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Molecular dynamics simulation on double-elastic deformation of zigzag graphene nanoribbons at low temperature

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ABSTRACT

Molecular dynamics simulation was performed to study the deformation behaviors of Zigzag Graphene Nano-Ribbons (ZGNRs) 150 Å × 150 Å in size, and double-elastic deformation was observed at temperatures lower than 90 K. Essentially, at such a low temperature, the lattice vibration was significantly weakened and thus the lifetime of C—C bonds was prolonged considerably. Moreover, it was difficult for broken bonds to accumulate and resulted in the destructive fracture of ZGNRs at low temperature. As a result, the "phase transformation" from hexagonal to quasi-rectangular and subsequently the second elastic deformation took place. However, at higher temperatures, says, 300 K, brittle fracture was observed and the fracture strength decreased with temperature, which was consistent with previously reported results. Additionally at higher strain rate, the atoms could not respond to the external loading in time, the fracture strain and fracture strength were enhanced.

1. Introduction

Because of the extremely high electron mobility (10^5 cm^2/Vs) [1] and excellent thermal conductivity (3–5 kW/mK) [2–5], graphene has potential applications in field effect transistors [1,6], Li-ion battery [7], supercapacitor [8], nano-electromechanical systems [9], and so on. Although graphene has the highest mechanical strength [10], the single-atom-layer nature makes it difficult to bear a considerably large external force. So the mechanical stability is a crucial issue for the practical applications of graphene. Previous investigations suggested that Stones–Wale (SW) defects, similar to the dislocations in three-dimensional bulk metals [11–13], dominate the plastic deformation of graphene. In a previous paper [14], we found that SW defects can be annihilated through the reverse rotation of C—C bonds under an appropriate stress. Hence, the mechanical strength of graphene with SW defects almost equals to that of ideal graphene. It resembles to the mechanical annealing observed in bulk metals [15]. Monte Carlo simulations on carbon nanotubes demonstrated that two SW defect arrays glided away from each other in a cooperative manner. The plastic elongation was significantly enhanced [16]. Grantab et al. [17] found that it was easier for the rotation of C—C bonds in large-angle tilt boundaries of graphene, and thus the graphene sheets with large-angle tilt boundaries were stronger than those with low-angle tilt boundaries. This is impossible in bulk metals. So the deformation mechanism should be special for this two-dimensional material, in spite of the similarity between SW defects and dislocations.

In essence, the deformation of graphene is dominated by the competition between bond fracture and bond rotation [18]. They are completely atomic behaviors, and hence should be extremely sensitive to the temperature and strain rate. For instances, Zhao et al. demonstrated through molecular dynamics (MD) simulation that the fracture strength of armchair graphene nanoribbons decreased significantly from 95 GPa to 40 GPa when the temperature was increased from 300 K to 2400 K, both fracture strength and fracture strain decreased slightly with stain rate at room temperature [19]. Min et al. investigated the mechanical properties of graphene under shearing and found that shear strength decreased from 60 GPa to 20 GPa as the temperature was increased from 100 K to 2000 K [20]. Similar to carbon nanotubes, the tensile yield strain linearly depends on the temperature but logarithmically depends on the strain rate, which is consistent with transition state theory [21]. However, most of the studies focused on the temperature range above room temperature. When the temperature is lowered even down to 10 K, most of the lattice vibration modes should be suppressed, and only a few acoustic vibration modes with extremely small amplitude are activated. This has been demonstrated by significantly reduced thermal conductivity as well as quantized thermal conductance [22,23]. In such a case, the lifetime of C—C bonds will be elongated and the fracture of C—C bonds becomes difficult. In the work of this paper, MD simulation is performed on the tensile loading process of graphene nanoribbons

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along the zigzag orientation to disclose the deformation mechanism at low temperature.

2. Simulation model

The simulation model of ZGNRs 150 Å × 150 Å in size is built up with 8540 atoms. In the MD simulation implemented in package LAMMPS [24], the interaction between carbon atoms are described by the adaptive intermolecular reactive bond order potential which could accurately capture the interactions between carbon atoms as well as bond breaking and re-forming [25,26]. The cutoff parameter describing the short-ranged C—C interactions is chosen to be 2.0 Å in order to avoid spuriously high bond forces and non-physical results at large deformation [27,28]. Before dynamics simulation, the graphene sheets with periodic boundary conditions in two in-plane directions are relaxed to an equilibrium state in the isothermal-isobaric ensembles at fixed temperature for 600,000 MD steps with a timestep of 1 fs. Then ZGNRs are created by deleting atoms outside part of the nanoribbons and a vacuum region 15 Å in width is added so that the atoms near one edge do not interact with those near the opposite edge.

MD simulation of uniaxial tensile loading is performed in the canonical ensemble using deformation-control method. Fig. 1(a) schematically shows the loading configuration. The loading stress is along the zigzag direction but perpendicular to the armchair one. For each atom, taking the yellow colored atom in Fig. 1(a) as an example, three chemical bonds are involved, but they can be classified into two kinds: the one perpendicular to the loading direction and denoted as "armchair" (colored red), the other having an angle of 30° with respect to the loading direction and denoted as "zigzag" (colored green), and the including bond angle is denoted as θ. It is not difficult to image that, as for the loading mode shown in Fig. 1(a), the armchair bonds could not be elongated considerably like the zigzag ones because of the extremely small stress resolved along the bond direction. Hence, the breakage should mainly occur on the zigzag bonds rather than the armchair ones, which will affect the deformation mechanism. The temperature in the range of 5–300 K is applied using the Nose–Hoover thermostat and the fracture stress and fracture strain are calculated according to Ref. [25]. The strain rate is 10^{-4} ps^{-1}. The layer separation of graphite, 3.4 Å, is taken as the effective thickness of the graphene monolayer and Poisson's ratio is chosen to be 0.165 [29,30].

3. Results and discussion

Fig. 1(b) presents the stress–strain curves of ZGNRs under tensile loading at the temperature ranging from 5 K to 300 K. The deformation behaviors depend on the temperature remarkably. At temperatures higher than 100 K, the tensile deformation process is as usually predicted. The stress increases linearly with the strain till 8% owing to the elastic response of the bonds, the stage is indicated by I. Then non-linear elasticity begins and continues up to a critical strain, which can be ascribed to the combined effect of bond elongation and bond angle variation. The stage is indicated by II. Finally, brittle fracture takes place as a result of bond rupture. Fig. 1(c) shows the fracture stress as a function of temperature. Apparently, the fracture strength increases with decreasing temperature and the value of about 120 GPa at room temperature is close to the reported theoretical result of 130 ± 10 GPa [27,31], indicated by the dashed red line in Fig. 1(b). However, at lower temperatures, another linear stress–strain region indicated by III appears after the critical strain of 35% and before the brittle fracture, similar to strain hardening in polycrystalline metals [32]. It is regarded as "The Second Linearly Elastic Deformation (SLED)". This improves the fracture strength and the fracture strain by about 50% and 36%, respectively, as displayed in Fig. 1(c).

The evolution of atomic configurations can be observed in Fig. 2. Fig. 2(a) presents the case at 5 K. The first and second deformation

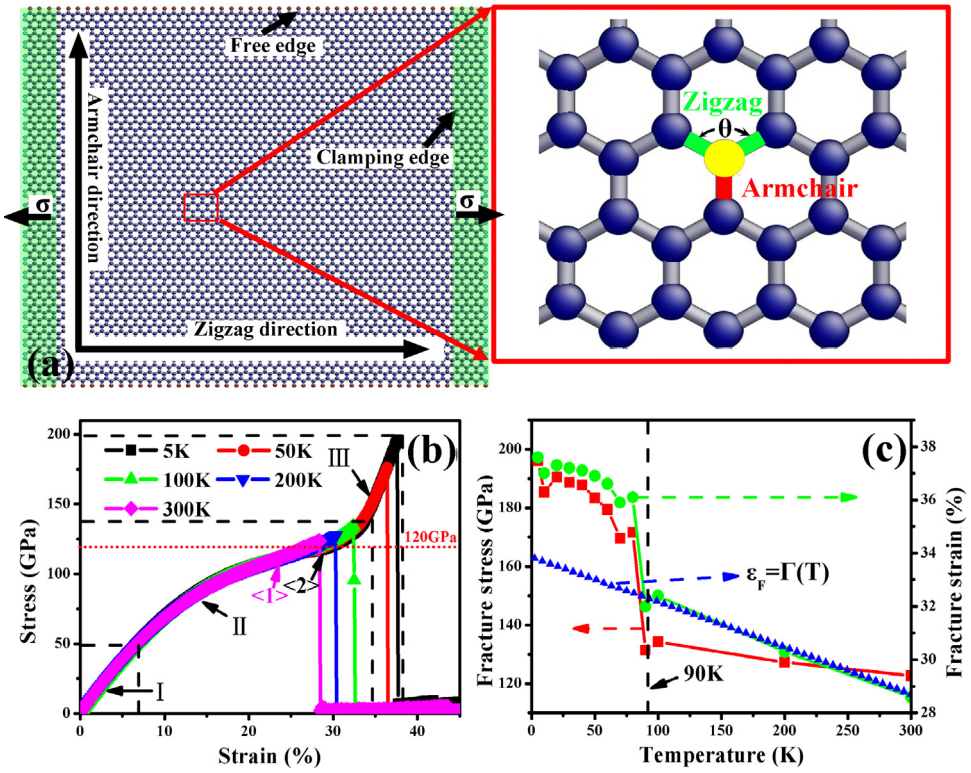

Fig. 1. (a) The simulation model of ZGNRs under tensile loading, (b) the stress–strain curves and (c) the fracture stress and fracture strain as a function of temperatures with a strain rate of 10^{-4} ps^{-1}. (For interpretation of the references to color in the text, the reader is referred to the web version of this article.)