

Article

The Effects of Dislocation Dipoles on the Failure Strength of Wrinkled Graphene from Atomistic Simulation

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Abstract: This research paper studies the fracture and mechanical properties of rippled graphene containing dislocation dipoles. The atomistic simulation is performed to study the deformation behavior of pristine and defective wrinkled graphene. Graphene wrinkling considerably decreases the ultimate tensile strength of graphene with and without defects but increases the fracture strain. For graphene with the dislocation dipoles, temperature increase slightly affects mechanical properties, in contrast to graphene and graphene with Stone–Wales defect. The extremely similar slopes of the stress-strain curves for graphene with the dislocation dipoles with different arms imply that the distance between dislocations in the dipole does not have noticeable effects on the elastic modulus and strength of graphene. Defects in graphene can also affect its wrinkling; for example, preventing wrinkle formation.

Keywords: graphene; dislocation dipole; mechanical properties; atomistic simulation



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1. Introduction

Defects of the crystal structure are naturally present in as-grown graphene, especially for large-scale growth methods. Defects can appear in response to external loads in order to relieve local stresses, during graphene syntheses, at high temperatures, and were extensively studied by different methods [1–4]. Defects in graphene can considerably affect different properties of graphene: mechanical [3–7], electronic and transport [8–10], chemical activity [11], to name a few.

One of the most common defects is the Stone–Wales (SW) defect which can appear due to the rotation of a C–C bond, with the transformation of the four adjacent hexagons into two pentagons and two heptagons [1,12]. From the other point of view, SW defect is a dislocation dipole in which two edge dislocations with opposite Burgers vectors are displaced by one lattice unit [13,14]. This pair of dislocations can be separated into a dislocation dipole with the dipole arm of different lengths. Usually, SW defects and dislocations result in graphene buckling which is also influenced by their special structure [13,15,16]. The strength of graphene is usually high, but it considerably depends on the presence of such topological defects and out-of-plane deformation. Defects change the mechanical properties of graphene [3–7,17–19]. For example, the fracture strength of defective graphene depends on temperature and strain rate [20]. The inverse effect of temperature increase on the mechanical properties of defective and perfect graphene was found [21]. In [22] the effects of defects and doping on the mechanical properties of graphene are studied. It is found that the location of defects and their concentration are important factors for understanding the mechanical properties of graphene.

The strength of graphene is highly important for the future development of high-performance graphene materials and devices for different areas, such as flexible electronics. One of the graphene structural peculiarities is wrinkling. The stability of graphene was discussed for a long time. The instability of two-dimensional (2D) structures at finite

temperatures were discussed first by Landau and Peirls [23,24] and further by Mermin [25]. According to the so-called Mermin–Wagner theorem [25], long-wavelength fluctuations destroy the long-range order of two-dimensional crystals. However, the stability of the 2D material is achieved by ripple formation [26]. Indeed, single-layered graphene may spontaneously develop thermal ripples at finite temperatures [27–29]. Defect-induced ripples were also observed in other studies [30,31].

The effect of ripples on graphene properties is not a trivial question. In [32,33], the stability of graphene was discussed. It was shown that even initially planar graphene can be transformed into rippled one under applied strain. Such ripples soften the elastic moduli, changing Poisson's ratio [34,35]. However, graphene with monotonously distributed corrugations also demonstrates high strength [34]. Interestingly, that wrinkled graphene can even be used to increase the strength of metal matrix composites [36,37].

In the present work, systematical MD simulations are carried out to investigate the fracture behavior of graphene with dislocation dipoles with different arm lengths at zero, room, and finite temperatures. The point of this work is to understand how the fracture process will develop in the presence of ripples and defects.

2. Materials and Methods

The graphene is modeled with a rectangular supercell, which contains 3100 carbon atoms in a two-dimensional x and y space with a 200 Å vacuum region along the z -axis. To prevent finite-size effects, the size of the simulation cells is approximately 103×74 Å, which is obtained from variable cell relaxation of graphene. In geometry optimization, all atoms are relaxed until the force on each atom is smaller than 0.01 eV/Å with an energy convergence of 10^{-4} eV. The internal strain field developed by defects such as dislocations in graphene results in the out-of-plane buckling [38]; however, in the present work periodic boundary conditions applied along x and y directions buckling is suppressed. Thus, the system moves to a mechanically stable state with a downward bubble around each dislocation. It was previously shown that dislocation dipole in graphene could induce such bubbles with an amplitude up to 3.3 Å.

A dislocation dipole (DD) consists of two dislocations divided by the different distance which is the dipole arm l . The part of the simulation cell with the DD is presented in Figure 1 for each considered defect. Here, the orientation angle of the dipoles is $\pi/6$, although it can be varied in a wide range [39]. The structures are named DD _{n} , where the subscript n indicates the distance between two 5–7 pairs in the hexagon units. The height h from the bottom of the basin to the top of the hillock changes as the distance between the two 5–7 pairs increases. The well-known SW defect in graphene may be viewed as a tightly bounded edge dislocation dipole in a 2D hexagonal lattice [39]. The Burgers vector of the dislocations comprising the SW defect and dislocation dipoles has magnitude $b = \sqrt{3}a$, where $a = 1.42$ Å is the C–C spacing in graphene. Values of dipole arms and buckling height for DD_{2–10} are presented in Table 1.

The defect structures are obtained with the help of a homemade program; the LAMMPS simulation package is employed to perform the tensile loading simulations. The adaptive intermolecular reactive bond order (AIREBO) potential [40] is used to describe the interaction between carbon atoms. The simulation cell is periodic along the x (armchair) and y (zigzag) directions.

Displacement-controlled uniaxial tension is applied to graphene at a constant temperature and strain rate 0.005 ps^{-1} , and the various stress components are calculated at each strain level to obtain the stress-strain curves. The tensile loading is applied by increasing the periodic simulation box size along the loading direction.

The Nose-Hoover thermostat is employed and the temperature is set to 0 K, 300 K, and 1000 K. All the values obtained at 300 K and 1000 K are averaged over at least 100 trials at given values of strain. Two criteria are used to identify the fracture of graphene: bond breaking and sharp reduction of the potential energy of the system. These two criteria give

close critical time since the large elastic strain and relatively low temperatures (lower than 1000 K) are considered. At these conditions, a brittle fracture is observed.

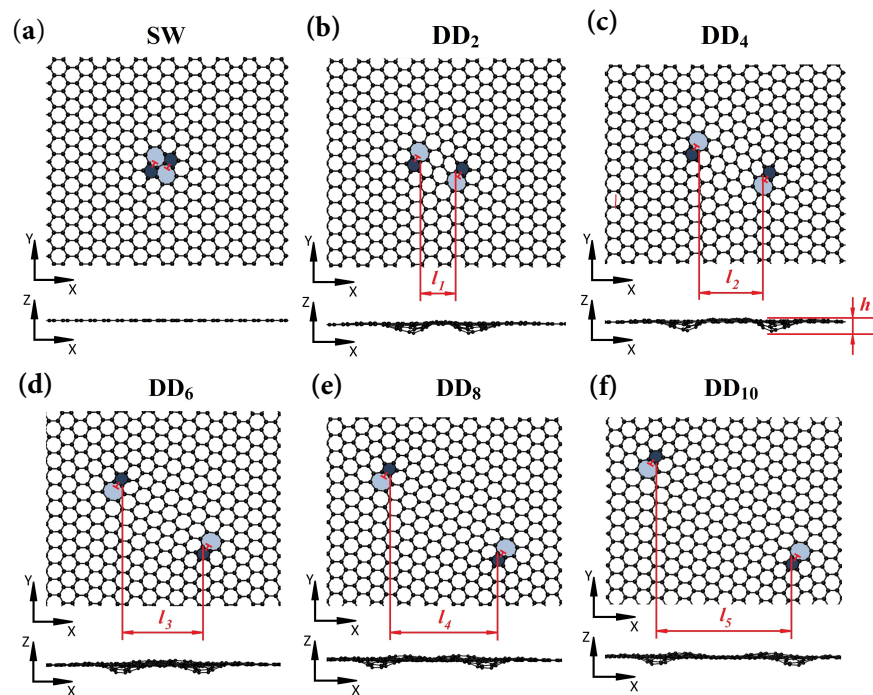


Figure 1. Typical structures of graphene in two projections: (a) graphene with SW defect, (b–f) graphene with dislocation dipole DD_n with the different arm. Geometrical parameters for dipoles are presented in Table 1. Pentagons and heptagons are colored in dark and light blue, respectively.

Table 1. Values of dipole arm l and buckling height h for graphene with SW and DD_n .

Defect	l , Å	h , Å
SW	0	0
DD_2	6	1.89
DD_4	11	2.0
DD_6	15	1.25
DD_8	20	1.22
DD_{10}	25	1.78

3. Results

3.1. Fracture Strength of Graphene with Defects

Figure 2 displays the course of the stress-strain curves for defect-free graphene and that featuring a number of different dislocation dipoles, under tension along armchair/zigzag orientations. For simplicity, all the values for tension along the zigzag direction will be defined by superscript z (zigzag) and, for tension along the armchair direction, by superscript a (armchair). All the critical values such as ultimate tensile strength σ_{UTS} , fracture strength ε_F and elastic modulus E for all considered structures under tension along armchair and zigzag direction are presented in Figure 3. Critical values for graphene under tension are shown by open circles. All the results are presented for three temperatures—0 K (theoretical strength), 300 K (room temperature), and 1000 K (finite temperatures). For a better understanding, both Figures 2 and 3 should be described in connection with each other.

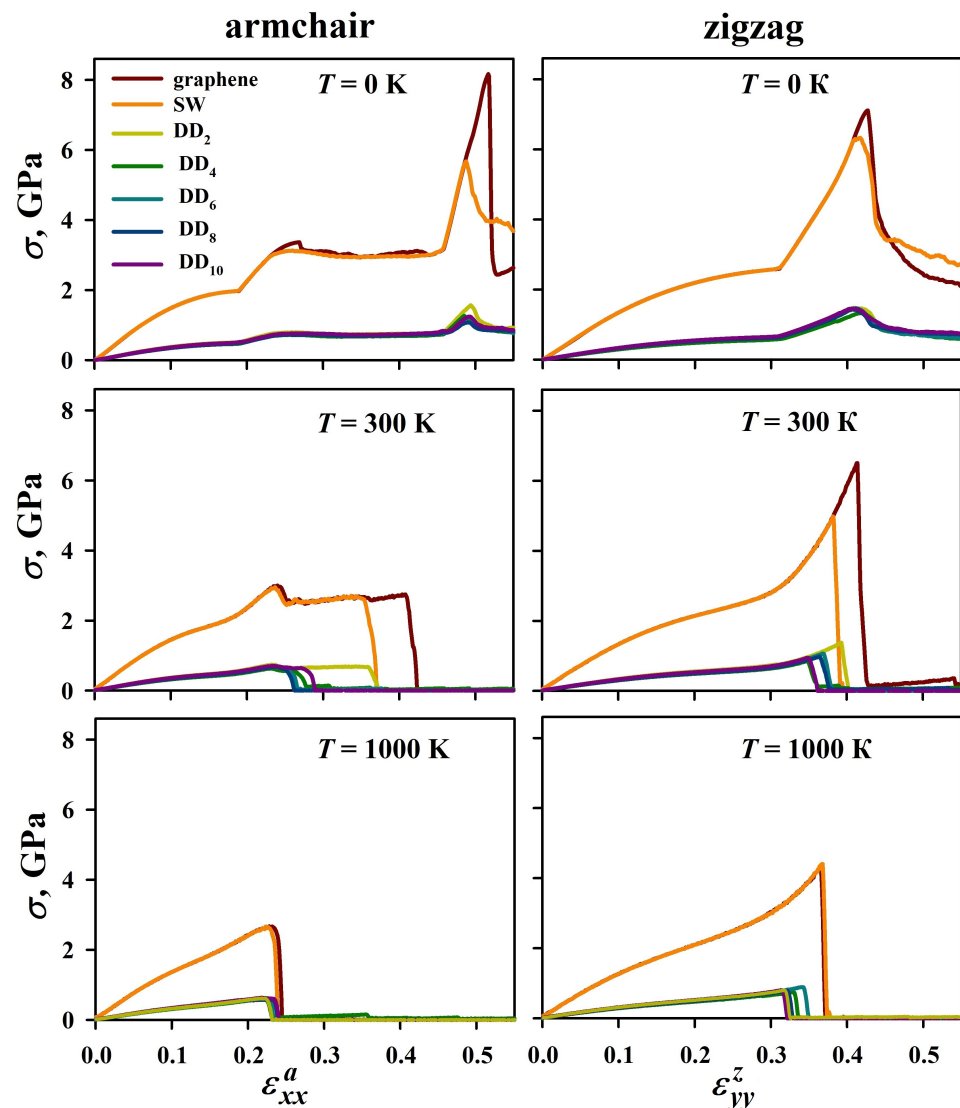


Figure 2. Stress-strain curves for graphene, graphene with SW defect and with DD_n under tension along armchair/zigzag direction at three temperatures.

First, let us discuss graphene strength. Commonly, in the literature, the graphene strength is very high, close to 100 GPa [19,41–43]. However, results obtained by different numerical methods are considerably dependent on the simulation technique, which is reviewed in [19]. For example, as it is mentioned in [44], under dynamic load covalent networks exhibit brittle fracture instead of ductile because of insufficient structure relaxation. How the tensile strain is applied results in a different scenario for the composites based on graphene network [45]: values of the fracture strength of covalent systems for dynamic loading can be overestimated. In the present work, crumpling of graphene is allowed with the aim to consider the effect of natural graphene rippling on fracture strength. It is known that the deformation energy in free-standing graphene can be easily released through the formation of out-of-plane wrinkles [31]. This is in line with [32,33], where it was shown that at positive strain values along one direction and negative strain values along the other direction, graphene loses its stability, and ripples with different orientations appear. In the present work, when graphene is stretched along one direction, it simultaneously can shrinkage along the normal direction, which results in positive stress along one axis (tension) and negative stress normal (compression). Thus, this scenario is known from the literature and in good agreement. It should be also mentioned, that type of ripples considerably affects the elastic modulus and fracture strain and strength [34,35]: if there

are small-amplitude corrugations of graphene, the fracture strength and elastic modulus are lower, but not so notably in comparison with the high-amplitude ripples.

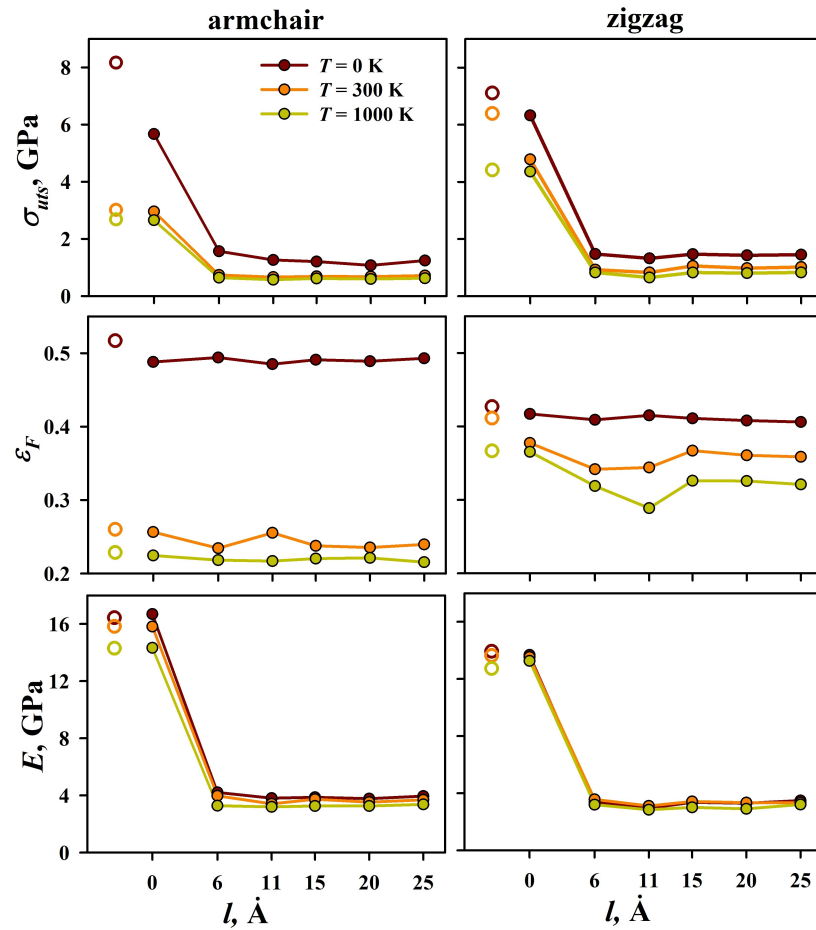


Figure 3. Variations of the ultimate strength σ_{UTS} , fracture strain ε_F and elastic modulus for defective graphene under tensile tests along the armchair/zigzag direction as the function of the dipole arm l . Open circles show these values for defect-free graphene.

Wrinkles and ripples can significantly reduce the magnitude of in-plane stresses, generated by the defects [38]. Thus, such a low $\sigma_{UTS}^a = 8.1$ GPa ($\sigma_{UTS}^z = 7.1$ GPa) and such a high $\varepsilon_F^a = 0.51$ ($\varepsilon_F^z = 0.43$) is quite understandable. Moreover, for graphene, fracture strength for tension along zigzag is higher than for tension along armchair. Here, it can be seen that $\varepsilon_F^z > \varepsilon_F^a$, which would be further described from the changes of the structural state of graphene under such tension technique. Elastic modulus can be defined from the slope of the stress-strain curves in the elastic regime. Here, in the presence of ripples, the elastic regime is considered only before the first ripples with an amplitude higher than 0.5 Å appeared.

Stress-strain curves for graphene and graphene with SW are closely matched before the fracture point. The same behavior was shown previously for a single SW defect in graphene [46,47]. The initial slope is significantly higher, indicating an increased elastic modulus of $E^a = 16.4$ GPa and $E^z = 13.9$ GPa. At the same time, the presence of any type of defect results in a considerable decrease of ε_F^a , which should be discussed in accordance with the structural transformations.

Temperature also plays a very important role in the degradation of the graphene strength with or without defects [48–50]. Thermal fluctuations drive the generation of atomic vacancies or dislocations since temperature increases the possibility of an atomic movement in the structure. For graphene, strength is considerably decreased by thermal fluctuations. Ultimate tensile strength and fracture strain of graphene under tension along armchair direction at room temperature is more than two times lower than at 0 K, while the further increase of temperature does not lead to a significant decrease of strength (see Figure 3a,b). Very similar results can be seen for graphene with SW. Elastic modulus E is almost not affected by the temperature increase, which is in line with the previous studies [51]. For tension along zigzag, the effect of temperature is not so significant. As can be seen, the increase of temperature considerably lowers the σ_{UTS}^a of graphene and graphene with SW, while almost not affecting these values for graphene with DD.

The extremely similar slopes of the stress-strain curves for all of the structures with the DD_n in Figure 2 imply that the distance between dislocations in the dipole does not noticeably affect the elastic modulus of graphene. The fitted elastic modulus is in the range of 3.76 to 4.14 GPa for tension along armchair and from 3.00 to 3.52 GPa for tension along zigzag. Hence, it can be concluded that the presence of DD does not have a significant effect on the elastic properties of graphene. Experimental and numerical observations showed the same results for grain boundaries [7,52]: elastic properties are not affected by the type of grain boundary. Despite, the value of fracture strength, the arm of dislocation dipole is not meaningful, but this issue is still important. The interesting point is that the dipole arm will affect the dislocation dynamics and, also, the wrinkling process. As a result, there is a correlation between wrinkling and fracture strain and stress.

In Figure 4 another critical issue is presented—simulation of graphene tension with another interatomic potential for comparison: stress-strain curves during tension at 0 and 300 K for graphene and graphene with DD₂ and snapshots of graphene after a fracture. Two interatomic potentials are compared—AIREBO and Tersoff. Tersoff interatomic potential is well-known for the simulation of physical and mechanical properties of graphene and other carbon structures [53]. As it is known, interatomic potential can considerably affect the simulation results [54]. As can be seen from Figure 4, before $\varepsilon = 0.25$ stress-strain curves are very close for graphene and graphene with the defects for both temperatures. Again, rippling is allowed in the model and it is the same as for structures simulated with AIREBO. Almost the same failure stress value for armchair and zigzag directions is obtained for Tersoff, which is not realistic. Tersoff also gives lower critical values of strain and stress. Fracture is brittle and it would be further compared with the snapshots of graphene simulated with AIREBO potential. However, for graphene in common, fracture occurs with the formation of carbon chains.

As it was previously shown, AIREBO potential is more suitable to describe the sp³ and sp² structures in comparison with Tersoff and Brenner [54]. The AIREBO potential correctly reproduces the overbinding effect of specific bonding configurations. Also, it was previously shown that AIREBO is successful in capturing the realistic mechanical behavior of graphene [55–57]. Tersoff is capable of accurately predicting phonon dispersion in graphene, but has been inaccurate in predicting the failure stresses when compared with experimental results [41]. Moreover, Tersoff predicted almost the same failure stress values for armchair and zigzag directions [58], which is also seen from Figure 4. Thus, it can be concluded that both potentials are not ideally describing the fracture process at high tensile strain, but AIREBO gives results much closer to the experiment and most of the numerical simulations. Further, only results obtained with AIREBO potential will be presented.

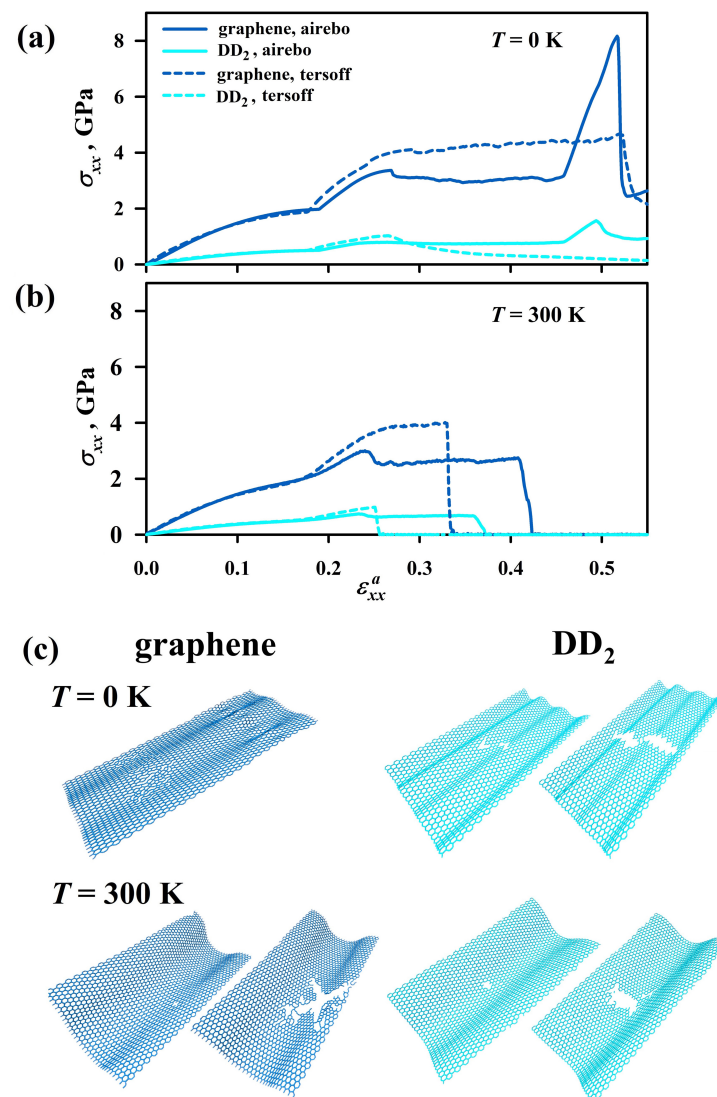


Figure 4. (a,b) Stress-strain curves for graphene and graphene with DD₂ under tension along armchair (a) and zigzag (b) direction at 0 and 300 K. (c) Snapshots of graphene after a fracture.

3.2. Analysis of the Fracture Mechanisms

The appearance of ripples during tension determines the course of the stress-strain curves at this deformation regime. In Figure 5a, the comparison between stress-strain curves (a) for tension at 0 K along armchair direction for graphene, graphene with SW and DD₂ is presented in comparison with the average amplitude of ripples (b) and bond length (c) as the function of strain. Only results for graphene with DD₂ under tension at 0 K are presented since the overall behavior of graphene with DD is the same. However, some differences will be discussed further in the text.

Average amplitude of ripples is calculated as $\bar{A} = 0.5(|A_{max}| + |A_{min}|)$, where A_{max} is the maximal amplitude and A_{min} is the minimal amplitude of the ripples. Obtained amplitudes are in good agreement with the literature [30,32]. Amplitude as the function of strain for one more defect is presented by green dots and dashed green approximation to show that graphene with any DD_n has almost the same behavior. As it was mentioned, a linear regime is a regime without ripples, when graphene is still planar. Small amplitude of the downward bubble around each dislocation as well as very small-amplitude ripples is neglected.

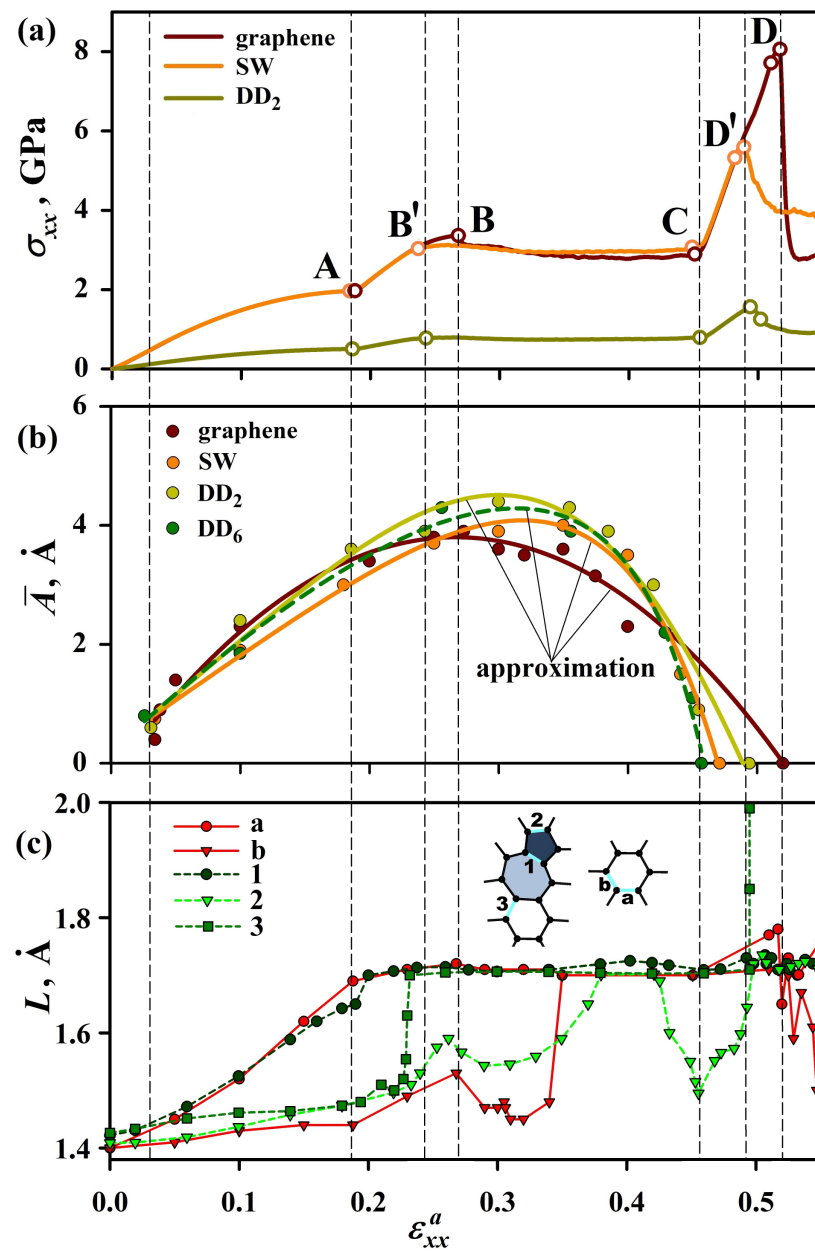


Figure 5. (a) Stress-strain curves for graphene, graphene with SW, and DD₂ under tension along armchair direction at $T = 0$ K. (b) Average amplitude $\bar{A}$ of ripples for defect-free graphene, graphene with SW, and DD₂ as the function of strain under tension along armchair direction at $T = 0$ K. Numerical data are shown by dots, while approximations are shown by solid lines. One more structure with the dipole (DD₆) is added for comparison with the approximation shown by a thick dashed line. The thin black dashed lines show different deformation regimes. (c) The bond length in graphene and graphene with DD₂ as the function of applied tensile strain.

Snapshots of the structure during tension along armchair and zigzag direction are presented for critical points on stress-strain curves in Figure 6. Let us consider tension in armchair direction first. As it can be seen, there are four different loading regimes: (i) after the elastic regime is over and before point A, (ii) between A and B (B' for graphene with SW and DD₂), (iii) from B (B') to C, and (iv) from C to D (D' for graphene with SW and DD₂). Almost the same deformation behavior at critical strains is observed for all structures. Point C can be considered as the pre-critical state.

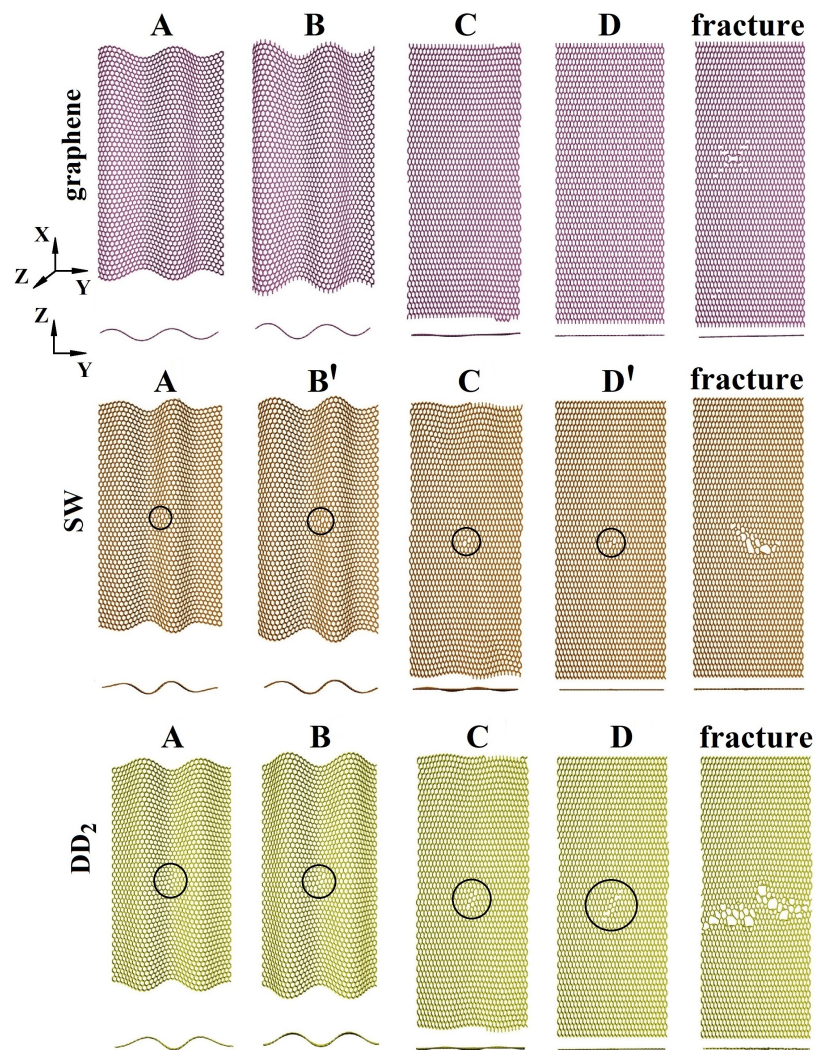


Figure 6. Snapshots of graphene, graphene with SW defect and with DD₂ under tension along armchair direction at $T = 0$ K. Snapshots are presented in a perspective view and in a projection on yz plane. The defect is shown by a black circle. Corresponding dots A–D, B', D' are from Figure 5.

Before point A, the amplitude of the ripples constantly increases for all structures. It should be mentioned that the size of the structure along x (armchair) direction is enough to obtain two ripples with the same parameters. Previously, in [32] it was shown that the amplitude and wavelength of ripples depend on the size of the graphene nanoribbon, which is also valid for graphene. The amplitude value achieves the maximum at point B for graphene and at about $\varepsilon_{xx}^a = 0.3$ —for graphene with SW and DD. In fact, the deformation is determined by two factors: changes in the lattice constant and the de-wrinkling of graphene.

Different bonds in the structure are analyzed during tension for graphene, graphene with SW, and DD. In Figure 5c, changes of the bonds in graphene and graphene with DD₂ have presented: two main bonds in graphene (a along armchair and b along zigzag) and three characteristic bonds near the dislocation—1, 2 and 3. Other different bonds in graphene are changing in a similar way to these three. To find equilibrium structures at different tensile strains and analyze the evolution of bond lengths, all structures are considered at 0 K. Small random perturbations to coordinates of all atoms with the magnitude 10^{-5} are introduced to check the structure for stability.

For graphene, before point A, bond a is continuously stretching and achieves a constant value of $1.7 \text{ \AA}$ until point C. In contrast, bond b almost not changed before point A, but increase until point B. After point B, bond a cannot be stretched more, and deformation took

place because of a further increase of the ripple amplitude and changes in the valent angles and bond b . Moreover, bond length can be decreased because of the transformation of valent angles. After point C, again bond a starts to increase and then break. From Figure 6 it is seen that graphene became a plane without any ripples and the prevailing deformation mechanism is bond stretching.

If structure with DD_n is considered, better to analyze all the bonds on the defect and also around it. However, for clearance, only three bonds are presented in Figure 5c—bond 1 between 5- and 7-atoms ring, bond 2 on the 5-atomic ring, and bond 3 near the defect DD_2 . As can be seen, bond 1 stretched before point A in the same way as bond a in graphene, while bonds 2 and 3 almost not changing. At B', the rapid increase of bond 3 took place which allow the further stretching of graphene. In fact, not only bond 3 is changing at this point. The same transformations appeared for some other orientations of the bonds in a hexagonal lattice. When the bonds are oriented along the tension direction (armchair in this case) they can provide tension along with the simultaneous ripple formation. However, when these bonds are critically strained, bonds with other orientations start to play the main role. These results are not trivial except for the case of defect-free graphene: it is expected that bond 1 in dislocation is the most strengthened, but the main changes in the lengths of the bonds took place near the defect, not right on it.

Interestingly, that defect position affects the ripple distribution. SW defect is set on the side of one of the ripples, while DD_2 is placed right between two ripples. The increase of the dipole arm results in a slight redistribution in the structure: each dislocation is placed on a different ripple, on the corresponding side. After the transition from rippled graphene to the plane, another structural transformation took place for all the considered graphenes at points C, C': almost equilibrium hexagons transform to elongated ones and this is a pre-critical transformation. In defect-free graphene, fracture starts at any place in its basal plane (an example is shown in Figure 6). For graphene with defects, ripples start to disappear right from the defect, and then the second transformation takes place. The fracture starts close to the defect and the crack extends diagonally from the 7-ring defect.

It should be mentioned that, for graphene with DD_6 , a third ripple tends to appear, but the presence of a defect prevents this. Moreover, for DD_6 – DD_{10} graphene does not transform to the totally planar before fracture. Also, the new defect appears under tension—defect 5-8-5, which is also well-known for graphene.

In Figure 7a, the comparison between stress-strain curves (a) for tension at 0 K along zigzag direction for graphene, graphene with SW and DD_2 is presented in comparison with the average amplitude of ripples (b) and bond length (c) as the function of strain. For tension along zigzag, the situation is a bit simpler: only two stages can be found—before the point I and point II (II' for graphene with SW and DD). Ripples did not disappear until the fracture and the elongation of graphene is much lower. From Figure 8 it can be seen that the length of the structure is not enough to obtain equilibrium ripples with the same parameters for graphene—there are three (at the point I) and two ripples of different amplitude. However, the presence of defects affects the ripple configuration and for graphene with SW and DD, ripples with close amplitude and wavelength appeared.

Again, a continuous increase in the ripple amplitude can be seen before the point I with a slow decrease until points II and II'. Bonds in graphene and defective graphene are also considered. For defect-free graphene, bond b , which is aligned in almost the same direction as tensile strain is weaker and rapidly increases before the point I. After that, the whole changes of the bonds and valent angles result in a continuous increase of both a and b bonds until the pre-critical stage. For graphene with DD, at the first deformation stage (even at $\epsilon^z = 0.1$), a sharp increase of the bond 3' which is also aligned in almost the same direction as tensile strain (as bond b in graphene). Since ripples did not totally disappear from the structure, no structural transformations to elongated hexagons took place. Bonds oriented along which the tensile strain is applied are the weakest bonds. Fracture starts near the defect (see Figure 8).

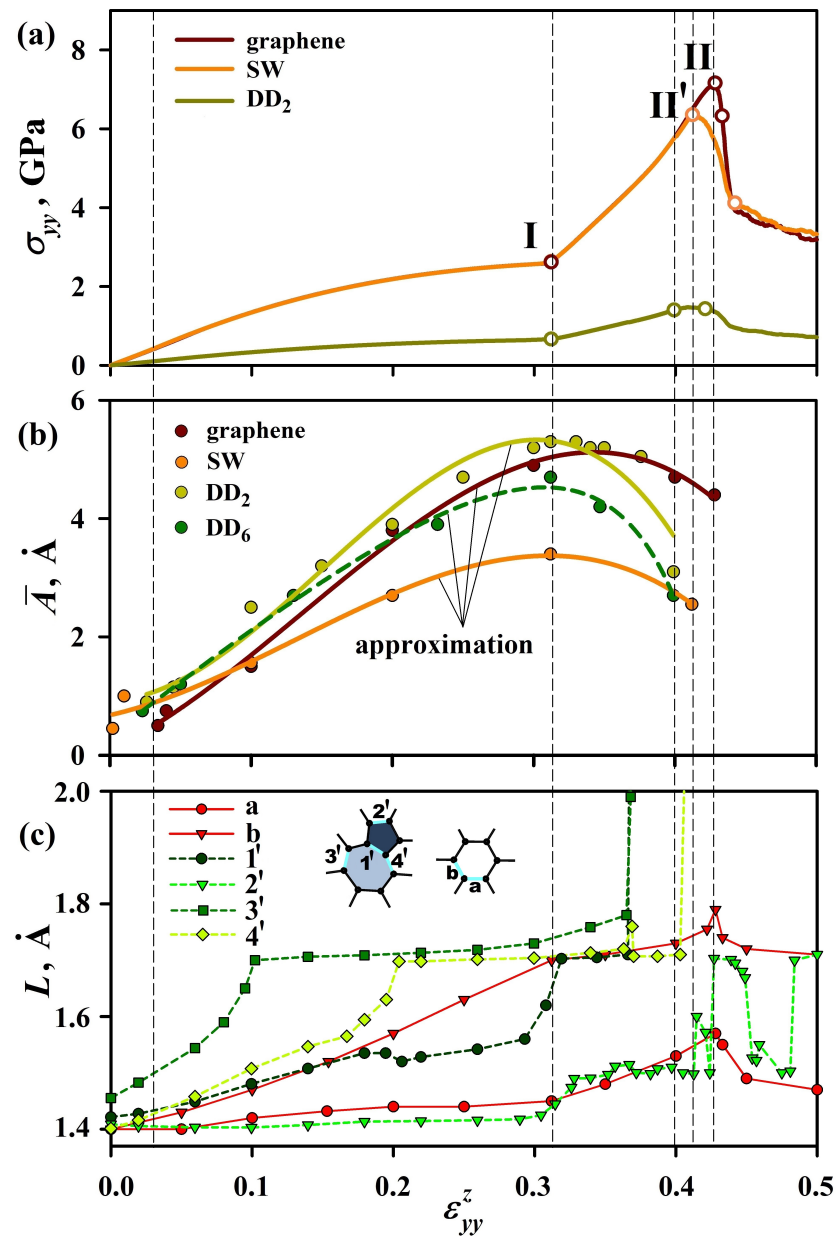


Figure 7. (a) Stress-strain curves for graphene, graphene with SW, and DD₂ under tension along zigzag direction at $T = 0$ K. (b) Average amplitude $\bar{A}$ of ripples for defect-free graphene, graphene with SW, and DD₂ as the function of strain under tension along zigzag direction at $T = 0$ K. Numerical data are shown by dots, while approximations are shown by solid lines. One more structure with the dipole (DD₆) is added for comparison with the approximation shown by a thick dashed line. The thin black dashed lines show different deformation regimes. (c) The bond length in graphene and graphene with DD₂ as the function of applied tensile strain.

The process of fracture of defect-free graphene and graphene with SW and DD is also analyzed at elevated temperatures. In common, the same situation took place: ripple formation under tension and transformation to the planar state at pre-critical strain, when the bonds are considerably stretched.

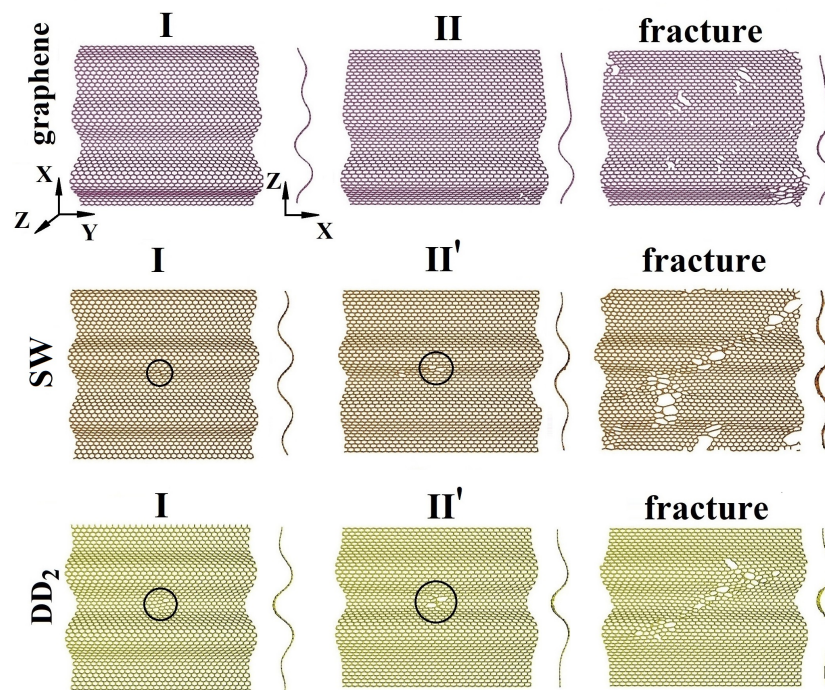


Figure 8. The same as in Figure 6, but for tension along zigzag direction. Corresponding dots I, II, II' are presented in Figure 7.

4. Conclusions

In conclusion, atomistic simulation is used to study the effect of dislocation dipole on the failure strength of graphene with ripples. Mechanical properties are obtained for graphene under tensile loading at 0 K, 300 K, and 1000 K. Fracture mechanisms are analyzed at zero temperature to exclude the effect of thermal fluctuations.

In the presence of ripples, the fracture process is quite complicated and involves graphene wrinkling with reverse transformation to the planar shape, continuous and very different changes in bond lengths, and the appearance of new defects. All these mechanisms are not contradictory, but act simultaneously, which results in quite a high fracture strain. However, the ultimate tensile strength and Young's modulus of rippled graphene are very low, since wrinkling makes graphene much weaker.

Temperature, graphene wrinkling, and the presence of defects are the main factors affecting the mechanical properties of graphene. The presence of dislocation dipole with the dipole arm greater than 15 Å can affect the special distribution of ripples, for example, prevent ripple formation. However, the increase in the length of the dipole arm does not lead to a considerable decrease in the ultimate tensile strength of graphene. SW defects do not lower strength to such a crucial extent, especially at room and finite temperatures. For graphene with dislocation dipole, temperature increase also does not result in a considerable decrease in the graphene strength.

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Abbreviations

The following abbreviations are used in this manuscript:

SW defect	Stone-Wales defect
2D	two-dimensional
MD	Molecular Dynamic
DD	dislocation dipole

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