



Self healing nature of bilayer graphene

Sanghamitra Debroy^a, V. Pavan Kumar Miriyala^a, K. Vijaya Sekhar^b,
Swati Ghosh Acharyya^{b,*}, Amit Acharyya^a

^a Department of Electrical Engineering, Indian Institute of Technology, Hyderabad, India

^b School of Engineering Sciences and Technology, University of Hyderabad, India

ARTICLE INFO

Article history:

Received 20 February 2016

Received in revised form 4 May 2016

Accepted 7 May 2016

Available online 8 May 2016

Keywords:

Bi-layer graphene sheet

Molecular dynamics simulation

Crack propagation

Self heal

ABSTRACT

The phenomenon of self healing of cracks in bilayer graphene sheet has been studied using molecular dynamics simulations. The bilayer graphene sheet was subjected to uniaxial tensile load resulting in initiation and propagation of cracks on exceeding the ultimate tensile strength. Subsequently, all forces acting on the sheet were removed and sheet was relaxed. The cracks formed in the graphene sheet healed without any external aid within 0.4 ps. The phenomenon of self healing of the cracks in graphene sheet was found to be independent of the length of the crack, but occurred for critical crack opening distance less than 5 Å for AA stacked sheet and 13 Å for AB stacked bilayer graphene sheet. Self healing was observed for both AB (mixed stacking of armchair and zigzag graphene sheet) and AA (both sheets of similar orientation i.e. either armchair-armchair or zigzag-zigzag) stacking of bilayer graphene sheet.

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1. Introduction

Ever since its discovery in 2004 [1], graphene has fascinated widespread research due to its unusual mechanical, thermal, chemical, electrical properties and relatively low chemical production cost [2–7] leading to potential applications in research and industry [8–15]. Recent investigations about graphene focuses greatly on single layer structure [16–25]. A transistor designed by means of a monolayer graphene follows the proportional size-to-interference problem, but if another sheet of graphene is stacked upon it, i.e. bilayer structure, then it has been shown to significantly stabilise the effect of the noise [26]. Moreover bilayer graphene displays unusual optical [27], electronic properties [28], high thermal conductivity at room temperature of about $2800 \text{ W m}^{-1} \text{ K}^{-1}$ [29,30], transparency with transmittance of white light of about 95% [31], impermeability to gases [32] and high mechanical stiffness, strength and flexibility (Young's modulus is estimated to be about 0.8 TPa) [33–35]. Bilayer graphene has immense potential for future applications in many research areas [36] including transparent, flexible electrodes for touch screen displays [37], high-frequency transistors [38], thermo electric devices [39], photonic devices including plasmonic devices [40], photo detectors [41] and energy applications including batteries [42,43]. Furthermore, bilayer graphene also holds potential for electronic application like in graphene based field effect transistors [44,45]. It is also possible to control both carrier density and energy band gap through doping or gating in bilayer graphene [36,46,47]. The mobility at room temperature is up to $40,000 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ in air for bilayer graphene [48] which may get affected by various types of scatterers, i.e., charge impurities and crystalline defects. Zhao et al. [49] has shown that as the

* Corresponding author.

E-mail address: sgase@uohyd.ernet.in (S.G. Acharyya).

crack length increases the fracture strength of graphene falls off drastically even by 56% for crack length of 10 Å resulting in significant impact in mechanical properties. Therefore, understanding the mechanical behavior of bilayer graphene and its inherent nature of self healing of cracks holds immense potential for its successful widespread application. Very limited information on the mechanical behavior of bilayer graphene is available at present [49,50]. The authors previously reported the self-healing phenomenon for single-layer graphene using molecular dynamics simulation [51]. The present study reports the phenomena of self-healing of cracks in bilayer graphene without the presence of any external stimulus at room temperature. The effect of chirality on (a) the mechanical properties of graphene and (b) the self healing behavior has also been reported in this paper.

2. Simulation method and modelling

The atomistic simulations in the present study were performed using LAMMPS [52] (Large-scale Atomic/Molecular Massively parallel simulator). REBO potential (Second generation reactive bond order potential) has been used to define force field of C–C atoms interaction in our simulation model which originated from Tersoff-Berner potential, that defines bond-bond interactions, bond breaking, bond reforming, inter molecular interactions between non-bonded atoms, as well as torsional angles formed by the sequence of three bonds [53,54]. The pristine bilayer graphene sheet contains 2016 carbon atoms with length of 50 Å and width of 50 Å. Periodic Boundary Condition (PBC) has been applied in two in-plane directions and a vacuum space of 100 nm is considered along z-direction to avoid edge effects and for considering it to have infinite length and width. The interlayer distance between the pristine bilayer graphene sheets has been assumed to be approximately 3.4 Å. According to the different chirality of each layer, three conditions of bilayer graphene have been considered which are as follows: armchair-armchair, zigzag-zigzag and armchair-zigzag.

The simulations have been carried out at constant room temperature $T = 300$ K, in the canonical ensemble (NVT), amount of substance (N), volume (V) and temperature (T). Nose-Hoover thermostat with Velocity-Verlet integration algorithm has also been implemented to solve the kinetic equation with a time step of 0.0005 ps and held at equilibrium for 30 ps to keep the system temperature at 300 K in all runs. Applying this thermostat method produces lesser instabilities in the system throughout the temperature stabilization process. Periodic Boundary Conditions are imposed on the system and allowed to relax for a period of 30 ps. The cracks initiated and propagated in the pristine sheets on applying uniaxial loading with constant strain rate of 0.001/ps exceeding the ultimate tensile strength.

In all the simulations reported here, the bonding atomic interaction in graphene is described by the reactive empirical bond order (REBO) potential [55]. REBO potential has been extensively accepted to study the mechanical properties of carbon-based nanomaterials such as CNTs, and graphene [53,56–60]. In order to limit the many body bond-order potential to nearest neighbour interactions, a cut-off function is used. In fracture studies, cut-off function plays a crucial role, inducing high bond order forces resulting in deviation from physical behavior. In the present study, the cut-off function has been fixed at 2 Å, eliminating non-physical ductile behavior in stretching process and to get accurate fracture behavior propagation distance of the crack. Several rows of atoms near the four edges are defined as boundaries. In order to study self-healing, all the forces acting on the deformed graphene sheet were removed once crack nucleation started. Once the cracks were self-healed the sheet was allowed to relax for a period of 150 ps. The interlayer cohesion is maintained by Van der Waals force and is characterized by the 12-6 Lennard-Jones potential [56].

$$V(r) = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right] \quad (1)$$

here r is the distance between a pair of atoms, ϵ is the depth of the potential well = 2.968 meV and σ is the finite distance at which the inter-particle potential is zero which in this case is 0.3407 nm.

3. Results

The convention used in the present study for loading graphene sheet is shown in Fig. 1. The bilayer graphene sheet was initially allowed to stabilise at 300 K for 30 ps. Tensile loading was thereafter applied to the sheet. The cracks were formed in the bilayer sheet by uniaxially loading the sheet in tension above its ultimate tensile strength. The bilayer sheet was then relaxed by removing all the forces acting on it at room temperature. The boundary atoms at edges parallel to the loading direction were kept unconstrained during deformation. Two different bilayer graphene models have been considered for self-healing studies i.e. (i) AB (armchair-zigzag) stacked pristine sheet and (ii) AA (armchair-armchair) stacked pristine sheet. The computational model used for the present study has been validated by comparing the fracture stress and strain with that of literature [34,61]. The stress and strain at fracture for AA stacked armchair and zigzag pristine bilayer sheets is 89 GPa at 0.14 and 100 GPa at 0.2 strain respectively, which is exactly at par with previously reported values [34,61] for bilayer graphene. The stress strain diagram of the AA and AB stacked bilayer graphene sheet is shown in Fig. 2. In the case of AB stacked bilayer graphene sheet the initial drop in strength occurred at a strain level of 0.14 where the stress level decreased from 87 GPa to an intermediate value of 40 GPa which is consistent with literature [61]. The visual images as shown in Fig. 3, indicated that at the strain of 0.14, the armchair constituent of the sheet failed. The zigzag constituent was still intact and continued to carry the external load on the sheet upto a stress value of 54 GPa following which the entire sheet had failed. The failure of armchair

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