Phonon modes in single-walled molybdenum disulphide nanotubes: lattice dynamics calculation and molecular dynamics simulation

Jin-Wu Jiang\textsuperscript{1}, Bing-Shen Wang\textsuperscript{2} and Timon Rabczuk\textsuperscript{3,4}

\textsuperscript{1} Shanghai Institute of Applied Mathematics and Mechanics, Shanghai Key Laboratory of Mechanics in Energy Engineering, Shanghai University, Shanghai 200072, People’s Republic of China
\textsuperscript{2} State Key Laboratory of Semiconductor Superlattice and Microstructure and Institute of Semiconductor, Chinese Academy of Sciences, Beijing 100083, People’s Republic of China
\textsuperscript{3} Institute of Structural Mechanics, Bauhaus-University Weimar, Marienstraße 15, D-99423 Weimar, Germany
\textsuperscript{4} School of Civil, Environmental and Architectural Engineering, Korea University, Seoul, South Korea

E-mail: jwjiang5918@hotmail.com and timon.rabczuk@uni-weimar.de

Received 24 October 2013, revised 17 December 2013
Accepted for publication 19 December 2013
Published 14 February 2014

Abstract
We study the phonon modes in single-walled MoS\textsubscript{2} nanotubes via lattice dynamics calculation and molecular dynamics simulation. The phonon spectra for tubes of arbitrary chiralities are calculated from a dynamical matrix constructed by the combination of an empirical potential with the conserved helical quantum numbers ($\kappa$, \(n\)). In particular, we show that the frequency ($\omega$) of the radial breathing mode is inversely proportional to the tube diameter ($d$) as $\omega = 665.3/d$ cm\textsuperscript{-1}. The eigenvectors of the twenty lowest-frequency phonon modes are illustrated. Based on these eigenvectors, we demonstrate that the radial breathing oscillation is initially disturbed by phonon modes of three-fold symmetry, then eventually the tube is squashed by modes of two-fold symmetry. Our study provides fundamental knowledge for further investigations of the thermal and mechanical properties of MoS\textsubscript{2} nanotubes.

Keywords: molybdenum disulfide, nanotube, lattice dynamics, phonon modes

(Some figures may appear in colour only in the online journal)

1. Introduction

Molybdenum disulfide (MoS\textsubscript{2}) is a semiconductor with a bulk bandgap above 1.2 eV \cite{1}, which can be further manipulated by changing its thickness \cite{2} or through application of mechanical strain \cite{3, 4}. This finite bandgap is a key reason for the excitement surrounding MoS\textsubscript{2} as compared to graphene, as graphene has a zero bandgap \cite{5}. Because of its direct bandgap and its well-known properties as a lubricant, MoS\textsubscript{2} has attracted considerable attention in recent years \cite{6, 7}. For example, Radisavljevic \textit{et al} \cite{8} demonstrated the application of single-layered MoS\textsubscript{2} (SLMoS\textsubscript{2}) as a good transistor. The strain and electronic noise effects were found to be important for SLMoS\textsubscript{2} transistors \cite{9–12}.

Besides the electronic properties, there has been increasing interest in the thermal and mechanical properties of MoS\textsubscript{2}. Several recent works have addressed the thermal transport properties of SLMoS\textsubscript{2} in both the ballistic and diffusive transport regimes \cite{13–16}. The mechanical behavior of SLMoS\textsubscript{2} has been investigated experimentally \cite{17–19}. For the theoretical part, we have examined the size and edge effects on the Young’s modulus of SLMoS\textsubscript{2} based on the Stillinger–Weber (SW) potential \cite{16}. Quite recently, we derived an analytic...
formula for the elastic bending modulus of $SLMoS_2$, where the importance of the finite thickness effect was revealed [20].

A fundamental property related to the thermal and mechanical behaviors is the lattice dynamics property of $MoS_2$, i.e. the phonon spectrum or phonon modes. The thermal conductivity in the semiconductor $MoS_2$ is dominated by the lattice thermal transport, which is contributed by the phonon modes. Different mechanical processes are governed by the corresponding phonon modes. For instance, the nanomechanical resonant oscillation takes advantage of the bending mode (flexure mode). Recently, there have been increasing experimental and theoretical studies on the lattice dynamics properties of single-layer or few-layer $MoS_2$ nanosheets [21–29]. However, to date, the lattice dynamics of single-walled $MoS_2$ nanotubes (SWMoS$_2$NTs) has been investigated only in a few works, which show different lattice properties in the tube structure from the planar sheet structure, because of the special line group in the nanotube [30, 31].

In this paper, we perform a lattice dynamics study and molecular dynamics simulation for the lattice properties of SWMoS$_2$NTs with arbitrary chiralities. The phonon spectrum is calculated from the dynamical matrix using the force constant matrix obtained from the SW potential. The helical quantum numbers are used to denote the phonon mode. The eigenvector of the twenty lowest-frequency phonon modes are presented. Furthermore, we show that the radial breathing mechanical oscillation is disturbed initially by three-fold modes and destroyed eventually by two-fold modes.

2. Structure and calculation details

The top view of $SLMoS_2$ is shown in figure 1 (top panel). The three arrows indicate three representative lattice directions: the armchair lattice direction ($n_1$, $n_1$), the zigzag lattice direction ($n_1$, 0), and a chiral lattice direction ($2n_2$, $n_2$). The lattice constant is $|\vec{a}_1| = 2.14 \text{ Å}$. The $SLMoS_2$ can be rolled up into tube structures, as shown in the bottom of figure 1.

Besides the two primitive vectors $\vec{a}_1$ and $\vec{a}_2$, the lattice structure can be described by any other pair of equivalent primitive lattice vectors which surround the same area $[\vec{a}_1 \times \vec{a}_2]$. A particular pair of such equivalent primitive lattice vectors are $\vec{R}_H$ and $\vec{R}_L$ [32], which have been used for SWMoS$_2$NTs [33]. The helical lattice vector $\vec{H} = p_1\vec{a}_1 + p_2\vec{a}_2$ describes the screw operation, with $n_1 p_2 - n_2 p_1 = N$. $N$ is the greatest common divisor of $n_1$ and $n_2$. A large translational cell along the axial direction can be produced by a proper application of the screw and rotational operations [32]. A unit cell in the $(n_1, n_2)$ tubule can be notated in two equivalent ways, either by the primitive vector $(\vec{H}, \vec{R}_L)$, or by $(\vec{a}_1, \vec{a}_2)$ as

$$\vec{r}_{m,l} = m\vec{H} + l\vec{R}_L,$$

or

$$\vec{r}_{q_1,q_2} = q_1\vec{a}_1 + q_2\vec{a}_2, \quad (1)$$

in which $(q_1, q_2)$ and $(ml)$ are related to each other by

$$m = (n_1 q_2 - n_2 q_1)/N, \quad l = q_1 p_2 - q_2 p_1. \quad (2)$$

Figure 1. The configuration of $MoS_2$. Mo atoms are represented by large balls (gray online). S atoms are represented by small balls (yellow online). Top panel: top view of the two-dimensional $MoS_2$ honeycomb lattice. Three lattice directions are depicted by arrows, $\vec{R}_{arm} = n_1\vec{a}_1 + n_2\vec{a}_2$, $\vec{R}_{zig} = n_1\vec{a}_1$, and $\vec{R}_{biral} = 2n_2\vec{a}_1 + n_2\vec{a}_2$. Bottom panels: three SWMoS$_2$NTs are obtained by rolling up the above $MoS_2$ sheet onto a cylindrical surface with the three corresponding lattice vectors as the circumference.

$$\vec{b}_H$$ and $\vec{b}_R$ are reciprocal unit vectors corresponding to $(\vec{H}, \vec{R}_L)$. Any wavevector in the reciprocal space can be written as

$$\vec{k} = \frac{\kappa}{2\pi} \vec{b}_H + \frac{n}{N} \vec{b}_R. \quad (3)$$

$\kappa$ and $n$ are the two helical quantum numbers. In the first Brillouin zone, $\kappa \in (-\frac{1}{2}, \frac{1}{2})$ and $n$ is an integer in $(-\frac{N}{2}, \frac{N}{2})$. A comprehensive description for the relationship between different sets of symmetric notations can be found in [34] and in the book chapter by Tang et al [35].

3. Phonon dispersion of SWMoS$_2$NT

All screw and rotational symmetry operations in SWMoS$_2$NTs form the space group of this tubal system, which is named a line group [33, 36–38]. According to the irreducible representation of the line group, we have the generalized Bloch theory for the vibration displacement of each atom $(mls)$ in the phonon mode $(\kappa n \tau)$ [34, 39–42],

$$\vec{u}(mls) = \frac{1}{\sqrt{MN}} \sum_{\kappa n \tau} e^{i(km+\frac{2\pi}{N}nl)} R(ml) \xi(\tau)(\kappa n)(00\tau) \vec{Q}_{kn}$$

where $\tau$ is the branch index. $M$ is the total number of the screw symmetry operation. $N$ is the greatest common divisor of $n_1$ and $n_2$. It gives the number of pure rotational symmetry operations. $M \times N$ gives the total number of unit cells in the
The axial direction by an angle in the unit cell. The magnitude but a negative sign. The spectrum is overall symmetric about $\kappa$ red lines, respectively. Other general curves are displayed by gray lines. In panel (d), only a single value for $n$, i.e. $n = 0$, is shown. The arrow in each figure depicts the position of one of the TA (flexure) modes. The other flexure mode is located at the $\kappa$ with the same magnitude but a negative sign. The spectrum is overall symmetric about $\kappa = 0$, so only curves in $\kappa \in [0, 0.5]$ are displayed.

![Figure 2. Phonon spectra in SWMoS$_2$NTs of different chiralities. (a) Armchair (15, 15), (b) zigzag (26, 0), (c) chiral (20, 10), (d) chiral (16, 13). The $x$ axis is the helical quantum number $\kappa$, corresponding to the screw symmetric operation. The number $n$ is the other quantum number, corresponding to the pure rotational symmetric operation. For panels (a), (b), and (c), $n = -1, 0, 1$ are shown by black, blue, and red lines, respectively. Other general curves are displayed by gray lines. In panel (d), only a single value for $n$, i.e. $n = 0$, is shown. The arrow in each figure depicts the position of one of the TA (flexure) modes. The other flexure mode is located at the $\kappa$ with the same magnitude but a negative sign. The spectrum is overall symmetric about $\kappa = 0$, so only curves in $\kappa \in [0, 0.5]$ are displayed.](image-url)
Figure 3. The twenty lowest-frequency phonon modes in the SWMoS₂NT (15, 15). Frequencies are given in units of cm⁻¹. Numbers in parentheses are the helical quantum numbers (κn) for each mode. The arrow attached to each atom represents the component of this atom in the eigenvector of the phonon mode. The view is along the axial direction.

Figure 3. The twenty lowest-frequency phonon modes in the SWMoS₂NT (15, 15). Frequencies are given in units of cm⁻¹. Numbers in parentheses are the helical quantum numbers (κn) for each mode. The arrow attached to each atom represents the component of this atom in the eigenvector of the phonon mode. The view is along the axial direction.

to the zero frequency of the TW mode. Furthermore, the helical quantum numbers correspond to the actual symmetric operations (screw and pure rotational symmetric operations) in the SWMoS₂NTs. Hence they are the good quantum numbers for the phonon modes in the system [34]. The phase ‘good’ means that these quantum numbers are conserved during the phonon-assisted physical process. For instance, it has been shown that these helical quantum numbers give a natural (the simplest) selection rule for the phonon–phonon scattering process in the lattice thermal transport of single-walled boron nitride nanotubes [43]. Here, we have successfully combined the helical quantum numbers with an empirical potential, thus taking advantage of both parts. Hence, figure 2 provides a ‘good’ recipe for further investigations of the phonon-assisted physical processes in SWMoS₂NTs.

We now pay attention to the low-frequency modes in SWMoS₂NTs, because these modes are easier to excite in practice. Figure 3 shows the twenty lowest-frequency modes in the armchair tube (15, 15). Three large translational cells are used in this calculation. A periodic boundary condition is applied in the axial direction. These modes are located in the Γ point in the Brillouin zone; i.e., the linear quantum number is zero. The linear quantum number is the wavevector corresponding to the large translational operation. Numbers in
Figure 4. The twenty lowest-frequency phonon modes in the SWMoS$_2$NT (26, 0). Frequencies are given in units of cm$^{-1}$. Numbers in parentheses are the helical quantum numbers ($\kappa n$) for each mode. The arrow attached to each atom represents the component of this atom in the eigenvector of the phonon mode. The view is along the axial direction.

The first four modes are the acoustic phonon modes with zero frequency. Their helical quantum numbers are ($\kappa n$) = (0, 0), ($\alpha$, 1), ($-\alpha$, -1), and (0, 0). In particular, the fourth mode is the TW mode, resulting from the particular hollow cylindrical structure of the SWMoS$_2$NTs. These four acoustic modes have important contributions to the thermal transport of SWMoS$_2$NTs. The fifth and sixth modes have two-fold symmetry, which is denoted by ($\kappa n$) = (0, 2). From their peculiar vibration morphology and their relatively low frequencies, it can be easily imagined that the vibration of these modes is likely to squash the tube configuration, leading to possible instability of the SWMoS$_2$NTs. The seventh and eighth modes have three-fold symmetry, which is denoted by ($\kappa n$) = (0, 3). The thirteenth mode is the radial breathing mode (RBM), which is denoted by ($\kappa n$) = (0, 0). The frequency of the RBM is sensitive to the tube diameter, due to its vibration morphology, and this mode is Raman active, so its frequency is usually used to estimate the tube diameter in the experiment. Figures 4 and 5 show the twenty lowest-frequency modes in tubes (26, 0) and (20, 10), respectively. In particular, the RBM has a close.
frequency among these three tubes of quite different chiralities, since the chirality only takes effect on the order of $1/r^3$ [41].

4. RBM mode

In the above, we have studied the full phonon spectrum for SWMoS$_2$NTs. The rest of this paper is devoted to the discussion of the RBM, since this mode plays an important role in the tubal structure. We will study the diameter dependence and nonlinear properties of the RBM. Figure 6 shows the frequency of the RBM in armchair, zigzag, and chiral tubes, i.e. $(n_1, n_1)$, $(n_1, 0)$, and $(2n_2, n_2)$. A periodic boundary condition is applied in the axial direction, since the tube length is longer than the interaction range. There are three large translational cells along the axial direction for the armchair $(n_1, n_1)$ and zigzag $(n_1, 0)$ tubes. One large translational cell is considered for the chiral tube $(2n_2, n_2)$, which has a length of 14.3 Å. This length is much larger than the interaction range of 4.27 Å for the SW potential used in the simulation; thus it is large enough to avoid possible edge effects.

The frequency of all tubes can be fitted to the function $\omega = 665.3/d$ cm$^{-1}$, where $d$ is the diameter. The frequency of the RBM in SWMoS$_2$NTs is much lower than that in single-walled carbon nanotubes with the same diameter. The coefficient here (665.3) is about one third of the value of 2295.6

Figure 5. The twenty lowest-frequency phonon modes in the SWMoS$_2$NT (20, 10). Frequencies are given in units of cm$^{-1}$. Numbers in parentheses are the helical quantum numbers $(\kappa n)$ for each mode. The arrow attached to each atom represents the component of this atom in the eigenvector of the phonon mode. The view is along the axial direction.
The diameter dependence of the frequency of the RBM in armchair, zigzag, and chiral tubes. The solid line (blue online) is the fitting function, \( y = \frac{665.3}{x} \), for all data.

in single-walled carbon nanotubes [40]. This is because the frequency of the RBM is related to the tensile mechanical properties [45], and the mechanical strength is weaker in SWMoS\(_2\)NTs [16]. Furthermore, Mo and S atoms are heavier than the C atom in carbon nanotubes. Figure 6 can be useful in the estimation of the diameter of SWMoS\(_2\)NTs in the experiment.

We further investigate the nonlinear effect on the RBM. The molecular dynamics is performed to simulate the radial breathing oscillation of the SWMoS\(_2\)NTs (15, 15), (26, 0), and (20, 10). The periodic boundary condition is applied in the axial direction. The tube is optimized to the energy minimum configuration. At the optimized configuration, the initial velocity distributions are set according to the vibration morphology of the RBM. The total kinetic energy corresponding to this initial velocity distribution is \( \Delta E = \alpha N E_0 \), where \( \alpha \) is the energy actuation parameter [46], \( N \) is the total atom number and \( E_0 = 0.54 \text{ meV} \) is introduced as the unit for energy. The tube is allowed to oscillate within the NVE ensemble with the initial velocity distribution. The total kinetic energy and the potential energy exchange with each other during this radial breathing oscillation.

In the initial oscillation stage, there is only a single oscillation mode, i.e. the radial breathing oscillation. If the oscillation is in the linear regime, i.e. it has a small amplitude, this radial breathing oscillation can be preserved for a very long time and other vibration modes are seldom excited. However, if the oscillation is in the nonlinear regime, i.e. with a larger actuation parameter \( \alpha \), then the other oscillation modes will be excited quickly. As a result, the radial breathing oscillation decays quickly, owing to the nonlinear induced phonon–phonon scattering between the RBM and the other excited modes.

Figure 7 shows the kinetic energy time history during the radial breathing oscillation of the three tubes. To study the nonlinear effect, we have shown only simulations with large actuation parameters \( \alpha = 10, 30, \) and 50 in the figure. The radial breathing oscillation will not decay if a very small actuation parameter is used, e.g. \( \alpha = 1.0 \), which would be similar to the graphene nanomechanical resonator [47]. Figure 7 shows that in the initial stage the total kinetic energy oscillates between zero and a maximum value, reflecting the good resonant oscillation of the SWMoS\(_2\)NT. After some time, the radial breathing oscillation starts to be disturbed by some other vibration modes, which are excited by the nonlinear effect relating to the large actuation energy. Arrows in the figure depict the lifetime at which the radial breathing oscillation starts to be disturbed. The inset in each panel shows the lifetime versus actuation parameter \( \alpha \). The inset shows that the lifetime decays exponentially with increasing actuation parameter \( \alpha \).
Figure 8. The evolution of the configuration for the SWMoS$_2$NT (20, 10) during the radial breathing oscillation with the actuation parameter $\alpha = 50.0$. The arrow attached to each atom represents the velocity of the atom. At $t = 0$ ps, the oscillation is actuated by adding an initial velocity distribution which follows the eigenvector of the RBM (thirteenth mode) in figure 5. Configurations at $t = 14.7$ and 16.0 ps show that the radial breathing oscillation is gradually disturbed by three-fold modes (seventh and eighth modes) in figure 5. The radial breathing oscillation is completely replaced by these three-fold modes after $t = 18.6$ ps. The three-fold oscillation is clearly demonstrated by the two configurations at $t = 21.0$ and 22.3 ps, which exactly follow the eigenvector of the two three-fold modes. After $t = 94.7$ ps, two-fold modes (fifth and sixth modes) in figure 5 start to be excited. The tube starts to be squashed by these two-fold modes after $t = 105.1$ ps.

5. Conclusion
In conclusion, we study the lattice dynamics properties of SWMoS$_2$NTs with arbitrary chiralities. In the construction parameter $\alpha$. The solid line is an exponential fitting to the calculated data. This set of simulations show that it is important to use a small actuation parameter for the radial breathing oscillation if this oscillation is used as a nanomechanical resonator [45].

In all three tubes, for very large actuation parameters such as $\alpha = 30$ and 50, the kinetic energy increases sharply after the radial breathing oscillation is disturbed. This indicates that these tubes undergo a structural transition that releases lots of potential energy. This potential energy is converted into kinetic energy in the system. Figure 8 shows the structural evolution during the radial breathing oscillation in the SWMoS$_2$NT (20, 10) with actuation parameter $\alpha = 50.0$. These snapshots are produced by OVITO [48]. Similar phenomena have been observed in the molecular dynamics simulation of tubes (15, 15) and (26, 0). The arrow attached to each atom represents the velocity of the atom at that moment. At $t = 0$ ps, the radial breathing oscillation is actuated by adding an initial velocity distribution which follows the eigenvector of the RBM (thirteenth mode) in figure 5. Configurations at $t = 14.7$ and 16.0 ps show that the radial breathing oscillation is disturbed gradually by the seventh and eighth modes (with three-fold symmetry) in figure 5 due to a nonlinear effect related to the large actuation energy. The radial breathing oscillation is completely replaced by these three-fold modes after $t = 18.6$ ps. These three-fold oscillations are clearly demonstrated by the two configurations at $t = 21.0$ and 22.3 ps, which exactly follow the eigenvector of the two three-fold modes. This shows that the three-fold mode is also a type of stable oscillation, i.e. this oscillation does not destroy the tubal structure. However, after $t = 94.7$ ps, the fifth and sixth modes (with two-fold symmetry) in figure 5 start to be excited. These two-fold modes are unstable due to their special vibration morphology and their low frequencies. A low frequency indicates that these modes are able to deform the tubal structure quite a lot with a small amount of energy. Indeed, the tube starts to be squashed by these two-fold modes after $t = 105.1$ ps.
of the $9 \times 9$ dynamical matrix, the force constant matrix is calculated from the SW potential and the phonon modes are denoted by helical quantum numbers which correspond to the line group in the system. The frequency and eigenvector of the low-frequency phonon modes are analyzed. The frequency of the RBM is found to be inversely proportional to the tube diameter as $\omega = 665.3/d$ cm$^{-1}$, where $d$ is the tube diameter. We perform a molecular dynamics simulation to investigate the radial breathing mechanical oscillation, and find that the lifetime of the radial breathing oscillation decays exponentially with increasing oscillation energy. More specifically, in the initial stage, this radial breathing oscillation is disturbed by three-fold modes. The SWMoS$_2$NTs are squashed by two-fold modes in the final stage if the oscillation is actuated into the nonlinear regime.

Acknowledgments

The work is supported by the Recruitment Program of Global Youth Experts of China (JWJ) and the German Research Foundation (DFG).

References

[1] Kam K K and Parkinson B A 1982 J. Phys. Chem. 86 463
[2] Mak K F, Lee C, Hone J and Heinz T F 2010 Phys. Rev. Lett. 105 136805
[3] Lu P, Wu X, Guo W and Zeng X C 2012 Phys. Chem. Chem. Phys. 14 13035
[4] Novoselov K S, Geim A K, Morozov S V, Jiang D, Katsnelson M I, Grigorieva I V, Dubonos S V and Firsov A A 2005 Nature 438 197
[5] Wang Q H, Kalantar-Zadeh K, Kis A, Coleman J N and Strano M S 2012 Nature Nanotechnol. 7 699
[6] Chhowalla M, Shin H S, Eda G, Li L, Loh K P and Zhang H 2013 Nature Chem. 5 263
[7] Radisavljevic B, Radenovic A, Brivio J, Giacometti V and Kis A 2011 Nature Nanotechnol. 6 147
[8] Conley H J, Wang B, Ziegler J I, Haglund R F, Pantelides S T and Bolotin K I 2013 Nano Lett. 13 3626
[9] Sangwan V K, Arnold H N, Jariwala D, Marks T J, Lauhon L J and Hershman M C 2013 Nano Lett. 13 4351
[10] Ghorbani-Asl M, Zibouche N, Wahiduzzaman M, Oliveira A F, Kuc A and Heine T 2013 Eur. Phys. J. B 87 136805
[11] Huang W, Da H and Liang G 2013 J. Appl. Phys. 113 104304
[12] Varshney V, Patnaik S S, Muratore C, Roy A K, Voevodin A A and Farmer B L 2010 Comput. Mater. Sci. 48 101
[13] Jiang J-W, Zhuang X-Y and Rabczuk T 2011 Sci. Rep. 3 2209
[14] Jiang J-W, Park H S and Rabczuk T 2013 J. Appl. Phys. 114 064307
[15] Bertolazzi S, Brivio J and Kis A 2011 ACS Nano 5 9703
[16] Cooper R C, Lee C, Marienotti C A, Wei X, Hone J and Kysar J W 2013 Phys. Rev. B 87 035423
[17] Cooper R C, Lee C, Marienotti C A, Wei X, Hone J and Kysar J W 2013 Phys. Rev. B 87 075991
[18] Jiang J-W, Qi Z, Park H S and Rabczuk T 2013 Nanotechnology 24 435705
[19] Jimenez Sandoval S, Yang D, Frindt R F and Irwin J C 1991 Phys. Rev. B 44 3955
[20] Molina-Sánchez A and Wirtz L 2011 Phys. Rev. B 84 155413
[21] Nakabayashi N, Smith H G and Nicklow R M 1975 Phys. Rev. B 12 659
[22] Lee C, Yan H, Brus L E, Heinz T F, Hone J and Ryu S 2010 ACS Nano 4 2695–700
[23] Zeng H, Zhu B, Liu K, Fan J, Cui X and Zhang Q M 2012 Phys. Rev. B 86 241301
[24] Zhao Y et al 2013 Nano Lett. 13 1007
[25] Rice C, Young R J, Zan R, Bangert U, Dolotin K I and Remskar M 2008 Mater. Manuf. Process. 23 579
[26] Dobardzic E, Milosevic I, Dakic B and Damnjanovic M 2006 Phys. Rev. B 74 033403
[27] White C T, Robertson D H and Mintmire J W 1993 Phys. Rev. B 47 5485
[28] Milosevic I, Vukovic T, Damnjanovic M and Nikolic B 2000 Eur. Phys. J. B 17 707
[29] Dobardzic E, Milosevic I, Nikolic B, Vukovi T and Damnjanovic M 2003 Phys. Rev. B 68 045408
[30] Tang H, Wang B-S and Su Z-B 2011 Graphene Simulation (Shanghai, China: InTech) Chapter 10 (Symmetry and Lattice Dynamics)
[31] Vujicic M, Bozovic I B and Herbut F 1977 J. Phys. A: Gen. Phys. 10 1271
[32] Bozovic I B, Vujicic M and Herbut F 1978 J. Phys. A: Math. Gen. 11 2133
[33] Bozovic I B and Vujicic M 1981 J. Phys. A: Math. Gen. 14 777
[34] Milosevic I and Damnjanovic M 1993 Phys. Rev. B 47 7805
[35] Popov V N, Vukovic T and Balkanski M 1999 Phys. Rev. B 59 8355
[36] Jiang J-W, Tang H, Wang B-S and Su Z-B 2006 Phys. Rev. B 73 235434
[37] Dakic B, Damnjanovic M and Milovic I 2009 J. Phys. A: Math. Theor. 42 125202
[38] Jiang J-W and Wang J-S 2011 Phys. Rev. B 84 085439
[39] Kokalj A 2003 Comput. Mater. Sci. 28 155
[40] Raravikar N R, Keblinski P, Rao A M, Dresselhaus M S, Schadler L S and Ajayan P M 2002 Phys. Rev. B 66 235424
[41] Jiang J-W and Wang J-S 2012 J. Appl. Phys. 111 054314
[42] Jiang J-W, Park H S and Rabczuk T 2012 Nanotechnology 23 475501
[43] Stukowski A 2010 Modell. Simul. Mater. Sci. Eng. 18 015012