rigidity( $E_T$ ) compared against the values from literature.  $E_{1T}$  and  $E_{2T}$  are tensile rigidities in two directions taken from the current work. Similar to the present results, Mukhopadhyay et al. [10] reported different values of Young's modulus in the longitudinal and transverse directions of MoS<sub>2</sub>.

Material	Present Results (TPa nm)	Reference results from literature ( $E_T$ in TPa nm)
Graphene	$E_{1T} = 0.296$ $E_{2T} = 0.282$	Experimental: 0.34 [50], 0.306 [51] <i>Ab initio</i> : 0.350 [52], 0.357 [18], 0.377 [53], 0.364 [54] Molecular Dynamics: 0.357 [55], 0.343 [56] Molecular Mechanics: 0.354 [24], 0.3604 [22], 0.354 [10]
hBN	$E_{1T} = 0.252$ $E_{2T} = 0.240$	Experimental: 0.251 [57] <i>Ab initio</i> : 0.271 [52], 0.272 [58] Molecular Dynamics: 0.236 [59], 0.278 [60] Molecular Mechanics: 0.269 [61], 0.322 [62], 0.265 [10]
MoS <sub>2</sub>	$E_{1T} = 0.080$ $E_{2T} = 0.180$	Experimental: 0.211 [63], 0.163 [64] <i>Ab initio</i> : 0.141 [65], 0.262 [66] Molecular Dynamics: 0.150 [67] Molecular Mechanics: 0.107 ( $E_{1T}$ ) and 0.214 ( $E_{2T}$ ) [10]

also found to be close to that of experimental works [57, 64]. Such a close correlation indicate that the present numerical results agree very well with experimental works obtained under more realistic conditions. The discrepancies between the current numerical results, and the MM/MD based results can be due to various reasons such as omission of non bonded energy terms in Equation 1 and presence of degrees of freedom including shearing effect within the Timoshenko finite elements representing covalent bonds.

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#### 4.2. Validation of natural frequencies of nano-heterostructures

After validating the developed atomistic finite element model with respect to the Young's moduli of 2D materials, here we present a further verification/ validation for the dynamic behaviour of nano-heterostructures considering a combination of graphene and hBN. This section involves dynamic analysis of graphene-hBN triple layer nano hetero-structure, wherein alternating graphene and hBN sheets have been overlapped into three layers. This configuration has been chosen to validate the present numerical model against the molecular dynamics (MD) model of similar configuration available in literature [37]. In order to validate the atomistic FE dynamic models, the modal analysis has been performed by constraining two edges of the multi-layer nano-heterostructures. Four separate finite element models have been constructed with sheet sizes  $5.534 \text{ nm} \times 12.121 \text{ nm}$ ,  $5.534 \text{ nm} \times 13.789 \text{ nm}$ ,  $5.534 \text{ nm} \times 18.101 \text{ nm}$  and  $5.534 \text{ nm} \times 20.112 \text{ nm}$ . For these four finite element models, the width has been kept constant at  $5.534 \text{ nm}$  and the length has been varied from  $12.121 \text{ nm}$  to  $20.112 \text{ nm}$ . These dimensions, boundary conditions and layer combinations have been chosen in order to replicate the MD simulations available in literature [37].

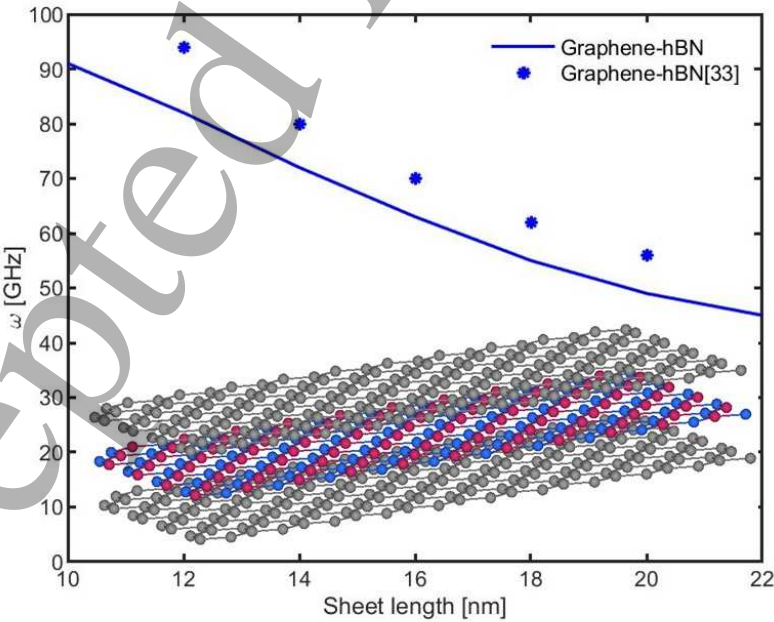


Figure 6: Comparison of natural frequency of current work against the values available in literature [37]. A schematic representation of the considered heterostructure is shown in the inset, wherein the two outer layers are graphene and the middle layer is hBN.



The variation of the natural frequency with respect to the sheet lengths is shown in figure 6. This plot presents two curves, a curve from the current atomistic FE simulations and a curve extracted from the MD results [37]. The trend of variation in the current work is comparable with that of the MD simulation [37]. Both atomistic FE and MD simulations predict a drop in natural frequency as the length of multilayer nano hetero-structure sheet is increased. However, the natural frequencies predicted by the atomistic FE simulations are found to be lower than those predicted by MD simulations. This is due to the fact that the number of numerical approximations happening within the finite element analysis including round off approximations and beam element six degrees of freedom (leading to sheet flexibility). Other reasons such as omission of non bonded energy terms in Equation 1 and shearing effect within the Timoshenko beam finite elements can also contribute to such discrepancies. At higher lengths, the results of atomistic FE simulations tend to converge towards those of MD simulations. Also, the curve of natural frequency between the lengths 18.101 nm and 20.112 nm appears to be relatively flat as compared to the rest of the curve. This further proves that, as the atomistic space frame lattice of nano-structures becomes larger in dimension, it simulates a continuous plate similar to earlier reports for bilayer and single layer graphene sheets [43]. It can be noted that the results presented in subsection 4.1 and 4.2 comprehensively establish the validity and confidence in the developed atomistic FE model. Hereafter new results on the dynamic behaviour of graphene based heterostructures are presented following the developed computational model.

#### 4.3. Higher order modal behaviour of nano hetero-structures

In this subsection we have studied three higher order modes of nano-heterostructures except the first mode of vibration. To understand the nature of dynamic features, mode shapes are required to be studied for a complex system. In order to demonstrate the mode shapes associated with natural frequencies, the 1st four mode shapes are presented in this section. Prior to enforcing boundary conditions, an initial free-free modal simulation has been carried out to verify the dynamic behaviour of the double-layer structures without the influence of external clamps and/or supports. A free-free run involves extracting and verifying rigid body mode shapes without any constraints, in order to ensure the integrity of the structure. The boundary condition used to perform modal analysis is cantilevered condition (Ref figure 7).

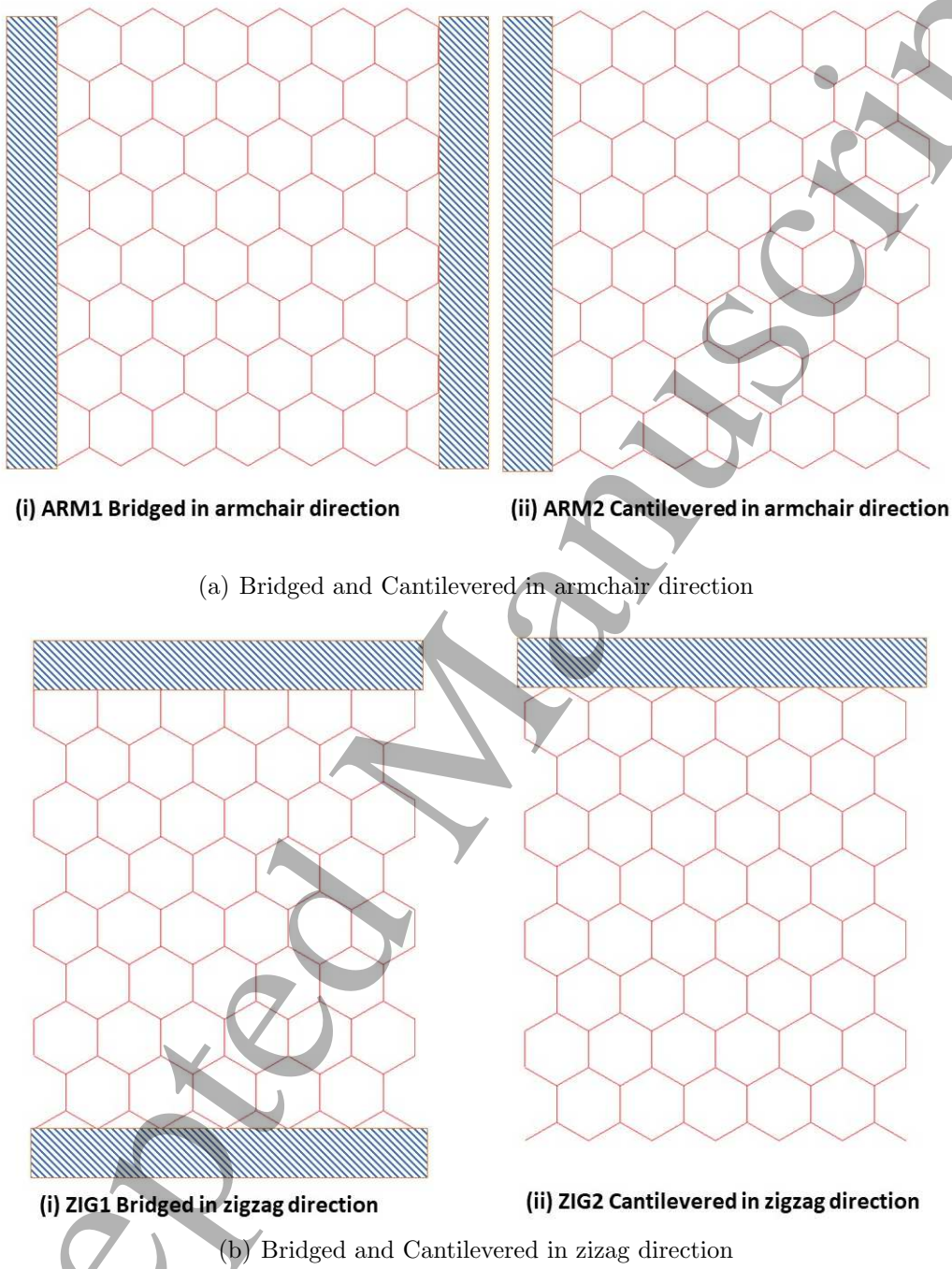


Figure 7: Depiction of bridged and cantilever boundary conditions (the marked edges are fully constrained in all six degrees of freedom).

Cantilever condition involves clamping at one edge and setting free other three edges of the nanostructures. Modal analysis has been performed on graphene-hBN and graphene-MoS<sub>2</sub> nano hetero-structures. Chosen size of both heterostructures is 10.5 nm × 3.5 nm. Such a dimension will lead to a nano ribbon type rectangular sheet with an aspect ratio 3. The

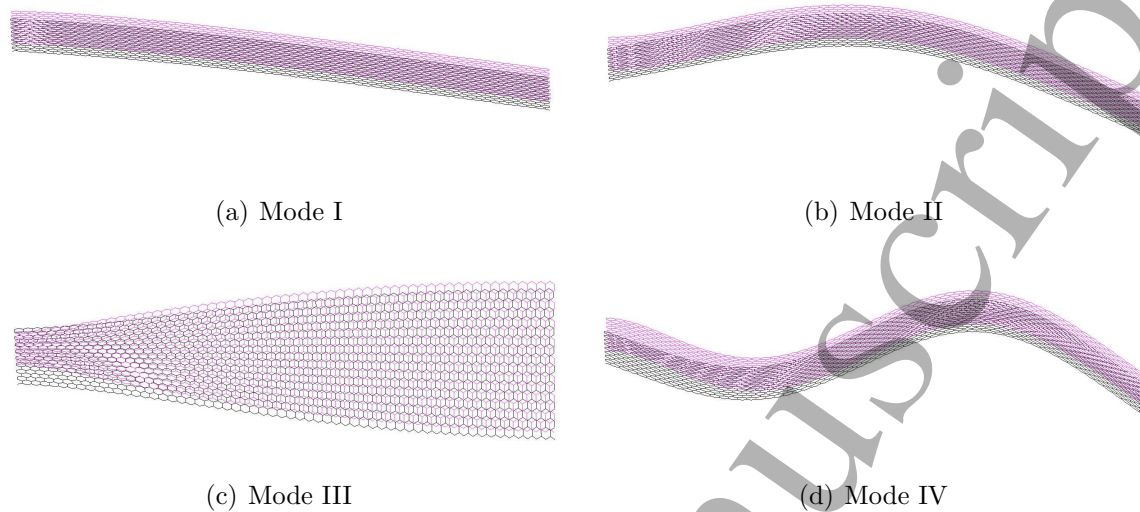


Figure 8: First four mode shapes of graphene-hBN nano hetero-structure.

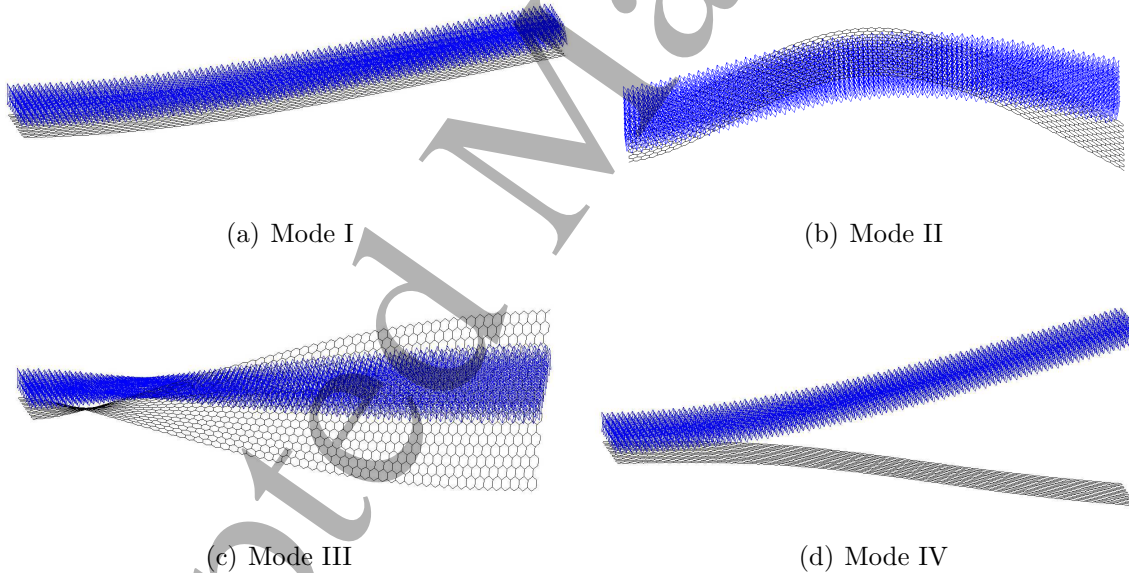


Figure 9: First four mode shapes of graphene-MoS<sub>2</sub> nano hetero-structure.

first four mode shapes for graphene-hBN and graphene-MoS<sub>2</sub> heterostructures are shown in figure 8 and figure 9. The first four natural frequencies for graphene-hBN heterostructure are 122 GHz, 144 GHz, 187 GHz and 202 GHz, while the corresponding values for graphene-MoS<sub>2</sub> heterostructure are 102 GHz, 131 GHz, 154 GHz and 190 GHz.

For the case of graphene-hBN, first mode shape is an out of plane bending with a cantilever tip motion, second mode shape is an out of plane bending with single waviness, third mode

shape is a torsional twisting mode and the fourth mode shape is an out of plane bending with double waviness. These mode shapes are comparable to that of bilayer graphene [43]. For the case of graphene-MoS<sub>2</sub>, first mode shape is an out of plane bending with a cantilever tip motion, second mode shape is a non-homogenous out of plane bending, third mode shape is a non-homogenous twist and fourth mode shape is an out of plane opening mode. Importantly, inter layer penetrative waviness has been observed in the second mode shapes of graphene-MoS<sub>2</sub>. Such a waviness and the presence of sheet separation modes (mode II, mode III and mode IV) in graphene-MoS<sub>2</sub>, indicates that the layer-layer interaction stiffness (weak van der Waals/L-J potentials) is lower in graphene-MoS<sub>2</sub> as compared to graphene-hBN. Thus under a dynamic condition, the graphene-MoS<sub>2</sub> heterostructure shows more susceptibility to a failure following this mechanism. Interestingly, the interlayer interaction plays an important role in case of dynamic analysis of heterostructures unlike the case of static elastic analyses, where the weak van der Waals effects have negligible contribution [30]. It is important to note that the presence of out of plane bond angle (Ref figure 2 and Table 1) in MoS<sub>2</sub> reduces the degree of interaction with any adjacent nanosheet. The first mode shapes for graphene-hBN and graphene-MoS<sub>2</sub> are similar. The other three higher order mode shapes for the two types of nano hetero-structures considered here differ from each other significantly. Such a difference indicate that the graphene-MoS<sub>2</sub> hetero-sheets are useful in nano oscillatory applications where sheet separation modes are needed.

#### 4.4. Size-dependence in natural frequency of nano-heterostructures

In this section, we investigate the effect of size of nanosheets on the first natural frequencies of heterostructures considering different boundary conditions with varying length. The results of fundamental natural frequency of armchair and zigzag graphene-hBN heterostructure is presented in figure 10, for bridged and cantilevered boundary conditions. It can be seen that for armchair graphene-hBN heterostructures (width = 4.08 nm) with the increasing length from  $\sim 11\text{\AA}$  to  $\sim 160\text{\AA}$  have fundamental frequencies in the range between 380 - 7 GHz for cantilever condition and 880 - 82 GHz for bridged condition. The zigzag graphene-hBN heterostructures (width = 4.1 nm) have their natural frequencies distributed between 330 - 5 GHz and 770 - 79 GHz for cantilevered and bridged boundary conditions respectively, with increasing lengths between  $12\text{\AA}$  to  $168\text{\AA}$ . The trend observed here (refer to figure 10)

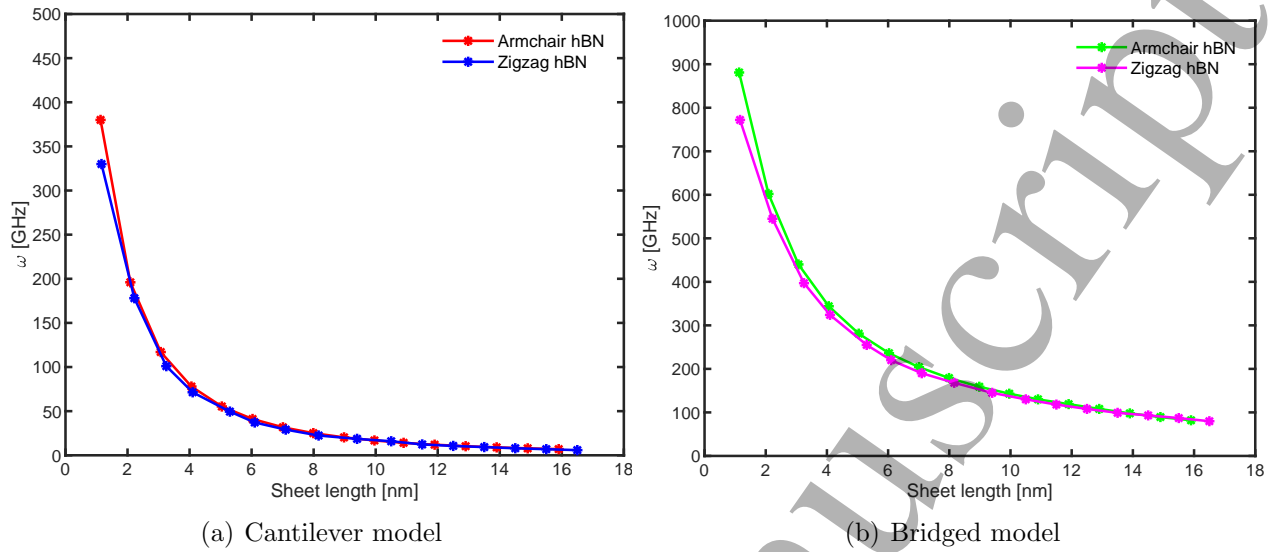


Figure 10: The dependence of natural frequency on sheet length: (a) Cantilevered boundary condition - fundamental natural frequency of armchair and zigzag graphene-hBN heterostructure as a function of sheet length. (b) Bridged boundary condition - fundamental natural frequency of armchair and zigzag graphene-hBN heterostructure as a function of sheet length.

is similar to the one identified for single layer graphene [68] and bi layer graphene [43]. The results of the fundamental frequencies of armchair and zigzag graphene-MoS<sub>2</sub> are presented in figure 11, for bridged and cantilevered boundary conditions. It can be seen that for armchair graphene-MoS<sub>2</sub> heterostructures (width = 4.08 nm) with the increasing length from  $\sim 11\text{\AA}$  to  $\sim 160\text{\AA}$  have fundamental frequencies in the range between 296 - 5 GHz for cantilever condition and 680 - 63 GHz for bridged condition; while the zigzag graphene-MoS<sub>2</sub> (width = 4.1 nm) have instead their natural frequencies distributed between 255 - 4 GHz and 598 - 58 GHz for cantilevered and bridged boundary conditions respectively, with increasing lengths between  $12\text{\AA}$  to  $168\text{\AA}$ . The trend observed (refer to figure 10) is again similar to the one identified for single layer graphene [68] and double layer graphene [43]. In general it can be concluded that an increase in sheet length leads to a reduction in natural frequency.

In figure 12 and figure 13, the variations of natural frequencies for graphene-hBN and graphene-MoS<sub>2</sub> heterostructures with respect to length at a given aspect ratio are presented. The pattern of variation here is qualitatively similar to that of single [68] and double layer [43] graphene. This is due to the fact that all nano sheets considered are 2D in nature and they have hexagonal cells. It can be observed from the figures that sheet length has a significantly more predominant effect on the natural frequency compared to aspect ratio. As per figure 12



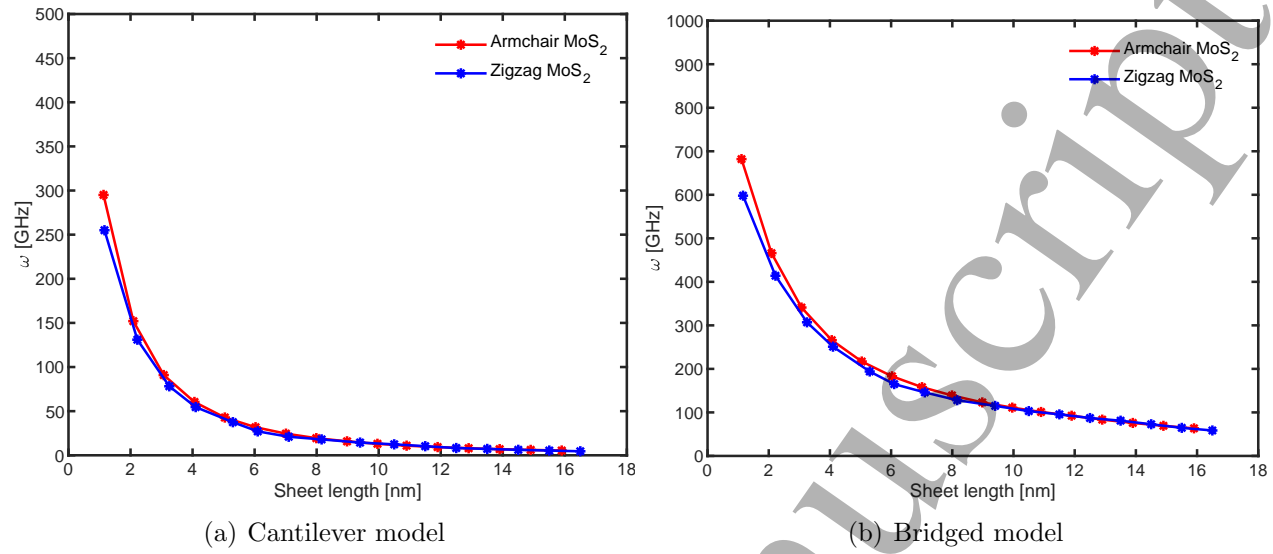


Figure 11: The dependence of natural frequency on sheet length: (a) Cantilevered boundary condition - fundamental natural frequency of armchair and zigzag graphene-MoS<sub>2</sub> heterostructure as a function of length. (b) Bridged boundary condition - fundamental natural frequency of armchair and zigzag graphene-MoS<sub>2</sub> heterostructure as a function of length.

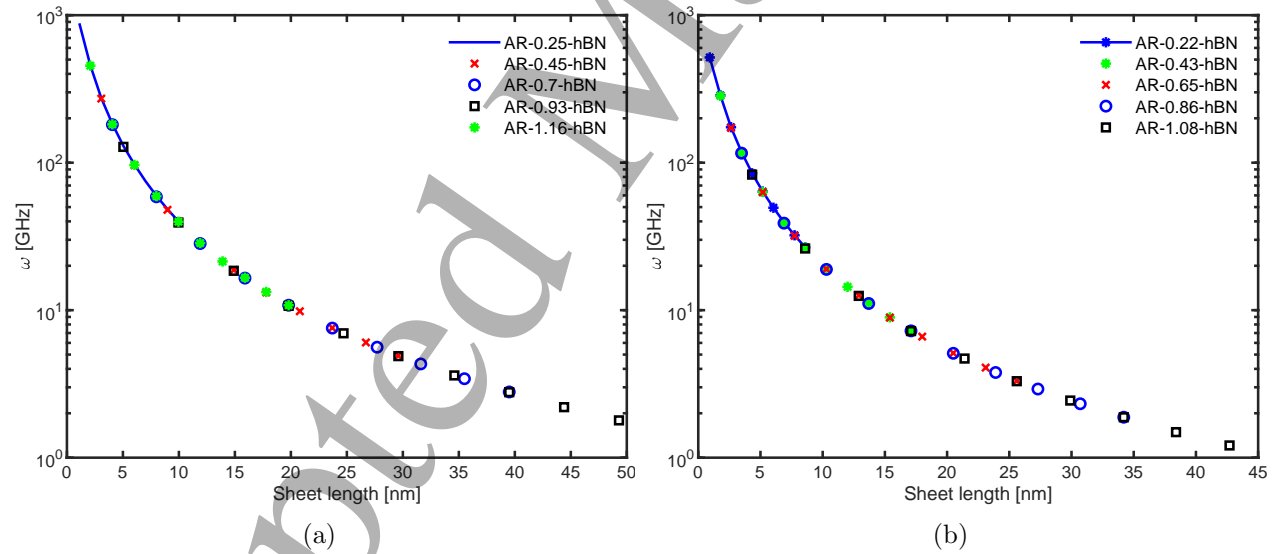


Figure 12: The variation of natural frequencies with sheet length at a given aspect ratio for graphene-hBN nano-heterostructure (a) Cantilevered graphene-hBN in armchair direction (b) Cantilevered graphene-hBN in zigzag direction

and figure 13, increase in sheet aspect ratio by keeping the sheet length constant will not lead to a significant change in natural frequency. In general, it is observed that graphene-hBN nano hetero-structure offers higher natural frequency as compared to graphene-MoS<sub>2</sub> for a given length and aspect ratio. This behaviour is in agreement with the stiffness (tensile rigidities) of nanosheets presented in figure 5.

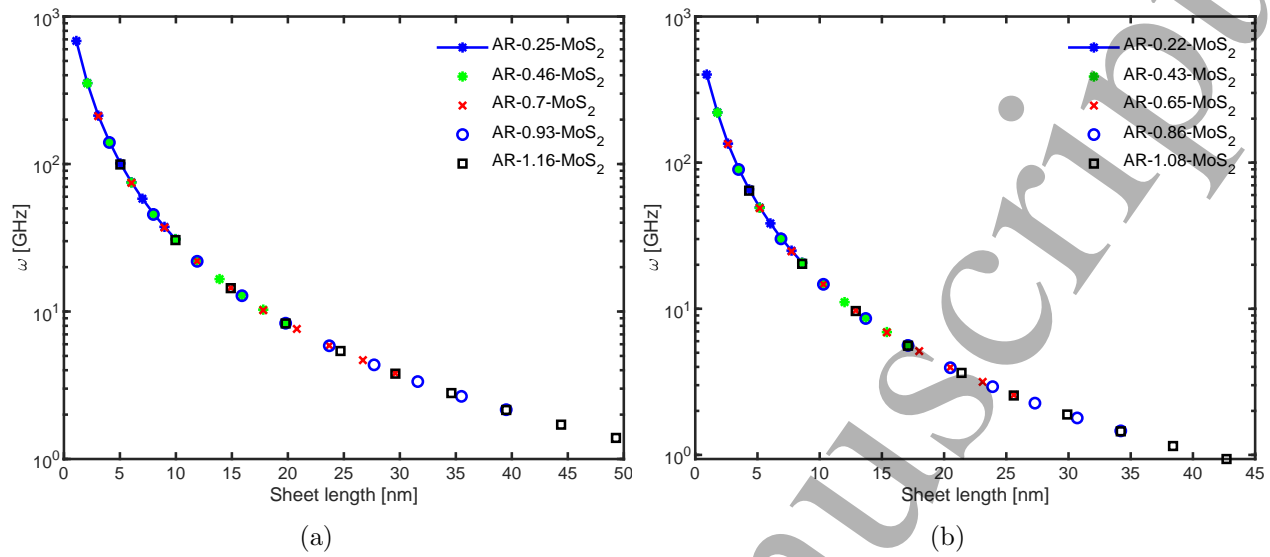


Figure 13: The variation of natural frequencies with sheet length at a given aspect ratio for graphene-MoS<sub>2</sub> nano-heterostructure (a) Cantilevered graphene-MoS<sub>2</sub> in armchair direction (b) Cantilevered graphene-MoS<sub>2</sub> in zigzag direction

#### 4.5. Dependence on the boundary condition

From the point of view of structural mechanics, a bridged structure is found to offer higher natural frequency [69] compared to the cantilever one due to more stiffness in the system. As per figure 10 and figure 11, the change of the boundary condition from one-edge-fixed to both-edge-fixed can enhance the natural frequency by upto 3 times. Such a boundary condition dependence was observed for the higher natural frequencies of both graphene-hBN and graphene-MoS<sub>2</sub>. Clamping the nano-heterostructure sheet at all edges will further enhance the stiffness, and subsequently increase the natural frequencies. Further, our study reveals that, as the aspect ratio is increased, the natural frequency of a cantilever model drops at higher rate as compared to a bridged model. From these observations, we can also conclude that the bridged topologies (refer to figure 7) are suitable for nanoelectromechanical system applications, where resonant frequencies are required to be very high, while the cantilever topologies (refer to figure 7) are suitable for low resonant frequency applications.

#### 4.6. Effect of chirality on the natural frequencies of heterostructures

From the results presented in the preceding subsections, it can be observed that chirality is an influential factor for the natural frequencies of vibration (refer to figure 10 and figure 11). For a given width and length, the fundamental frequencies of armchair nano-heterostructure



sheets are higher than those of zigzag ones. This difference can be attributed to the higher tensile rigidity in the armchair direction for graphene, as shown in figure 5. The maximum relative difference calculated as  $(\omega_{armchair} - \omega_{zigzag})/\omega_{armchair}$  is found to be in the order of 0.14 and 0.12 for cantilevered and bridged boundary conditions, respectively. A similar trend can also be noticed from figure 12 - 13 for the zigzag and armchair directions. However, increasing the sheet length diminishes the difference caused by chirality. In other words, there is a size effect on the effect of chirality and it is more prominent for nano-sheets with smaller dimension.

## 5. Summary and perspective

The area of two-dimensional (2D) materials, which started with the synthesis of graphene, has received a wide range of attention from the engineering and science community. After several years of intensive investigation, research concerning graphene has logically reached to a rather matured stage. Thus, investigation of other two dimensional and quasi-two-dimensional materials have started receiving the due attention recently. However, the possibility of combining single layers of different two dimensional materials (heterostructures) has expanded this field of research dramatically; well beyond the scope of considering a simple single layer graphene or other 2D material. The interest in such heterostructures is growing very rapidly with the advancement of synthesizing such materials in laboratory, as the interest in graphene did few years ago. The attentiveness is expected to expand further in coming years with the possibility to consider different tunable nanoelectromechanical properties of the prospective combination (single and multi-layer structures with different stacking sequences) of so many two dimensional materials.

The current article presents an efficient atomistic finite element-based modelling framework for the dynamic analysis of such nano-heterostructures. Here the contribution is two-fold: I. Insightful new results unravelling the dynamic behaviour of graphene based heterostructures including the effects of dependence on size, chirality and boundary conditions II. Development of the generic atomistic finite element framework for efficient dynamic analysis of heterostructures. The physics-based atomistic finite element framework is applicable to multiple 2D materials with any stacking sequence and number of layers. Adoption of the atomistic finite element approach instead of conventional simulation methods such as molecular dynamics

simulation brings significantly more computational efficiency in the analysis and the proposed approach is a panacea in situations where interatomic potentials required for carrying out molecular dynamics simulations are unavailable in case of many complex heterostructures.

The unique capability of these heterostructures to achieve a range of simultaneously tunable multifunctional properties is expected to have a wide appeal across different disciplines of research concerning nanotechnology. Vibrational characteristics of nanostructures are of utmost importance in order to access their performance as structural members for adoption in nano-scale devices and systems. However, the dynamics and vibration of nano-heterostructures have not received the required attention yet. Thus, here we have focused on investigating the size-dependent dynamic behavior of nano hetero-structures by developing a generic atomistic finite element model.

## 6. Conclusions

The vibrational characteristics of graphene based nano-heterostructures are investigated in this article considering the dependence on size, chirality and boundary conditions. A generic atomistic finite element based approach has been developed for the static and dynamic analysis of nano-heterostructures by considering the mechanical equivalence of atomic bonds, interlayer interactions and atomic masses. Within the atomistic finite element model, the inter atomic bonds are represented by equivalent structural beams with stretching and bending mechanisms, while the interlayer interaction between two adjacent layers are modelled using equivalent non-linear spring elements based on L-J potentials. The atomic masses are modelled as lumped mass system in the dynamic analysis framework. The developed atomistic finite element model is validated extensively with available literature for effective elastic properties and vibrational frequencies. After gaining adequate confidence on the proposed computational model, insightful new results on dynamic properties are presented for graphene-hBN and graphene-MoS<sub>2</sub> heterostructures. Natural frequencies and mode shapes are investigated up to the fourth mode explaining their fundamental characteristics. The study reveals that the weak van der Waals interactions between the layers assume an important role in the dynamics of heterostructures unlike the case of static elastic analysis. Depending on the modulus of elasticity, graphene-hBN shows a higher bending stiffness compared to graphene-MoS<sub>2</sub> heterostructure, leading to higher natural frequencies. Similar to the behaviour of single

and bilayer graphene sheets, the fundamental natural frequency of hetero-structures reduces with increasing length and aspect ratio. The nano hetero-structures with bridged boundary conditions are found to have higher natural frequencies compared to their cantilevered counterpart, making them more appropriate for high-resonance applications. A size effect is unravelled concerning the influence of chirality on the natural frequencies and it is found to be more prominent for nano-sheets with smaller dimension.

In summary, we have investigated the dynamic behaviour of graphene based heterostructures considering two different configurations with monoplanar and multi-planar 2D nano materials. Such graphene based heterostructures are ideal candidates for multi-synchronous modulation of a wide range properties for the application-specific requirements of various nanoelectromechanical devices and systems. In-depth characterization of the vibrational characteristics of these nano-heterostructures would assume a cardinal role in accessing their suitability as structural members for adoption in such nano-scale objects. Moreover, the generic atomistic finite element approach developed in this study would be useful to efficiently explore the dynamic properties of various other nano-heterostructures with multiple number of 2D materials and their stacking sequences in the future investigations.

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## References

- [1] Y. Gan, W. Chu, L. Qiao, STM investigation on interaction between superstructure and grain boundary in graphite, *Surface Science* 539 (1) (2003) 120 – 128.
- [2] K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, Y. Zhang, S. V. Dubonos, I. V. Grigorieva, A. A. Firsov, Electric field effect in atomically thin carbon films, *Science* 306 (5696) (2004) 666–669.
- [3] S. Balendhran, S. Walia, H. Nili, S. Sriram, M. Bhaskaran, Elemental analogues of graphene: Silicene, germanene, stanene, and phosphorene, *Small* 11 (6) (2015) 640–652.

- [4] M. Xu, T. Liang, M. Shi, H. Chen, Graphene-like two-dimensional materials, *Chemical Reviews* 113 (5) (2013) 3766–3798.
- [5] S. Das, J. A. Robinson, M. Dubey, H. Terrones, M. Terrones, Beyond graphene: Progress in novel two-dimensional materials and van der waals solids, *Annual Review of Materials Research* 45 (1) (2015) 1–27.
- [6] R. K. Zahedi, A. Shirazi, P. Alimouri, N. Alajlan, T. Rabczuk, Mechanical properties of graphene-like bc<sub>3</sub>; a molecular dynamics study, *Computational Materials Science* 168 (2019) 1 – 10.
- [7] A. K. Geim, I. V. Grigorieva, Van der waals heterostructures, *Nature* 499 (419).
- [8] Y. J. Zhang, M. Yoshida, R. Suzuki, Y. Iwasa, 2d crystals of transition metal dichalcogenide and their iontronic functionalities, *2D Materials* 2 (4) (2015) 044004.
- [9] A. Mahata, T. Mukhopadhyay, Probing the chirality-dependent elastic properties and crack propagation behavior of single and bilayer stanene, *Phys. Chem. Chem. Phys.* 20 (2018) 22768–22782.
- [10] T. Mukhopadhyay, A. Mahata, S. Adhikari, M. A. Zaeem, Effective elastic properties of two dimensional multiplanar hexagonal nanostructures, *2D Materials* 4 (2) (2017) 025006.
- [11] A. A. Balandin, S. Ghosh, W. Bao, I. Calizo, D. Teweldebrhan, F. Miao, C. N. Lau, Superior thermal conductivity of single-layer graphene, *Nano Letters* 8 (3) (2008) 902–907.
- [12] P. Ball, Why nature prefers hexagons, *Nautilus* 035.  
URL [nautil.us/issue/35/boundaries/why-nature-prefers-hexagons](http://nautil.us/issue/35/boundaries/why-nature-prefers-hexagons)
- [13] T. Mukhopadhyay, S. Adhikari, A. Batou, Frequency domain homogenization for the viscoelastic properties of spatially correlated quasi-periodic lattices, *International Journal of Mechanical Sciences* 150 (2019) 784 – 806.
- [14] T. Mukhopadhyay, S. Adhikari, Effective in-plane elastic moduli of quasi-random spatially irregular hexagonal lattices, *International Journal of Engineering Science* 119 (2017) 142 – 179.

- [15] T. Mukhopadhyay, S. Adhikari, A. Alu, Theoretical limits for negative elastic moduli in subacoustic lattice materials, *Phys. Rev. B* 99 (2019) 094108.
- [16] V. Zolyomi, J. R. Wallbank, V. I. Falko, Silicane and germanane: tight-binding and first-principles studies, *2D Materials* 1 (1) (2014) 011005.
- [17] T. Lorenz, J.-O. Joswig, G. Seifert, Stretching and breaking of monolayer MoS<sub>2</sub>—an atomistic simulation, *2D Materials* 1 (1) (2014) 011007.
- [18] F. Liu, P. Ming, J. Li, Ab initio calculation of ideal strength and phonon instability of graphene under tension, *Phys. Rev. B* 76 (2007) 064120.
- [19] R. Grantab, V. B. Shenoy, R. S. Ruoff, Anomalous strength characteristics of tilt grain boundaries in graphene, *Science* 330 (6006) (2010) 946–948.
- [20] E. W. Bucholz, S. B. Sinnott, Mechanical behavior of Mos<sub>2</sub> nanotubes under compression, tension, and torsion from molecular dynamics simulations, *Journal of Applied Physics* 112 (12) (2012) 123510.
- [21] E. W. Bucholz, S. B. Sinnott, Structural effects on mechanical response of Mos<sub>2</sub> nanostructures during compression, *Journal of Applied Physics* 114 (3) (2013) 034308.
- [22] T. Chang, H. Gao, Size-dependent elastic properties of a single-walled carbon nanotube via a molecular mechanics model, *Journal of the Mechanics and Physics of Solids* 51 (6) (2003) 1059 – 1074.
- [23] F. Scarpa, S. Adhikari, A. S. Phani, Effective elastic mechanical properties of single layer graphene sheets, *Nanotechnology* 20 (6) (2009) 065709.
- [24] M. M. Shokrieh, R. Rafiee, Prediction of youngs modulus of graphene sheets and carbon nanotubes using nanoscale continuum mechanics approach, *Materials & Design* 31 (2) (2010) 790 – 795.
- [25] L. Boldrin, F. Scarpa, R. Chowdhury, S. Adhikari, Effective mechanical properties of hexagonal boron nitride nanosheets, *Nanotechnology* 22 (50) (2011) 505702.

- [26] Y. Chandra, R. Chowdhury, S. Adhikari, F. Scarpa, Elastic instability of bilayer graphene using atomistic finite element, *Physica E: Low-dimensional Systems and Nanostructures* 44 (1) (2011) 12 – 16.
- [27] Y. Chandra, R. Chowdhury, F. Scarpac, S. Adhikarib, J. Sienza, C. Arnold, T. Murmu, D. Bouda, Vibration frequency of graphene based composites: A multiscale approach, *Materials Science and Engineering B* 177 (2012) 303–310.
- [28] T. Mukhopadhyay, S. Adhikari, Stochastic mechanics of metamaterials, *Composite Structures* 162 (2017) 85 – 97.
- [29] T. Mukhopadhyay, S. Adhikari, A. Alu, Probing the frequency-dependent elastic moduli of lattice materials, *Acta Materialia* 165 (2019) 654 – 665.
- [30] T. Mukhopadhyay, A. Mahata, S. Adhikari, M. A. Zaeem, Effective mechanical properties of multilayer nano-heterostructures, *Scientific reports* 7 (1) (2017) 15818.
- [31] T. Mukhopadhyay, A. Mahata, S. Adhikari, M. Asle Zaeem, Probing the shear modulus of two-dimensional multiplanar nanostructures and heterostructures, *Nanoscale* 10 (2018) 5280–5294.
- [32] J.-W. Jiang, H. S. Park, Mechanical properties of  $\text{MoS}_2$ /graphene heterostructures, *Applied Physics Letters* 105 (3) (2014) 033108.
- [33] R. M. Elder, M. R. Neupane, T. L. Chantawansri, Stacking order dependent mechanical properties of graphene/  $\text{MoS}_2$  bilayer and trilayer heterostructures, *Applied Physics Letters* 107 (7) (2015) 073101.
- [34] A. Wei, Y. Li, D. Datta, H. Guo, Z. Lv, Mechanical properties of graphene grain boundary and hexagonal boron nitride lateral heterostructure with controlled domain size, *Computational Materials Science* 126 (2017) 474 – 478.
- [35] Y. Li, W. Zhang, B. Guo, D. Datta, Interlayer shear of nanomaterials: Graphene/graphene, boron nitride/boron nitride and graphene/boron nitride, *Acta Mechanica Sinica* 30 (3) (2017) 234 – 240.

- [36] J. E. Barrios-Vargas, B. Mortazavi, A. W. Cummings, R. Martinez-Gordillo, M. Pruneda, L. Colombo, T. Rabczuk, S. Roche, Electrical and thermal transport in coplanar polycrystalline graphene/hBN heterostructures, *Nano Letters* 17 (3) (2017) 1660–1664.
- [37] J. Zhang, Vibrations of van der Waals heterostructures: A study by molecular dynamics and continuum mechanics, *Journal of Applied Physics* 125 (2) (2019) 025113.
- [38] B. Gelin, *Molecular modeling of polymer structures and properties*, Hanser Gardner Publications,.
- [39] C. Li, T.-W. Chou, A structural mechanics approach for the analysis of carbon nanotubes, *International Journal of Solids and Structures* 40 (10) (2003) 2487 – 2499.
- [40] Y. Chandra, F. Scarpa, R. Chowdhury, S. Adhikari, J. Sienz, Multiscale hybrid atomistic-continuum approach for the nonlinear tensile behaviour of graphene nanocomposites, *Composites Part A* 46 (2013) 147–153.
- [41] Y. Chandra, F. Scarpa, S. Adhikari, J. Zhang, E. S. Flores, H.-X. Peng, Pullout strength of graphene and carbon nanotube/epoxy composites, *Composites Part B: Engineering* 102 (2016) 1 – 8.
- [42] Y. Chandra, E. S. Flores, F. Scarpa, S. Adhikari, Buckling of hybrid nano composites with embedded graphene and carbon nanotubes, *Physica E* 83 (2016) 434–441.
- [43] Y. Chandra, R. Chowdhury, F. Scarpa, S. Adhikari, Vibrational characteristics of bilayer graphene sheets, *Thin Solid Films* 519 (18) (2011) 6026 – 6032.
- [44] Optistruct 14.0 reference guide, Altair Engineering, Inc.
- [45] F. Scarpa, S. Adhikari, R. Chowdhury, The transverse elasticity of bilayer graphene, *Physics Letters A* 374 (19) (2010) 2053 – 2057.
- [46] A. J. Pak, G. S. Hwang, Theoretical analysis of thermal transport in graphene supported on hexagonal boron nitride: The importance of strong adhesion due to  $\pi$ -bond polarization, *Phys. Rev. Applied* 6 (2016) 034015.



- [47] M. Neek-Amal, F. M. Peeters, Graphene on boron-nitride: Moiré pattern in the van der Waals energy, *Applied Physics Letters* 104 (4) (2014) 041909.
- [48] L. A. Girifalco, M. Hodak, R. S. Lee, Carbon nanotubes, buckyballs, ropes, and a universal graphitic potential, *Phys. Rev. B* 62 (2000) 13104–13110.
- [49] P. L. Montgomery, A block lanczos algorithm for finding dependencies over  $GF(2)$ , in: L. C. Guillou, J.-J. Quisquater (Eds.), *Advances in Cryptology — EUROCRYPT '95*, Springer Berlin Heidelberg, Berlin, Heidelberg, 1995, pp. 106–120.
- [50] C. Lee, X. Wei, J. W. Kysar, J. Hone, Measurement of the elastic properties and intrinsic strength of monolayer graphene, *Science* 321 (5887) (2008) 385–388.
- [51] B. Demczyk, Y. Wang, J. Cumings, M. Hetman, W. Han, A. Zettl, R. Ritchie, Direct mechanical measurement of the tensile strength and elastic modulus of multiwalled carbon nanotubes, *Materials Science and Engineering: A* 334 (1) (2002) 173 – 178.
- [52] K. N. Kudin, G. E. Scuseria, B. I. Yakobson,  $c_2F$ , bn, and c nanoshell elasticity from ab initio computations, *Phys. Rev. B* 64 (2001) 235406.
- [53] G. V. Lier, C. V. Alsenoy, V. V. Doren, P. Geerlings, Ab initio study of the elastic properties of single-walled carbon nanotubes and graphene, *Chemical Physics Letters* 326 (1) (2000) 181 – 185.
- [54] D. Sánchez-Portal, E. Artacho, J. M. Soler, A. Rubio, P. Ordejón, Ab initio structural, elastic, and vibrational properties of carbon nanotubes, *Phys. Rev. B* 59 (1999) 12678–12688.
- [55] J.-W. Jiang, J.-S. Wang, B. Li, Young's modulus of graphene: A molecular dynamics study, *Phys. Rev. B* 80 (2009) 113405.
- [56] H. Zhao, K. Min, N. R. Aluru, Size and chirality dependent elastic properties of graphene nanoribbons under uniaxial tension, *Nano Letters* 9 (8) (2009) 3012–3015.
- [57] L. Song, L. Ci, H. Lu, P. B. Sorokin, C. Jin, J. Ni, A. G. Kvashnin, D. G. Kvashnin, J. Lou, B. I. Yakobson, P. M. Ajayan, Large scale growth and characterization of atomic hexagonal boron nitride layers, *Nano Letters* 10 (8) (2010) 3209–3215.

- [58] Q. Peng, W. Ji, S. De, Mechanical properties of the hexagonal boron nitride monolayer: Ab initio study, *Computational Materials Science* 56 (2012) 11 – 17.
- [59] S. Zhao, J. Xue, Mechanical properties of hybrid graphene and hexagonal boron nitride sheets as revealed by molecular dynamic simulations, *Journal of Physics D: Applied Physics* 46 (13) (2013) 135303.
- [60] M.-Q. Le, Young's modulus prediction of hexagonal nanosheets and nanotubes based on dimensional analysis and atomistic simulations, *Meccanica* 49 (7) (2014) 1709–1719.
- [61] L. Jiang, W. Guo, A molecular mechanics study on size-dependent elastic properties of single-walled boron nitride nanotubes, *Journal of the Mechanics and Physics of Solids* 59 (6) (2011) 1204 – 1213.
- [62] E.-S. Oh, Elastic properties of various boron-nitride structures, *Metals and Materials International* 17 (1) (2011) 21–27.
- [63] A. Castellanos-Gomez, M. Poot, G. A. Steele, H. S. J. van der Zant, N. Agrat, G. Rubio-Bollinger, Elastic properties of freely suspended  $\text{MoS}_2$  nanosheets, *Advanced Materials* 24 (6) (2012) 772–775.
- [64] S. Bertolazzi, J. Brivio, A. Kis, Stretching and breaking of ultrathin  $\text{MoS}_2$ , *ACS Nano* 5 (12) (2011) 9703–9709.
- [65] T. Lorenz, D. Teich, J.-O. Joswig, G. Seifert, Theoretical study of the mechanical behavior of individual  $\text{TiS}_2$  and  $\text{MoS}_2$  nanotubes, *The Journal of Physical Chemistry C* 116 (21) (2012) 11714–11721.
- [66] E. Scalise, M. Houssa, G. Pourtois, V. Afanas'ev, A. Stesmans, Strain-induced semiconductor to metal transition in the two-dimensional honeycomb structure of  $\text{MoS}_2$ , *Nano Research* 5 (1) (2012) 43–48.
- [67] J.-W. Jiang, Z. Qi, H. S. Park, T. Rabczuk, Elastic bending modulus of single-layer molybdenum disulfide ( $\text{MoS}_2$ ): finite thickness effect, *Nanotechnology* 24 (43) (2013) 435705.

- [68] A. Sakhaee-Pour, M. T. Ahmadian, R. Naghdabadi, Vibrational analysis of single-layered graphene sheets, *Nanotechnology* 19 (8) (2008) 085702.
- [69] G. B. Warburton, The vibration of rectangular plates, *Proceedings of the Institution of Mechanical Engineers* 168 (1) (1954) 371–384.