Computational Materials Science xxx (2013) xxx–xxx

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

The size effect in mechanical properties of finite-sized graphene nanoribbon

Yanbiao Chu [a], Tarek Ragab [a,b], Cemal Basaran [a,*]

[a] Electronic Packaging Laboratory, University at Buffalo, SUNY, NY 14260, USA
[b] Nanotechnology Research Laboratory, University of Tabuk, Saudi Arabia

ARTICLE INFO

Article history:
Received 19 June 2013
Accepted 11 August 2013
Available online xxxx

Keywords:
Graphene nanoribbon
Mechanical properties
Size effects

ABSTRACT

Size effect in mechanical behavior of finite-sized graphene nanoribbons (GNRs) under uniaxial tension is studied using Molecular Dynamics (MD) simulations. The size effect and aspect ratio effect are significant in zigzag GNRs (ZGNRs), while their influence on the mechanical behavior of armchair GNRs (AGNRs) is negligible. For square shaped ZGNRs of increasing size, the elastic modulus increases while the ultimate failure stress and strain decrease. For rectangular shaped ZGNRs, the aspect ratio effects are especially predominant in those with fixed length. Wider ZGNRs have higher elastic modulus but lower failure stress and strain. For GNRs of fixed width, neither ZGNRs nor AGNRs show significant aspect ratio effect when length increases. The results show that ZGNRs are generally stronger than AGNRs under the same loading conditions. A new concept Density of Weakness (DOW) has been proposed to explain the size effect of ZGNRs.

1. Introduction

Graphene, a single layer of carbon atoms arranged in honeycomb lattice, has promising applications in nanoelectronics [1], nano-electromechanical systems [2], and nanocomposites [3]. Especially, graphene nanoribbon (GNR), tailored from the 2D graphene lattice with finite size, has been found to possess interesting electronic structures based on its width and edge shape [4]. These material properties open an opportunity to construct electronic devices made completely of graphene [5].

The ultimate use of graphene will likely require an understanding of the mechanical properties that affect the device performance and reliability. The mechanical properties of bulk graphene have been extensively studied both experimentally [6,7] and theoretically [8,9]. For GNRs, although precise fabrication methods have been developed recently [10,11], there are still very few experimental results available in the literature. Thus, valuable exploratory studies in this field are currently done by theoretical and computational methods based on molecular dynamics (MD) [9,12–14], structural or continuum mechanics [15,16], and quantum mechanics [17,18] methods.

Most computational studies concentrate on the uniaxial tensile behavior of GNRs. The edges of GNRs can be zigzag (ZGNR), armchair (AGNR), or at other chiral angles. The following literature review focuses on pristine GNRs without any functionalization. Zhao et al. [9] studied square AGNRs and ZGNRs by MD with AIREBO potential, which is the most commonly used and accurate potential for C-C bond in graphene. They reported increasing Young's modulus and decreasing Poisson's ratio as the diagonal length of GNRs becomes larger. When the diagonal length of nanoribbon is over 10 nm, both parameters converged slowly to those of bulk graphene. However, results about failure stress and failure strain are not presented. Based on Tersoff potential, Bu et al. [12] report studies only for fix-length AGNRs. The results also show the increasing Young's modulus for wider AGNRs, and the size effect is appreciable only when width is smaller than 2 nm. Lu et al. [13] studied infinitely long AGNRs and ZGNRs by molecular statics (i.e. no temperature presents). They use the second-generation reactive empirical bond-order (REBO) potential, which is an earlier version of AIREBO potential. As shown in their paper, both types of GNRs have a decreasing Young's modulus and decreasing failure strain as width increases, while the failure stress increases at the same time. Xu [14] studied nanoribbon of the size 20 nm by 10 nm with second generation REBO potential as well, with chiral angles of 0, 15, 30. A brittle failure mechanism is observed at room temperature. Using structural mechanics based on modified Morse potential, Georgantiznos et al. [16] studied both AGNRs and ZGNRs of various sizes. For fixed width, longer GNRs of both types have smaller Young's modulus, and slightly smaller failure stress and failure strain. While for both type GNRs with fixed length, narrower ones have higher failure stress and higher failure strain. However, the Young's modulus of ZGNRs increase while decrease for AGNRs as the width of nanoribbon decreases. By using

* Corresponding author. Tel.: +1 716 645 3667.
E-mail address: cjb@buffalo.edu (C. Basaran).

0927-0256/$ - see front matter © 2013 Elsevier B.V. All rights reserved.
http://dx.doi.org/10.1016/j.commatsci.2013.08.016

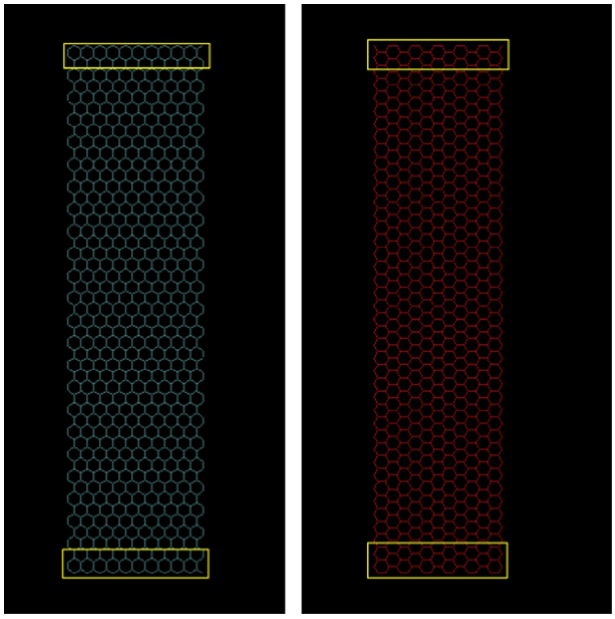

Fig. 1. Typical AGNR and ZGNR. Deformation is applied in axial direction.

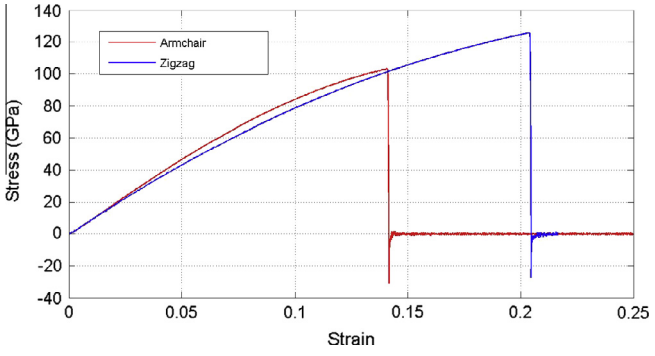

Fig. 2. Uniaxial tensile behavior of graphene.

quantum mechanics and quantum molecular dynamics, Gao et al. [17] reported that ZGNRs have higher failure stress than AGNRs, but the failure strain is lower. Based on first principle density functional theory, Faccio et al. [18] reported that the elastic modulus of ZGNRs is considerably higher than bulk graphene. They also reported that fewer atoms would harden the material, or small size would be stronger.

Each of the above publication discusses some aspect of GNR's mechanical properties and gives us some insight in that direction. However, as shown above, we cannot combine them to get a consistent picture. The reason could be the usage of different potentials, different simulation methods, different loading conditions, etc.

To get a more comprehensive picture of this topic, this paper presents a systematic study of GNRs under uniaxial tension at room temperature. Besides the chirality as AGNR and ZGNR, we also focus on the size and aspect ratio effects on elastic modulus, failure stress and failure strain. In this study, molecular dynamic simulations were performed by LAMMPs [19] with AIREBO [20] potential to run extensive parametric studies in order to resolve this inconsistency. In the second section, we discuss simulation models and methods in detail. In the third section we present the parametric studies for ZGNRs and AGNRs of various sizes and aspect ratios.

2. Simulation models and methods

The size of GNR is defined by the length L (in loading direction) and the width W. The initial C–C bond length (a_{C-C}) to start the computation is set as 1.4 Angstrom. The typical configurations of AGNR and ZGNR are shown in Fig. 1.

In all simulations, a 2.5 Å wide strip at each end (the region within the yellow box shown in Fig. 1) is constrained as a boundary condition. Before loading, the system is relaxed to reach a thermodynamic equilibrium state. Then the system is deformed by displacing fixed boundary regions at each end by a strain rate of 0.001/ps. With a time step of 0.1 fs, the system is subjected to the strain increment of 0.01% and then relaxed for 1000 steps. This procedure is repeated until complete failure of GNRs. All the molecular dynamics simulations are carried out at 300 K with NVT ensemble by LAMMPs [19].

The Adaptive Intermolecular Reactive Empirical Bond Order (AIREBO) [20] potential was used for molecular interaction, as it allows for covalent bond breaking and reforming. The potential consists of three terms,

$$E = \frac{1}{2}\sum_{i}\sum_{j\neq i}[E_{ij}^{REBO} + E_{ij}^{LJ} + \sum_{k\neq i,jl\neq i,j,k}\sum E_{ijkl}^{TORSION}] \quad (1)$$

E_{ij}^{REBO} stands for the hydrocarbon REBO potential; E_{ij}^{LJ} includes long range interactions similar to standard Leonard–Jones potential; $E_{ijkl}^{TORSION}$ is an explicit 4-body potential that describes various dihedral angle preferences in hydrocarbon configurations. All three terms are included in our calculations.

For the REBO part of potential, a switching (cut off) function is defined to limit the interaction among the nearest neighbors,

$$f_c(r) = \begin{cases} 1 & r < D_{\min} \\ \frac{1}{2}\left[1 + \cos\left(\frac{r - D_{\min}}{D_{\max} - D_{\min}}\pi\right)\right] & D_{\min} < r < D_{\max} \\ 0 & D_{\max} < r \end{cases} \quad (2)$$

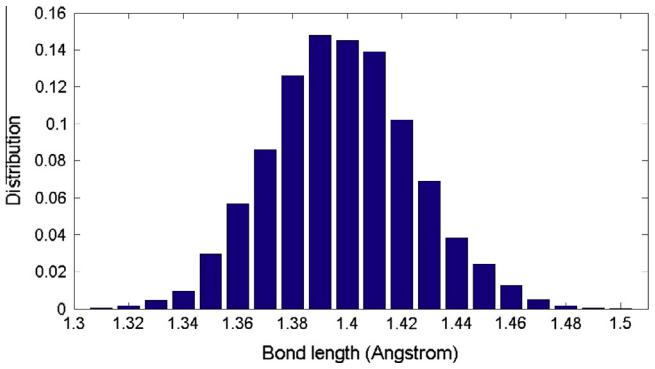

Fig. 3. Distribution of bond length in equilibrium.

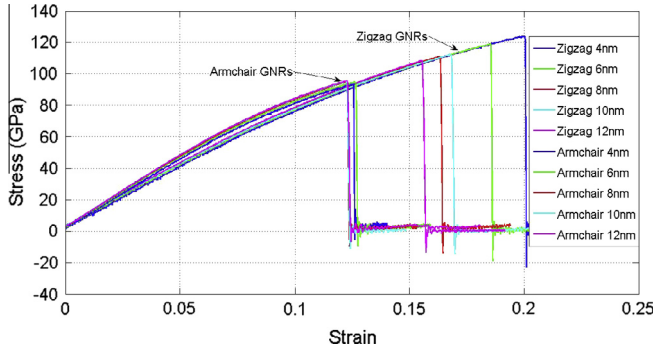

Fig. 4. Uniaxial behavior of square shaped AGNRs and ZGNRs with different size.