Effect of temperature and strain-rate on mechanical properties of defected graphene sheet: A molecular dynamics study

Aniyush Juneja¹ and G Rajasekaran²

¹Department of Mechanical Engineering, SRM Institute of Science and Technology, Chennai, TN, India.

²Research Assistant Professor, Department of Mechanical Engineering, SRM Institute of Science and Technology, Chennai, TN, India.

Corresponding authors: junejaaniyush@gmail.com; rajasekaran.ed@gmail.com

Abstract. Graphene, a one atom thick sheet of carbon exhibits outstanding mechanical properties, but defects which are unavoidable at the time of synthesis may strongly affect such as intrinsic properties and fracture toughness of graphene can be altered by topological defects such as vacancy, Stone-Thrower-Wales (STW) defects, dislocations and grain boundaries. In this research article, authors have extensively studied the effect of Stone-Thrower-Wales defect on mechanical properties of a single layer of graphene sheet at different temperature and strain-rates using classical molecular dynamics (MD) based simulations. Also, authors have studied the effect of defect-concentration on the mechanical properties of graphene at different temperature and strain rates. It has been observed that fracture strength and strain is not varying with temperature for STW-1 in zigzag direction and STW-2 in armchair direction respectively. Also, the same scenario was observed for different strain-rate values. Further-more it was observed that at 1K both STW-1 and STW-2 defects shows almost same fracture strength and strain in armchair and zigzag directions for higher strain-rates. On the other hand, at lower strain-rates both STW-1 and STW-2 defects showed different fracture strength and strain at 1K. Also, it was observed that at higher temperatures STW-1 in armchair direction and STW-2 in zigzag direction shows enormous decrease in mechanical properties, it shows STW-1 and STW-2 are not favourable in armchair and zigzag directions respectively. In addition, the effect of defects at different strain-rates and concentration on the fracture strength and failure morphology of graphene sheet has also been studied.

1. Introduction
Graphene, the two-dimensional (2D) monolayer of carbon atoms organized in a honeycomb lattice structure was revealed and effectively secluded from bulk graphite [1-2]. Due to its fascinating mechanical, thermal, electromechanical and magnetic [3] properties, it is being used in developing new nano technological devices for several applications ranging from biomedical to aerospace [4]. In addition to numerous applications, graphene is also listed among the very effective nano fillers for designing nano composites with improved mechanical properties [5-9]. To design reliable nano technological graphene based devices, a thorough understanding of their mechanical behaviour as individual element is critically important under different boundary conditions. Since graphene have been considered for
application in numerous fields, researchers are now directing towards on synthesizing industrial-scale graphene sheets. Synthesizing industrial scale graphene sheets by various methods such as chemical vapour deposition (CVD) and mechanical exfoliation usually results in a graphene with topological defects such as 5-7 defects [10-13], vacancies [3], 5-7-7-5 defects which is also known as Stone-Thrower-Wales (STW) defects [3], 5-8-5 defects [14], impurities, adatoms, substitution atoms [15] and crack like flaws such as slits and holes [16-17]. In addition to the topological defects that are associated with the synthesise techniques, structural defects can also be produced intentionally for enhancing functionality of graphene sheet in terms of ideal shape, orientation and structure for desired properties [18].

It is understandable from the literature that, defect engineering is one of the popular techniques which have been extensively used by researchers to tailor various properties of metals [19-20], ceramics [21] and diamond like materials [22]. In addition, structural and topological defects have also unlocked the possibilities to alter both intrinsic and fracture properties of graphene. Several studies have been conducted to investigate the effect of structural and topological defects on the intrinsic properties such as fracture strength and strain and Young’s modulus of graphene sheet. Wang et al. [23] studied the influence of Stone-Thrower-Wales defects and vacancy defects on the fracture strength of graphene sheet. It was concluded from their atomistic model that the fracture strength of graphene sheet was affected by chirality as well as temperature, but they have calculated all the intrinsic properties at higher temperature, i.e. 300 K to 900 K. Jing et al. [6] examined the influence of vacancies and STW-1 defects on modulus of elasticity of graphene and they noticed an overall decrease in the modulus of elasticity with an increase in defects concentration. Xiao et al. [24] investigated the effect of multiple STW defects on mechanical properties of graphene sheets and CNT’s using atomistic based finite bond element model. Recent research on 5-7 (pentagon-heptagon) defects [25-27] have been conducted to show that higher concentration of grain boundary (GB) defects can instinctively give increase to higher intrinsic strength in tilt grain boundaries. Wei et al. [28] predicted that strength of grain boundary (GB) can either increase or decrease with tilt angle. Also, Yang et al. [29] investigated the effect of temperature and strain-rate on nano-crystalline graphene sheets, and it was noticed that the atomic behaviour in the GBs was a crucial factor deciding the intrinsic strength of the sheet. In addition to atomistic based numerical simulations, various means of experimental techniques [30-31] also been carried out to investigate the fundamental importance of the effect of above discussed topological defects on the intrinsic properties of graphene.

![Figure 1](image1.png)

**Figure 1.** STW defects are generated by rotating the C-C bond by $\pi/2$ about the midpoint of the bond. (a) Blue C-C bond rotates by $\pi/2$ to form STW-1 defect. (b) Blue C-C bond rotates by $\pi/2$ to form STW-2 defect.

From the literature it is very clear that topological defects can be effectively used for tailoring intrinsic as well as fracture properties of graphene. The Stone-Thrower-Wales defects are the most significant defective structure in graphene. It has been understandable from Tserpes et al. [32] that interfacial bonding in nanocomposites with graphene and CNT as nanofillers may preferably take place at STW defected regions. Investigations have been shown that besides the impact that may have on the intrinsic and fracture behaviour of graphene, STW defects also affects their magnetic, electronic and
hybridization characteristics of graphene sheet [32]. Even though several research works have been conducted to understand the effect of structural defects on mechanical properties of graphene sheet, still it needs to understand clearly that how the STW defects effect the mechanical properties of graphene sheet. On the other hand, Baimova et al. [33] studied the effect of STW-1 and STW-2 on structural stability at zero temperature using MD simulation and investigated that STW-1 and STW-2 defects have no effect on the graphene strength along zigzag direction, but at the same time reduction of critical strain by STW-1 and STW-2 defects are maximal along armchair direction, which is greater for STW-1 in comparison to STW-2 defect. Due to temperature and strain rate dependent annihilation nature of STW defects, and previous studies on STW-1 and STW-2 defects were carried out in their favourable directions at 300 K and above, so it is necessary to understand the effect of STW-1 and STW-2 defects at different boundary conditions such as at lower temperature, different loading directions and strain rates.

In addition to mechanical properties, strain rate also affects fracture mechanism. Zhao and his team [34] studied the relation between fracture strength and time to failure with strain rate for pristine graphene sheet and graphene with atomic-scale slit. Their investigation showed that, increasing the temperature or decreasing the strain-rate could lead to decrease in the strength of the sheet. Also, at higher temperature the effect of strain-rate was more dominant. Mortazavi et al [35] investigated the effect of STW defects concentration on the failure strength of the graphene sheet with mixed proportion of STW-1 and STW-2 defects. So far, no research study has been conducted on the effect of strain rate on intrinsic properties of graphene sheet with STW-1 and STW-2 in their favourable (i.e. STW-1 in zigzag and STW-2 in armchair) and non-favourable (i.e. STW-2 in zigzag and STW-1 in armchair) directions. Furthermore, it needs to study the synchronized effects of operating parameters such as temperature and strain rate in applications were both factors may exist. Also, while producing large area graphene sheets the intrinsic strength of the sheet also depends on the concentration of the STW defects in their favourable directions. Hence, the aim of this research article is to illuminate the influence of STW-1 and STW-2 defects on the mechanical properties and failure morphology of graphene under various temperatures, strain rate and defect concentration along their favourable as well as non-favourable directions. It is proposed that both STW-1 and STW-2 defects can be used in either zigzag and/or armchair directions at 1 K without sacrificing their strength which is equal to that of in their favourable directions. A good resistance against the temperature and strain-rate has been observed when STW-1 and STW-2 defects are loaded in their favourable direction than compared to a drastic drop in strength in their non-favourable direction. Also, a change in fracture morphology is observed which is both strain-rate and concentration dependent.

2. Modeling Details and Methodology

In this article, atomistic models of graphene sheets were developed in the environment of molecular dynamics (MD). All the MD simulations were carried out in open source code LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) package [36]. In this atomistic model, the interatomic interactions between carbon atoms were simulated by using AIREBO (adaptive intermolecular reactive empirical bond order) potential [37]. AIREBO potential contains three major components, which are the REBO (reactive empirical bond order) potential [38], the torsional component and the Lennard-Jones (LJ) component. The REBO potential estimates energy stored in C-C bonds, the torsional component evaluates the energy due to torsional interactions between carbon atoms and the LJ component reflects the non-bonded interactions between carbon atoms. To eliminate unwanted behaviour of interatomic potential in estimating the failure properties of graphene, constant cut-off distance value of 1.92 Å was employed in the simulations [39-41].

To avoid finite size effect, all the MD simulations were carried out by keeping the dimensions of the graphene sheet as 9 nm x 9 nm which contains 3024 carbon atoms. Thickness of the sheet was taken as 0.34 nm [39-40]. Simulations are run at different temperatures with an integration time-step of 0.5 fs. Unit lattice vector was kept high so as to eliminate the formation of bi-layer graphene. Periodic boundary
conditions (PBCs) were applied in all directions, fixing the out of plane boundary condition to eliminate the van-der-Waals interaction between the sheet and its periodic image. Initially the system was relaxed for 30 ps at isothermal and isobaric conditions using NPT ensemble. After that a force was applied on the defected sheet in both zigzag and armchair directions at different strain-rates and temperature. Fracture stress was calculated at the time-step of first bond rupture with the help of virial-stress [18] method that averages of the stresses on all the carbon atoms in the model. The equation is defined as

\[
\sigma_{ij} = \frac{1}{\Omega^a} \left( \frac{1}{2} m^a v_i^a v_j^a + \sum_{\beta=1,n} r_{\alpha\beta} f_{\alpha\beta} \right)
\]

(1)

Where \( i \) and \( j \) represents indices in Cartesian coordinate system; \( \alpha \) and \( \beta \) are the atomic indices; \( m^a \) and \( v^a \) are mass and velocity of atom \( \alpha \); \( r_{\alpha\beta} \) is the distance between atoms \( \alpha \) and \( \beta \); \( \Omega^a \) is the atomic volume of atom \( \alpha \). The atomic volume can be calculated from the relaxed graphene sheet with a thickness of 0.34 nm.

3. Results and Discussion

3.1 Effect of Temperature and strain-rate on mechanical behavior and failure morphology of graphene with STW defects

Stone-Thrower-Wales (STW) defects are formed by rotating a C-C bond by 90°, which transforms 4 hexagonal unit cells into 2 heptagons and 2 pentagons as shown in figure 1. Due to hexagonal lattice structure and symmetric geometry of graphene system, it is possible to form only two types of STW defects namely STW-1 and STW-2 defects which are explained with the help of figure 1. The important feature of graphene with STW defects is that it retains the same number of atoms as the pristine graphene and it will form without creating any dangling bonds.

As mentioned earlier in this article, it is very clear that many of the previous studies on graphene with STW-1 and STW-2 defects has been carried out in zigzag and armchair directions respectively at higher temperatures of 300 K and above and at the strain rate of 0.001 ps\(^{-1}\). Since the mechanical properties of graphene depends on numerous factors such as loading direction, temperature, strain rate and so on. Hence, in order to use the advantages of STW-1 and STW-2 defects for various functional aspects, one need to understand the effect of these defects in their favourable (i.e. STW-1 is favourable in zigzag and STW-2 is favourable in armchair directions) and non-favourable directions at various temperatures and strain rates. Hence, in this section, authors have conducted the simulations of defected graphene sheet at different temperatures ranging from 1 K to 600 K and at different strain rates from 0.0001 ps\(^{-1}\) to 0.01 ps\(^{-1}\).

Initially, to validate AIREBO potential and our large-scale atomistic model, simulations were performed with pristine graphene sheet as well as graphene sheet with STW-1 and STW-2 defects along the zigzag and armchair directions at 300 K and at a strain rate of 0.001 ps\(^{-1}\). Stress-strain response of graphene sheet with STW-1 and STW-2 defects with respect to different tensile loading directions is depicted in figure 2. It can be understandable from the stress-strain response plotted in figure 2b and figure 2c that STW-1 and STW-2 defects are important to tailor mechanical properties. On the other hand, STW-1 and STW-2 are considered highly detrimental for the graphene sheet along the armchair and zigzag directions respectively. An anisotropic stress-strain response plotted in figure 2 for pristine as well as STW defected graphene sheet are in good agreement with the experimental values [42] and other atomistic simulation results [18].
After validating the model through examining the stress-strain response of pristine as well as STW defected graphene at 300 K, MD simulations were performed to study the effect of temperature and strain rate on mechanical properties of graphene sheet. Figure 3 illustrates the stress-strain response of graphene sheet with STW-1 and STW-2 defects in both zigzag and armchair directions at various temperatures and strain rates. It can be inferred from figure 3 that the fracture strength and strain of graphene sheet with STW-1 and STW-2 defects are gradually decreasing with respect to the studied temperature range in zigzag and armchair directions respectively.

Whereas, the strength and strain of graphene sheet with STW-1 and STW-2 defects are erratically decreasing in armchair and zigzag directions respectively in the temperature range of 1 K to 150 K. It is also observed from figure 3 that at lower temperature i.e. at 1 K, the strength and strain of graphene sheet with STW-1 and STW-2 defects are almost same in zigzag and in armchair directions at higher strain rate (0.001 ps\(^{-1}\) and 0.01 ps\(^{-1}\)). At lower strain rate (figure 3c) one can find a mild change in
mechanical properties of graphene with STW-1 and STW-2 defects at 1 K in both zigzag and armchair directions. It can be inferred from figure 3 that the effect of temperature on the fracture strength is more significant at a low strain rate than at high strain rate.

**Figure 3.** Illustration of failure strength and strain plots against temperatures at different strain rates in both zigzag and armchair directions. (a) at strain rate of 0.01 ps\(^{-1}\) (b) at strain rate of 0.001 ps\(^{-1}\) (c) at strain rate of 0.0001 ps\(^{-1}\).
When temperature increases from 1 K to 600 K, the fracture strength of graphene with STW-1 defect drops 28 % and 99 % in zigzag and armchair directions respectively and the fracture strength of graphene with STW-2 defect drops 99 % and 27 % in zigzag and armchair directions respectively at the low strain rate of 0.0001 ps\(^{-1}\), while it only drops 20 % and 92 % for graphene with STW-1 defects in zigzag and armchair directions respectively and 53 % and 18 % for graphene with STW-2 defects in zigzag and armchair directions respectively at the higher strain rate of 0.01 ps\(^{-1}\).

**Figure 4.** Illustration of failure morphology of graphene sheet with STW defects during tensile deformation at 1K. (a) STW-1 defect in zigzag direction before crack nucleation. (b) STW-1 defect in zigzag direction during crack nucleation. (c) STW-2 defect in zigzag direction before crack nucleation. (d) STW-2 defect in zigzag direction during crack nucleation. (e) STW-1 defect in armchair direction before crack nucleation. (f) STW-1 defect in armchair direction during crack nucleation. (g) STW-2 defect in armchair direction before crack nucleation. (h) STW-2 defect in armchair direction during crack nucleation.

To understand the failure morphology of graphene sheet at 1K, MD simulations were carried out for graphene sheets with STW-1 and STW-2 defects in zigzag and armchair directions at the strain rate of 0.001 ps\(^{-1}\) and plotted in figure 4. It is understandable from figure 4b and figure 4d that the failure pattern (i.e., failure triggering from defects and propagating with multiple branches as shown in figure 4b and
figure 4d) of graphene sheet in zigzag direction is same for both STW-1 and STW-2 defects. Similarly, it can also be understandable from figure 4f and figure 4h that the failure pattern (i.e., failure triggering from defects and propagating perpendicular to the loading direction with chain formation) is same for STW-1 and STW-2 defects in armchair direction. This clearly shows that, in addition to identical fracture strength at lower temperature the failure morphology of graphene sheet with STW-1 and STW-2 defects are also similar at such cryogenic temperature.

3.2 Effect of defect concentration and strain rate on failure morphology of graphene sheet with STW defects

To study the effect of defect concentration and strain rate on failure morphology of graphene sheets, authors have carried out set of MD simulations for graphene sheet with different concentration of STW-1 defects in zigzag direction and STW-2 defects in armchair direction at the temperature of 300K. Figure 5 illustrates the failure morphology of graphene sheet with STW defects at different strain rates. It can be observed from figure 5b and figure 5f that at lower strain rate of 0.0001 ps\(^{-1}\) the failure initiates from one STW defect and crack nucleates and complete rupture take place. Whereas on the other hand, it was observed from figure 5d and figure 5h that at higher strain rate value of 0.01 ps\(^{-1}\) the failure initiates from different STW defects and crack nucleates and complete rupture take place. It is understandable that at higher strain rates the bond rotation and reformation was not accomplished completely whereas at lower strain rate the bonds get sufficient time to re-orient themselves [29]. Due to this incomplete bond rotation and reformation, multiple stress concentrated regions are found on the sheet around these defects, which leads to multiple breakages at higher strain-rate. Further it was observed that, at higher defect concentration, the initiation of failure at multiple locations was transformed into a single point failure at SW defect even at higher strain-rate. This is due to the position of STW defects with respect to each other over the graphene sheet. From this section it can be concluded that failure morphology of graphene sheet with STW defects is a function of defect-concentration as well as the strain-rate.

4. Conclusions

In this research article, systematic MD simulations were carried out to study the effect of temperature and strain-rate on the mechanical strength and failure morphology of a STW defected graphene sheet in both the zigzag and armchair directions. With the help of Stress distribution diagrams, it was proposed that identical fracture strength of STW-1 and STW-2 defects in both the zigzag and armchair direction was observed at 1K. Whereas a slight change in strength was observed on decreasing the strain-rate. Further, identical failure morphology of STW-1 and STW-2 defects in both zigzag and armchair directions were observed at the temperature of 1K. As the temperature was increased, the fracture strength decreased drastically for STW-1 and STW-2 defects in armchair and zigzag direction respectively. On the other hand, it was observed that the fracture strength decreased moderately when the tensile load was applied in their favourable directions (i.e. STW-1 in zigzag direction and STW-2 in armchair direction). Failure Morphology of STW-1 in zigzag direction and STW-2 in armchair direction was observed as a function of strain-rate and defect concentration. Where single to multiple point fracture was observed on increasing the strain-rate. After a certain limit of defect concentration, a change in the trend of multiple to single point fracture was observed at high strain-rate of 0.01/ ps\(^{1}\). These results can help in designing graphene based materials at large scale, which could be used in harsh environment and in areas which exploits such property of this material. Also, it provides a precise knowledge of enhancing mechanical strength of graphene by exploiting the novel effects of STW-1 and STW-2 defects when exposed to different boundary conditions.
Figure 5. Illustration of failure morphology of graphene sheet with different STW defects concentration during tensile deformation at different strain rate at 300K. (a),(b) STW-1 defect in zigzag direction before and after crack nucleation at strain rate of 0.0001ps\(^{-1}\). (c),(d) STW-1 defect in zigzag direction before and after crack nucleation at strain rate of 0.01ps\(^{-1}\). (e),(f) STW-2 defect in armchair direction before and after crack nucleation at strain rate of 0.0001ps\(^{-1}\). (g),(h) STW-2 defect in armchair direction before and after crack nucleation at strain rate of 0.01ps\(^{-1}\).

5. Acknowledgements
This work is supported by the SRM Institute of Science & Technology (SRMIST) Chennai, India. We thank High Performance Computing Centre (HPCC), SRMIST for providing computational facility and support for this project.

6. References
[1] K.S.Novoselov, A.K.Geim, S.V.Morozov, D.Jiang, Y.Zhang, S.V.Dubonos, I.V.Grigorieva, A.A.Firsov 2004 Electric Field Effect in Atomically Thin Carbon Films Science 306 666-669
[2] A.K.Geim, 2009 Graphene: Status and Prospects Science 324 1530-1534
[3] G. Rajasekaran, P. Narayanan, A. Parashar 2016 Effect of point and line defects on mechanical and thermal properties of graphene: a review Crit. Rev. Solid State Mater. Sci. 41(1) 47-71
[4] M.A.N. Dewapriya S.A. Meguid, 2017 Atomistic simulations of nanoscale crack-vacancy interaction in graphene Carbon 125 113-131
[5] G. D. Zhan, J. D. Kuntz, J. Wan, and A. K. Mukherjee 2003 Single-wall carbon nanotubes as attractive toughening agents in alumina-based nanocomposites Nat. Mater. 2 38–42
[6] N. Jing, Q. Xue, C. Ling, M. Shan, T. Zhang, X. Zhou, and Z. Jiao 2012 Effect of defects on Young’s modulus of graphene sheets: a molecular dynamics simulation RSC Adv. 2 9124–9129
[7] T. Kuila, S. Bhadra, D. Yao, N. H. Kim, S. Bose, and J. H. Lee 2010 Recent advances in graphene based polymer composites Prog. Polym. Sci. 35 1350–1375
[8] T. K. Das and S. Prusty 2013 Graphene-based polymer composites and their applications Polymer-Plastics Technol. Eng. 52 319–331
[9] R. Verdejo, M. M Bernal, L. J Romasanta, and M. A. Lopaz-Manchado 2011 Graphene filled polymer nanocomposites J. Mater. Chem. 21 3301–3310
[10] Jannik C. Meyer, C. Kisielowski, R. Erni, Marta D. Rossell, M.F. Crommie, A. Zettl 2008 Direct imaging of lattice atoms and topological defects in graphene membranes Nano Lett. 8 (11) 3582–3586
[11] Maria P. Lopez-Sancho, Fernando de Juan, Maria A.H. Vozmediano 2009 Magnetic moments in the presence of topological defects in graphene Phys. Rev. B Condens. Matter 79 075413
[12] J. Wu, Y. Wei 2013 Grain misorientation and grain-boundary rotation dependent mechanical properties in polycrystalline graphene J. Mech. Phys. Solids 61 1421–1432
[13] Y.I. Jhon, S.E. Zhu, J.H. Ahn, M.S. Jhon 2012 The mechanical responses of tilted and nontilted grain boundaries in graphene Carbon 50 3708–3716
[14] J. Kotakoski, A.V. Krasheninnikov, U. Kaiser, J.C. Meyer 2011 From point defects in graphene to two-dimensional amorphous carbon Phys. Rev. Lett. 106 105505
[15] F. Banhart, J. Kotakoski, A.V. Krasheninnikov 2011 Structural defects in graphene ACS Nano 5 (1) 26–41
[16] T. Zhang, H. Gao 2015 Toughening graphene with topological defects: a perspective J. Appl. Mech. 82 051001 (3pp)
[17] R. Khare, S.L. Mielke, J.T. Paci, S. Zhang, R. Ballarini, G.C. Schatz, T. Belytschck 2007 Coupled quantum mechanical/molecular mechanical modelling of the fracture of defective carbon nanotubes and graphene sheets Phys. Rev. B Condens. Matter 75 075412 (12pp)
[18] G. Rajasekaran, A. Parashar 2016 Molecular dynamics study on the mechanical response and failure behaviour of graphene: performance enhancement via 5-7-7-5 defects RSC Adv. 6 26361
[19] K.S. Kumar, H. Van Swygenhoven, S. Suresh 2003 Mechanical behavior of nanocrystalline metals and alloys Acta Mater. 51 5743–5774
[20] K. Lu, L. Lu, S. Suresh 2009 strengthening materials by engineering coherent internal boundaries at the nanoscale Science 324 349–352
[21] Y. Tian, B. Xu, D. Yu, Y. Ma, Y. Wang, Y. Jiang, W. Hu, C. Tang, Y. Gao, K. Luo, Z. Zhao, Li-Min Wang, B. Wen, J. He, Z. Liu 2013 Ultrahard nanotwinned cubic boron nitride Nature 493 385–388
[22] Q. Huang, D. Yu, B. Xu, W. Hu, Y. Ma, Y. Wang, Z. Zhao, B. Wen, J. He, Z. Liu, Y. Tian 2014 Nanotwinned diamond with unprecedented hardness and stability Nature 510 250–253
[23] M. C. Wang, C. Yan, L. Ma, N. Hu, and M. W. Chen 2012 Effect of defects on fracture strength of graphene sheets Comput. Mater. Sci. 54 236–239
[24] J. R., B. Bhattacharyya 2005 Effect of randomly occurring Stone-Wales defects on mechanical properties of carbon nanotubes using atomistic simulation Nanotechnology 16 555-566
[25] R. Grantab, V. B. Shenoy, R. S. Ruoff 2010 Anomalous strength characteristics of tilt grain boundaries in graphene Science 330 946-948
[26] Y. I. Jhon, S. E. Zhu, J. H. Ahn, M. S. Jhon 2012 The mechanical responses of tilted and non-tilted grain boundaries in graphene Carbon 50 3708-3716
[27] J. Wu, Y. Wei 2013 Grain misorientation and grain-boundary rotation dependent mechanical properties in polycrystalline graphene J. Mech. Phys. Solids 61 1421-1432
[28] Y. Wei, J. Wu, H. Yin, X. Shi, R. Yang, M. Dresselhaus 2012 The nature of strength enhancement and weakening by pentagon-heptagon defects in graphene Nat. Mater. 11 759-763
[29] Z. Yang, Y. Huang, F. Ma, Y. Sun, K. Xu, and Paul K. Chu 2015 Temperature and strain-rate effects on the deformation behaviour of nano-crystalline graphene sheets Eur. Phys. J. B 88:135
[30] A. Zandiatashbar, G. H. Lee, S. J. An, S. Lee, N. Mathew, M. Terrones, T. Hayashi, C. R. Picu, J. Hone, N. Koratkar 2014 Effect of defects on the intrinsic strength and stiffness of graphene Nat. Commun. 5 3186
[31] A. W. Robertson, G. D. Lee, K. He, E. Yoon, A. I. Kirkland, J. H. Warner 2014 Stability and dynamics of the tetravacancy in graphene Nano Lett 14 1634-1642
[32] K. I. Tserpes, P. Papanikos 2007 The effect of Stone-Wales defect on the tensile behaviour and fracture of single-walled carbon nanotubes Compos. Struct 79 581-589
[33] J. A. Baomova, L. Bo, S. V. Dmitriev, K. Zhou, A. A. Nazarov 2013 Effect of Stone-Thrower-Wales defect on structural stability of graphene at zero and finite temperatures EPL 103 46001
[34] H. Zhao and N. R. Aluru 2010 Temperature and strain-rate dependent fracture strength of graphene J. Appl. Phys. 108 064321
[35] B. Mortazavi, S. Ahzi 2013 Thermal conductivity and tensile response of defective graphene: A molecular dynamics study carbon 63 460-470
[36] S. Plimpton 1995 Fast Parallel Algorithms for Short-Range Molecular Dynamics J. Comput. Phys. 117 1-19
[37] S. J. Stuart, A. B. Tutein, J. A. Harrison 2000 A reactive potential for hydrocarbons with intermolecular interactions J. Chem. Phys. 112 6472-6486
[38] D. W. Brenner, O. A. Shenderova, J. A. Harrison, S. J. Stuart, B. Ni, S. B. Sinnott 2002 A second-generation reactive empirical bond order (REBO) potential energy expression for hydrocarbons J. Phys.: Condens. Matter 14 783-802
[39] G. Rajasekaran, A. Parashar 2016 Anisotropic compressive response of Stone-Thrower-Wales defects in graphene: A molecular dynamics study Mater. Res. Express 3 095015
[40] R. Kumar, G. Rajasekaran, A. Parashar 2016 Optimized cut-off function for Tersoff-like potentials for a BN Nanosheet: a molecular dynamics study Nanotechnology 27 085706
[41] G. Rajasekaran, R. Kumar, A. Parashar 2016 Tersoff potential with improved accuracy for simulating graphene in molecular dynamics environment Mater. Res. Express 3 035011
[42] C. Lee, X. Wei, J. W. Kysar, J. Hone 2008 Measurement of the elastic properties and intrinsic strength of monolayer graphene Science 321 (5887) 385-388