Graphene nanoribbon as an elastic damper

Iman Evazzade\textsuperscript{1}, Ivan P Lobzenko\textsuperscript{2,3}, Danial Saadatmand\textsuperscript{4}, Elena A Korznikova\textsuperscript{2,5}, Kun Zhou\textsuperscript{5,6}, Bo Liu\textsuperscript{5,6} and Sergey V Dmitriev\textsuperscript{2,7}

\textsuperscript{1} Department of Physics, Faculty of Science, Ferdowsi University of Mashhad, Mashhad, Iran
\textsuperscript{2} Institute for Metals Superplasticity Problems RAS, Ufa 450001, Russia
\textsuperscript{3} Toyota Technological Institute, 2-12-1 Hisakata, Tempaku-ku, Nagoya, 468-8511 Japan
\textsuperscript{4} Department of Physics, University of Sistan and Baluchestan, Zahedan, Iran
\textsuperscript{5} School of Mechanical and Aerospace Engineering, Nanyang Technological University, 639798, Singapore
\textsuperscript{6} Environmental Process Modeling Center, Nanyang Environment and Water Research Institute, Nanyang Technological University, 50 Nanyang Avenue, 639798, Singapore
\textsuperscript{7} National Research Tomsk State University, Tomsk 634050, Russia

E-mail: i.evazzade@mail.um.ac.ir

Received 1 December 2017, revised 2 February 2018
Accepted for publication 28 February 2018
Published 27 March 2018

Abstract

Heterostructures composed of dissimilar two-dimensional nanomaterials can have nontrivial physical and mechanical properties which are potentially useful in many applications. Interestingly, in some cases, it is possible to create heterostructures composed of weakly and strongly stretched domains with the same chemical composition, as has been demonstrated for some polymer chains, DNA, and intermetallic nanowires supporting this effect of two-phase stretching. These materials, at relatively strong tension forces, split into domains with smaller and larger tensile strains. Within this region, average strain increases at constant tensile force due to the growth of the domain with the larger strain, at the expense of the domain with smaller strain. Here, the two-phase stretching phenomenon is described for graphene nanoribbons with the help of molecular dynamics simulations. This unprecedented feature of graphene that is revealed in our study is related to the peculiarities of nucleation and the motion of the domain walls separating the domains of different elastic strain. It turns out that the loading–unloading curves exhibit a hysteresis-like behavior due to the energy dissipation during the domain wall nucleation and motion. Here, we put forward the idea of implementing graphene nanoribbons as elastic dampers, efficiently converting mechanical strain energy into heat during cyclic loading–unloading through elastic extension where domains with larger and smaller strains coexist. Furthermore, in the regime of two-phase stretching, graphene nanoribbon is a heterostructure for which the fraction of domains with larger and smaller strain, and consequently its physical and mechanical properties, can be tuned in a controllable manner by applying elastic strain and/or heat.

Keywords: two-dimensional nanomaterial, graphene nanoribbon, two-phase stretching, heterostructure, molecular dynamics

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

1. Introduction

Two-dimensional (2D) nanomaterials, due to the combination of their unusual mechanical and physical properties, have attracted great interest from researchers over the last decade (see [1] and references therein). The combination of dissimilar 2D materials in various heterostructures is another way to achieve new properties and find new applications. Such heterostructures can be created in a number of different ways including through chemical modification, partial hydrogenation of graphene [2–5], by assembling layered heterostructures using weak van der Waals interactions [6–10], or by edge-to-edge stacking of dissimilar 2D materials [5, 11–13].
The synthesis of heterostructures is not easy [7, 14–17] and it would be helpful to find new methods of creation. Savin et al [18] have uncovered a general mechanism of two-phase stretching, experimentally observed for DNA [19–22], polypeptides [23], and some polymer chains [18]. There exists numerical evidence that NiAl, FeAl, and CuZr intermetallic nanowires also split into domains with smaller and larger strain, and stretching occurs due to the growth of the domain with larger strain at the expense of the domain with smaller strain. Within the range \( \varepsilon_1 < \varepsilon < \varepsilon_2 \) force is constant (red dashed line) since \( F = dP/d\varepsilon \), and \( P(\varepsilon) \) is linear. Outside the range \( \varepsilon_1 < \varepsilon < \varepsilon_2 \) stretching is homogeneous.

Figure 1. Schematic dependence of the potential energy \( P \) of a translational unit of a material (black solid line) and applied force \( F \) (red solid line) as the functions of tensile strain. The \( P(\varepsilon) \) curve features the concave down region in the range \( \varepsilon_1 < \varepsilon < \varepsilon_2 \) [18]. The presence of such a concave down region on the \( P(\varepsilon) \) function is the necessary condition for two-phase stretching. This is because within the range \( \varepsilon_1 < \varepsilon < \varepsilon_2 \) there exists a path with lower potential energy, shown by the black dashed line, which is the tangent of the \( P(\varepsilon) \) function at the points \( \varepsilon_1 \) and \( \varepsilon_2 \). When the system moves along this low energy path, the material splits into domains with tensile strain \( \varepsilon_1 \) and \( \varepsilon_2 \), and stretching occurs due to the growth of the domain with larger strain at the expense of the domain with smaller strain. Outside the range \( \varepsilon_1 < \varepsilon < \varepsilon_2 \) stretching is homogeneous. Tensile force as the function of \( \varepsilon \) is shown in figure 1 by the red solid line. During the two-phase stretching the force is constant within the domain of \( \varepsilon_1 < \varepsilon < \varepsilon_2 \) (see red dashed line), since \( F = dP/d\varepsilon \) and \( P(\varepsilon) \) is linear.

From the picture described above it can be seen that two-phase stretching occurs through the motion of domain walls (DWs) separating domains with different tensile strain. To have the possibility of witnessing two-phase stretching, the size of the material should be sufficiently large to host at least one DW generated at the surface, or at least two DWs (positive and negative) if they are generated in the bulk. Actually, the generation and motion of DWs in two-phase stretching may have interesting consequences on the behavior of materials; e.g. resulting in negative stiffness within the strain range \( \varepsilon_1 \) and \( \varepsilon_2 \) [25, 26] or in strong hysteresis of the stress-strain response [30, 32, 35].

In the present study, with the help of molecular dynamics simulations, we demonstrate that the armchair graphene nanoribbons go through two-phase stretching. Furthermore, we show that the nucleation and motion of DWs produces considerable dissipation of elastic strain energy so that the nanoribbon combines the properties of elasticity and damping. A similar combination of elasticity and damping is demonstrated by such macroscopic materials as rubber or porous metallic rubber, which find many engineering applications [47, 48]. To the best of our knowledge, such analogs have not been proposed for 2D nanomaterials.

2. Materials and methods

The uniaxial tension of graphene nanoribbons is studied by molecular dynamic simulations using the LAMMPS program package [49] with the use of AIREBO (adaptive intermolecular reactive empirical bond order) potentials [50]. The initial graphene nanoribbon structure is schematically shown in figure 2. The armchair (zigzag) graphene direction is along the x- (y-) axis. We consider a rectangular translational cell with four atoms, as shown by the dashed line. The initial size of this cell is \( L_0 = 4.26 \text{Å} \) and \( h_0 = 2.46 \text{Å} \). To simulate the nanoribbons, a rectangular computational cell consisting of \( M \times N \) translational cells is built. The translational cells are thus numbered by the indices \((m, n)\). In figure 2, the nanoribbon with \( M = 10 \) and \( N = 3 \) is shown, but in our simulations the computational cell has \( M = 40 \) cells along the x-axis and \( N = 3, 6, \) or \( N = 12 \) cells along the y-axis. The actual dimensions of the studied nanoribbons are: the three different initial widths \( H_0 = N_0 - h_0/2 = 6.07, 13.41, \) and \( 28.03 \text{Å} \), with the same initial length of \( L_0 = M_0 = 166.05 \text{Å} \). The total number of atoms in
the computational cell is equal to $4MN$. To apply strain-controlled tension, two zigzag chains at each end of the nanoribbon are assumed to be free. The nanoribbon is subjected to quasi-static stretching (unstretching) along the $x$-axis by a stepwise increase (decrease) of the axial strain followed by structure relaxation after each increment. The search for the energy minimum stops when the maximal force acting on the atoms is less than $10^{-3}$ (g/mole) $\times$ (Å fs$^{-2}$). The averaged longitudinal and transverse strains are defined as $\varepsilon_{xx} = (L - L_0)/L_0$ and $\varepsilon_{yy} = (H - H_0)/H_0$, respectively, where $L$ is the current distance between the nanoribbon ends and $H$ is the current nanoribbon width. The local axial strain is calculated for the translational cells with the numbers $m = 1, \ldots, M$, $n = N/2$ ($n = 2$ for $N = 3$) as $\varepsilon_{xx}(m) = (l_m - l_0)/l_0$, where $l_m$ is the current length of the cell. Most of the results are obtained for zero temperature. However, the effect of temperature is discussed in the section Temperature Effect. When solving numerically the equations of atomic motion, the Verlet algorithm of fourth order of accuracy was used with the time step of 0.5 fs.

3. Numerical results

Here we present the simulation results for the stretching/unstretching of graphene nanoribbons schematically shown in figure 2.

3.1. Relaxational dynamics

In figure 3 tensile membrane force as a function of averaged tensile strain for the nanoribbons of different widths: $N = 3$ (blue solid line), $N = 6$ (red dashed line), and $N = 12$ (black dash-dotted line). Note that axial force $F$ applied to the nanoribbon is measured in nanonewtons and normalized by the initial nanoribbon width $H_0$, measured in angstroms. At small strain ($\varepsilon_{xx} < 0.05$), membrane force increases linearly with strain, and then in the domain $0.05 < \varepsilon_{xx} < \varepsilon_{xx}^{(1)}$ the tensile stiffness of the nanoribbon gradually reduces with increasing strain. For all three curves $\varepsilon_{xx}^{(1)}$ equals 0.19. Then each curve features a hump, whose height increases with increasing nanoribbon width, followed by a plateau at the level of 0.006 nN Å$^{-1}$. For the narrowest nanoribbon the plateau is at a slightly smaller value due to the more pronounced effect of free edges. The plateau ends at $\varepsilon_{xx} = \varepsilon_{xx}^{(2)} = 0.375$ (this value is given for $N = 3$ and slightly increases with increasing $N$), and for larger average strain the membrane force increases until it reaches the maximal value (at about $\varepsilon_{xx} = 0.45$) where nanoribbon rupture begins, resulting in a sudden drop in the membrane force.

Potential energy per atom for the three studied nanoribbons is shown in figure 4 as a function of the averaged tensile strain $\varepsilon_{xx}$ for the nanoribbons of different widths: $N = 3$ (blue solid line), $N = 6$ (red dashed line), $N = 12$ (black dash-dotted line). Results are presented in figure 5, where the values of the averaged tensile strain $\varepsilon_{xx}$ are
given in the insets for each curve. As one can see from figure 5(a), at \( \varepsilon_{xx} = 0.19 \) the two domains with \( \varepsilon_{xx} = 0.375 \) appear at the two ends of the nanoribbon and they grow with increasing averaged strain at the expense of the domain with \( \varepsilon_{xx} = 0.19 \). The appearance of the domains at the nanoribbon ends is explained by the clamped boundary conditions producing strain gradients near the ends. For \( \varepsilon_{xx} > 0.375 \) the domain with the smaller value of \( \varepsilon_{xx} \) disappears and further stretching is homogeneous until the rupture point. The local lateral strain shown in figure 5(b) is also inhomogeneous within the range of the average strain \( \varepsilon_{xx}^{(1)} < \varepsilon_{xx} < \varepsilon_{xx}^{(2)} \). At

**Figure 4.** Potential energy per atom as a function of averaged tensile strain for the nanoribbons of different widths: \( N = 3 \) (blue solid line), \( N = 6 \) (red dashed line), \( N = 12 \) (black dash-dotted line). Sudden drop of energy corresponds to nanoribbon rupture.

**Figure 5.** Distribution of (A) axial and (B) lateral strain in the nanoribbon with \( N = 3 \) at different levels of the averaged tensile strain \( \varepsilon_{xx} \), as indicated in the insets.

\( \varepsilon_{xx} = 0.19 \) in the domain of \( e_{yy} = -0.01 \), the two domains with \( e_{yy} = -0.175 \) appear near the ends of the nanoribbon and grow with increasing average strain until \( \varepsilon_{xx} = 0.375 \). At higher average strain, stretching is homogeneous. The result is given in figure 5 for the narrowest nanoribbon (\( N = 3 \)) but the same was observed for the two wider nanoribbons.

Note that the presence of a plateau on the stress-strain curves in the range \( \varepsilon_{xx}^{(1)} < \varepsilon_{xx} < \varepsilon_{xx}^{(2)} \) (see figure 3) as well as the linear energy-strain dependence in this range (see figure 4) are the features of the two-phase stretching related to the presence of a concave down region on the energy-strain dependence for a single translational cell, as described in [18] and schematically illustrated in figure 1. Let us check if this is the case for the graphene nanoribbon considered here. In figure 6 we plot the energy-strain dependence for the translational cell containing four atoms (see figure 2) subject to periodic boundary conditions. Loading (red solid) and unloading (blue dashed) curves are presented. The concave down regions are clearly seen for both curves. Note that the formation of domains with different strain is suppressed by the small volume of the translational cell, which is why the system follows the concave down curve rather than the tangent straight line schematically shown in figure 1 by the black dashed line. Remarkably, the concave down regions are observed in the range of strain where two-phase stretching of the nanoribbons takes place, namely, in the range \( \varepsilon_{xx}^{(1)} < \varepsilon_{xx} < \varepsilon_{xx}^{(2)} \) with \( \varepsilon_{xx}^{(1)} = 0.19 \) and \( \varepsilon_{xx}^{(2)} = 0.375 \).

The microscopic origin of the appearance of the concave down region on the energy-strain curve is related to the competition between the potential energy of the valence bonds and the potential energy of valence angles. The many-body nature of the AIREBO interatomic potentials does not allow us to separate these two energies for graphene, but this was done for the model of 2D zigzag molecular chain considered in [18]. In that work, it was shown that two-phase
stretching of the molecular chain is a result of the proper combination of the bonds and valence angles deformation.

3.2. Hysteresis loop

It is instructive to study the behavior of the nanoribbon during unloading starting from the strain level $\varepsilon_{xx} > 0.375$, when the entire nanoribbon is homogeneously stretched (except for the regions near the clamped nanoribbon ends). The result is shown in figure 7, where the dependence of the tensile membrane force as a function of averaged tensile strain $\varepsilon_{xx}$ during loading (red solid line) and unloading (blue dashed line) of the nanoribbons with width (A) $N = 3$, (B) $N = 6$, and (C) $N = 12$.

Figure 7. Membrane tensile force $F/H_0$ as a function of averaged tensile strain $\varepsilon_{xx}$ during loading (red solid line) and unloading (blue dashed line) of the nanoribbons with width (A) $N = 3$, (B) $N = 6$, and (C) $N = 12$.

Figure 8. DW motion during (A) loading and (B) unloading of the nanoribbon of width $N = 12$. Values of averaged tensile strain are given for each panel. In (A) the DW moves to the right, it is tilted, and its propagation begins at the bottom edge of the nanoribbon. In (B) the DW moves to the left, it is pointed, and its motion is initiated in the middle of the nanoribbon.
DW dynamics are different for loading and unloading, as can be seen in figure 8, and this difference explains why the loading and unloading curves do not coincide. Atoms belonging to the domain with larger (smaller) tensile strain are shown in red (blue). Some atoms are colored in yellow, and they belong to the strongly distorted translational cells located either at the nanoribbon edges or at the DWs. During loading, shown in figure 8(a) (values of the averaged tensile strain are indicated for each panel), the DW moves to the right, converting the domain with larger tensile strain into the domain with smaller tensile strain, and it is tilted. Motion of this DW begins at the bottom edge of the nanoribbon. During unloading, (see figure 8(b)), the DW moves to the left, it has a pointed shape, and its propagation starts from the middle of the nanoribbon. The results in figure 8 are given for the widest studied nanoribbon with \( N = 12 \). A similar picture is observed for the nanoribbons with smaller widths.

A careful look at figure 7 reveals that the height of the plateau on the loading curve is almost the same for the nanoribbons of different widths and comprises about 0.006 nN Å\(^{-1}\). On the contrary, the plateau level on the unloading branch noticeably increases with increasing \( N \), being equal to 0.0035, 0.0039, and 0.0043 nN Å\(^{-1}\) for \( N = 3, 6, \) and 12, respectively. This result is understandable, taking into account the aforementioned fact that during loading DW motion starts at the nanoribbon edge, while during unloading it starts in the middle of the nanoribbon.

The reduction of the unloading plateau level with decreasing \( N \) explains the increase in the hysteresis loop area with decreasing \( N \).

3.3. Temperature effect

Finally, the nanoribbon is heated up to 300 K then cooled down to 0 K in order to see the effect of temperature on the DW behavior in the narrowest nanoribbon with \( N = 3 \). The Langevin thermostat [51] is used for temperature control. A temperature increment of 10 K (positive on heating and negative on cooling) was followed by thermalization for 20 ps and then the positions of the DWs were determined. Two equilibrium states with DWs are considered: one on the loading branch \( (\varepsilon_{xx} = 0.21, F/H_0 = 0.0059 \text{ nN} \text{ Å}^{-1}) \) and the other one on the unloading branch \( (\varepsilon_{xx} = 0.24, F/H_0 = 0.0035 \text{ nN} \text{ Å}^{-1}) \), see figure 7(a). Note that both initial structures are on the plateaus of the force-strain curves, which means that they contain domains with local tensile strain equal to \( \varepsilon_{xx}^{(1)} = 0.19 \) and \( \varepsilon_{xx}^{(2)} = 0.375 \). Let \( L^{(1)} \) and \( L^{(2)} \) be the lengths of the domains with local tensile strain \( \varepsilon_{xx} = \varepsilon_{xx}^{(1)} = 0.19 \) and \( \varepsilon_{xx} = \varepsilon_{xx}^{(2)} = 0.375 \), respectively. Note that \( L^{(1)} + L^{(2)} = L \), where \( L \) is the current length of the nanoribbon. We introduce relative lengths of the domains, \( C^{(1)} = L^{(1)}/L \) and \( C^{(2)} = L^{(2)}/L \) with \( C^{(1)} + C^{(2)} = 1 \). In figure 9, \( C^{(i)} \) is shown as a function of temperature for the structure on the loading (A) and unloading (B) branch. As can be seen, in figure 9(a), \( C^{(i)} \) decreases with temperature on heating and does not change on subsequent cooling. In contrast to that, in figure 9(b), \( C^{(i)} \) increases with temperature on heating and, similarly to the previous case, remains unchanged on cooling.

From this result it is clear that not only stretching/unstretching, but also heating can be used to control the DW motion in the two-phase state. We have also demonstrated that the highly stretched nanoribbon survives heating up to room temperature. According to our simulations, fracture of the highly stretched nanoribbon takes place at about 500 K. It is worth noting that the melting temperature of graphene in the absence of loading is about 5000 K [52, 53].

4. Discussion and conclusions

A study of the molecular dynamics of the uniaxial, strain-controlled tension of graphene nanoribbons with armchair edges is carried out. It is found that when tensile strain reaches the value of \( \varepsilon_{xx}^{(1)} = 0.19 \), two domains with the larger tensile strain of \( \varepsilon_{xx}^{(2)} = 0.375 \) appear near the clamped edges of the nanoribbon. Stretching within the range of the average tensile strain \( \varepsilon_{xx}^{(1)} < \varepsilon_{xx} < \varepsilon_{xx}^{(2)} \) occurs through the growth of the domain with larger strain at the expense of the domain with smaller strain.

Similar two-phase stretching has been experimentally observed for DNA [19–22], polypeptides [23], and some
polymer chains [18]. This effect is attributed to the presence of a concave down region on the dependence of the potential energy of the unit cell as a function of tensile strain [18], see figure 6. However, for the 1D materials, such as DNA and polymer chains, the loading and unloading curves coincide. In the present study of 2D material (graphene nanoribbon) an elastic hysteresis loop is revealed by simulating loading and unloading through the range of strain with two-phase stretching, see schematic figure 1 for a 1D chain and figure 7 for the graphene nanoribbon considered here. A structure analysis presented in figure 8 has shown the difference in the DW profile and kinematics during loading and unloading. Nucleation of DWs and their motion are accompanied by dissipation of the elastic energy. Thus, the nanoribbon can be used as an elastic damper, efficiently converting mechanical strain energy into heat during cyclic loading–unloading through the strain range where domains with larger and smaller strain coexist.

On the other hand, 2D materials supporting two-phase stretching allow for the new way of creating heterostructures. The fraction of differently strained domains can be controlled by strain-controlled loading or/and by heating, which would result in tuning physical and mechanical properties of the heterostructure.

Acknowledgments

The work of IPL was supported by the Russian Foundation for Basic Research, grant no. 17-02-00984-A. EAK thanks the Russian Science Foundation, grant no. 16-12-10175, for their financial support. SVD gratefully acknowledges financial support provided by the Russian Science Foundation, grant no. 14-13-00982.

ORCID iDs

Iman Evazzade @ https://orcid.org/0000-0002-9070-8565
Elena A Kozrnikova @ https://orcid.org/0000-0002-5975-4849

References

[1] Kong X, Liu Q, Zhang C, Peng Z and Chen Q 2017 Chem. Soc. Rev. 46 2127–57
[2] Melnick C and Kaviani M 2016 Phys. Rev. B 93 125203
[3] Yang M, Nurbawono A, Zhang C, Feng Y P and Ariando 2010 Appl. Phys. Lett. 96 193115
[4] Xiang H, Kan E, Wei S H, Whangbo M H and Yang J 2009 Nano Lett. 9 4025–30
[5] Liu B, Baimova J A, Reddy C D, Law A W K, Dmitriev S V, Wu H and Zhou K 2014 ACS Appl. Mater. Interfaces 6 18180–8
[6] Geim A K and Grigorieva I V 2013 Nature 499 419–25
[7] Novoselov K S, Mishchenko A, Carvalho A and Castro Neto A H 2016 Science 353 64
[8] Li C, Zhou P and Zhang D W 2017 J. Semicond. 38 031005
[9] Zhang J, Wang X, Hong Y, Xiong Q, Jiang J and Yue Y 2017 Nanotechnology 28 035404
[10] Chen Y, Zhang Y, Cai K, Jiang J, Zheng J C, Zhao J and Wei N 2017 Carbon 117 399–410
[11] Chen X K, Liu J, Peng Z H, Du D and Chen K Q 2017 Appl. Phys. Lett. 110 091907
[12] Liu B, Baimova J A, Reddy C D, Dmitriev S V, Law W K, Feng X Q and Zhou K 2014 Carbon 79 236–44
[13] Kistanov A A, Cai Y, Zhang Y W, Dmitriev S V and Zhou K 2017 J. Phys.: Condens. Matter. 29 095302
[14] Ai R, Guan X, Li J, Yao K, Chen P, Zhang Z, Duan X and Duan X 2017 ACS Nano 11 3413–9
[15] Luo B, Liu G and Wang L 2016 Nanoscale 8 6904–20
[16] Zhang X Q, Lin C H, Tseng Y W, Huang K H and Lee Y H 2015 Nano Lett. 15 410–5
[17] Tongay S et al 2014 Nano Lett. 14 3185–90
[18] Savin A V, Kikut I P, Mazo M A and Onufriev A V 2013 Proc. Natl Acad. Sci. USA 110 2816–21
[19] Ikai A 2017 Single-molecule DNA and RNA mechanics The World of Nano-Biomechanics (Amsterdam: Elsevier) pp 133–45
[20] King G A, Gross P, Bockelmann U, Modesti M, Wuite G J L and Peterman E J G 2013 Proc. Natl Acad. Sci. USA 110 3859–64
[21] Zhang X, Chen H, Le S, Rouzina I, Doyle P S and Yan J 2013 Proc. Natl Acad. Sci. USA 110 3865–70
[22] Smith S B, Cui Y and Bustamante C 1996 Science 271 795–9
[23] Afrin R, Takahashi I, Shiga K and Ikai A 2009 Biophys. J. 96 1105–14
[24] Babicheva R I, Bukreeva K A, Dmitriev S V, Mulyukov R R and Zhou K 2013 Intermetallics 43 171–6
[25] Bukreeva K A, Babicheva R I, Dmitriev S V, Zhou K and Mulyukov R R 2013 Phys. Solid State 55 1963–7
[26] Bukreeva K A, Babicheva R I, Sultanguzhina A B, Dmitriev S V, Zhou K and Mulyukov R R 2014 Phys. Solid State 56 1157–62
[27] Bukreeva K A, Babicheva R I, Dmitriev S V, Zhou K and Mulyukov R R 2013 JETP Lett. 98 91–5
[28] Sutrakar V K and Mahapatra D R 2010 Intermetallics 18 679–87
[29] Sutrakar V K and Mahapatra D R 2010 Intermetallics 18 1565–71
[30] Ma F, Sun Y J, Ma D Y, Xu K W and Chu P K 2011 Acta Mater. 59 6783–9
[31] Sun Y J, Huang Y H, Ma F, Ma D Y, Hu T W and Xu K W 2014 Mater. Sci. Eng. B 190 1–6
[32] Sun Y J, Ma F, Huang Y H, Hu T W, Xu K W and Chu P K 2013 Appl. Phys. Lett. 103 191906
[33] Yang Z, Huang Y, Ma F, Miao Y, Bao H, Xu K and Chu P K 2015 RSC Adv. 5 105194–6
[34] Zhao J, Yang Z, Wei N and Kou L 2016 Sci. Rep. 6 23233
[35] Bao H, Huang Y, Yang Z, Miao Y, Chu P K, Xu K and Ma F 2017 Appl. Surf. Sci. 404 180–7
[36] Zhao J, Kou L, Jiang J W and Rabczuk T 2014 Nanotechnology 25 295701
[37] He X, Li H, Zhu Z, Dai Z, Yang Z, Yang P, Zhang Q, Li P, Schwingenschlogl U and Zhang X 2016 Appl. Phys. Lett. 109 173105
[38] Yang S, Liu F, Wu C and Yang S 2016 Small 12 4028–47
[39] Kalikka J, Zhou X, Dilcher E, Wall S, Li J and Simpson R E 2016 Nat. Commun. 7 11983
[40] Quereda J, San-Jose P, Parente V, Vaquero-Garzon L, Molina-Mendoza A, Agrait N, Rubio-Bollinger G, Guine E, Roldan R and Castelanos-Gomez A 2016 Nano Lett. 16 2931–7
[41] Si C, Sun Z and Liu F 2016 Nanoscale 8 3207–17
[42] Xie H, Ouyang T, Germaneau E, Qin G, Hu M and Bao H 2016 Phys. Rev. B 93 075404
[43] Qi J, Qian X, Qi L, Feng J, Shi D and Li J 2012 Nano Lett. 12 1224–8
[44] Li J, Shan Z and Ma E 2014 *MRS Bull.* **39** 108–14
[45] Zhu T and Li J 2010 *Prog. Mater. Sci.* **55** 710–57
[46] Baimova J A, Dmitriev S V, Zhou K and Savin A V 2012 *Phys. Rev.* B **86** 035427
[47] Paimushin V N, Firsov V A, Gyunal I and Shishkin V M 2016 *Mech. Compos. Mater.* **52** 435–54
[48] Ponomarev Y K, Ermakov A I, Simakov O B and Mikhalkin I K 2013 *Met. Sci. Heat Treat.* **55** 8–13
[49] http://lammps.sandia.gov/
[50] Stuart S J, Tutein A B and Harrison J A 2000 *J. Chem. Phys.* **112** 6472–86
[51] Grest G S and Kremer K 1986 *Phys. Rev.* A **33** 3628–31
[52] Los J H, Zakharchenko K V, Katsnelson M I and Fasolino A 2015 *Phys. Rev.* B **91** 045415
[53] Ganz E, Ganz A, Yang L M and Dornfeld M 2017 *Phys. Chem. Chem. Phys.* **19** 3756