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Mechanical and electronic properties of graphene nanomesh heterojunctions

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ABSTRACT

It is well known that introducing periodic holes into graphene can be used to obtain semiconducting graphene nanomeshes (GNM). Using Molecular Dynamics (MD) simulations as well as semi-empirical Extended Hückel (EH) method, the mechanical and electronic properties of GNM heterojunction are studied. In this study the mechanical and electronic properties of graphene nanoribbons with different hole sizes and different hole shapes (circular, square and equilateral triangle) were studied. Midgap states were observed near the Fermi level, which are also affected by the geometries of the holes. Dependence of the properties on the density (ρ) was also investigated for each geometry. It has been found that GNM is significantly brittle compared to pristine graphene nanoribbons. It is observed that the relationship between the hole shape and size and the band gap is different for armchair and zigzag chirality.

1. Introduction

Graphene is single layer of carbon atoms that arranged in a hexagonal honeycomb lattice. It is a material that has a great potential to revolutionize electronics due to its excellent mechanical properties with high failure strength that is in the order of 100 GPa [1,2] and high flexibility [3,4]. Also it has extraordinary thermal properties (about $(4.84 \pm 0.44) \times 10^3$ to $(5.30 \pm 0.48) \times 10^3$ W/mK) [5–7] and extremely high electron mobility (about 200,000 cm^2/Vs) [8]. Recent development of highly flexible electronics [9] and the ever growing requirement on the current density capacity of materials make graphene a good candidate to replace traditional metallic and semiconductor materials, especially in power electronic devices where very high electrical current is essential [10].

A graphene sheet intrinsically has no energy bandgap [11] thus introducing a band gap into this material is essential in semiconductor applications [12–15]. The methods of introducing an energy band gap include cutting graphene sheets into graphene nanoribbons (GNR) [16–19], application of either a tensile or shear strain on the lattice [17,20–25], processing graphene sheet into graphene nanomesh (GNM) by introducing periodic nano holes [26–33], hydrogenating graphene with a certain pattern [34,35], and growth of graphene on various substrates [3,4]. Using the above method realized the application of graphene as semiconductor, but they may alter the properties and behavior of graphene [36–40]. The purpose of this study is to verify the viability of the graphene nanomesh in high current density power electronics applications, thus it is important to understand the effect the nano hole patterns on its energy dispersion relations.

Graphene heterojunctions, where metallic and semiconducting regions are connected [41–44], is an essential component for nanoelectronics. The metallic regions can be obtained by fabricating GNR with specific widths such that there is no energy bandgap [19] or using an graphene sheet. The semiconducting regions can be obtained by introducing nano holes [27]. It has been proven that the band gap can be tuned by the hole dimensions and the geometry of the hole [26,29,45]. However, introducing these periodic holes may largely degrade the material strength and ductility. Under high electrical current density, there will be electron migration forces acting on the lattice which is generated by the electron scattering with phonons, impurity and edges [46,47]. Under high electrical current density, current crowding around these nano holes will lead to an increased electron wind forces [48] leading to disintegration of the graphene nanoribbons [49]. In order to better understand the influence of periodic nano holes on the current capacity of graphene, it is necessary to study the fracture strength of GNM under uniaxial tensile loading [12,49–54].

Previous studies [55,56] on mechanical behavior of GNM only focused on the response or mechanical properties of one unit lattice where the interaction of the metallic and semiconducting regions in the heterojunctions are ignored. Hu, Wyant [55] studied the mechanical behavior and fracture of graphene nanomesh with circular pores, in which the simulation was performed to hexagonal lattice. Comparison has been made between the results of Hu, Wyant [55] and this study and they are discusses further in the next section.

Although some study has been done, the simulation directly

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performed to the graphene heterojunctions is still necessary. In graphene heterojunctions, the metallic regions and semiconducting regions act together thus only studying the mechanical behavior of a unit lattice is not sufficient when assessing the viability of GNM heterojunctions. In this study, the mechanical properties of GNM heterojunctions with circular, square, and equilateral triangular holes under uniaxial tension are studied using Molecular Dynamics (MD) simulations because of the good performance and low computational cost [1,2,12,49,54,57–64].

Moreover, for every hole geometry studied mechanically, the energy dispersion relation is studied to quantify the effect of the hole geometry and hole size on the induced band gap. In the literature previous studies focuse on the band structure of GNM. For example, Ouyang et al. [65] have studied the electronic structure and chemical modification of GNM using spin-polarized density functional theory (DFT). They found that the energy band gap of GNM is sensitive to the hole shape and size, in which GNM with hexagonal holes is typical semiconductor and GNM with triangular holes present semiconducting behavior with some localized states. Pedersen et al. [66] have studied the electronic properties of GNM using finite-element method, Tight Binding (TB) scheme as well as DFT. They show that using all three methods, band gap of a few hundred meVs is opened in GNM and the presence of carbon vacancies along the hole edges induce midgap bands. Yu et al. [67] studied the influence of edge imperfections on the transport behavior of GNM using DFT. They observed that edge imperfection of the GNM nano holes would induce localized edge state which contributes to the metallic conducting behavior of the GNM; by decorating the hole edge with Oxygen-containing group, the Fermi level will shift to the valence band and make the GNM p-doped. Chandratre and Sharma [32] showed that by introducing holes of the right geometry graphene can be tuned into piezoelectric material.

Previous studies have shed light on the development of GNM based nano-devices. It is worth mentioning that all these researchers used hexagonal or rhombus shape supercell for GNM energy band gap calculations, which the same reciprocal lattice as graphene was used and give rise to A-B-A stacking of the nano holes. In this study, however, rectangle supercell was used, which lead to A-A-A stacking of the nano hole and an orthorhombic Brillouin zone. In addition, both armchair and zigzag supercell were also considered.

2. Molecular dynamics simulations

Graphene Nanoribbons (GNRs) can be metallic and semiconducting depending on the chirality and the width of the GNR. For instance, armchair GNR can be both metallic and semiconducting depending on the number of atoms along the width of the GNR, while zigzag GNR is always metallic [3]. In this paper, both armchair and zigzag GNR were studied. The semiconducting region in the middle was produced through the introduction of the holes (see Fig. 1).

Three unit cells at each end of the nanomesh which is enclosed by the blue[1] rectangles were used to apply a prescribed uniaxial tensile displacement as shown in Fig. 2. The prescribed displacement is applied at constant a speed of 0.25 Å/picosecond until complete fracture of the GNM. The width of the simulated graphene heterojunctions is 10.0 nm and the overall length is 25.0 nm. The metallic region is 4.5 nm long on each side and the semiconducting region is 16.0 nm. Periodic boundary conditions along the width direction were applied for the unit cell in the energy bandgap calculations. In the MD simulations periodic boundary condition along the width direction was also applied. As shown in Fig. 3, the result shows that using periodic boundary condition along the width direction of the GNM has very little effect on the stress-strain diagram compared to the simulations using shrink-wrapped boundary conditions. The dimensions of the circular, square and triangular holes

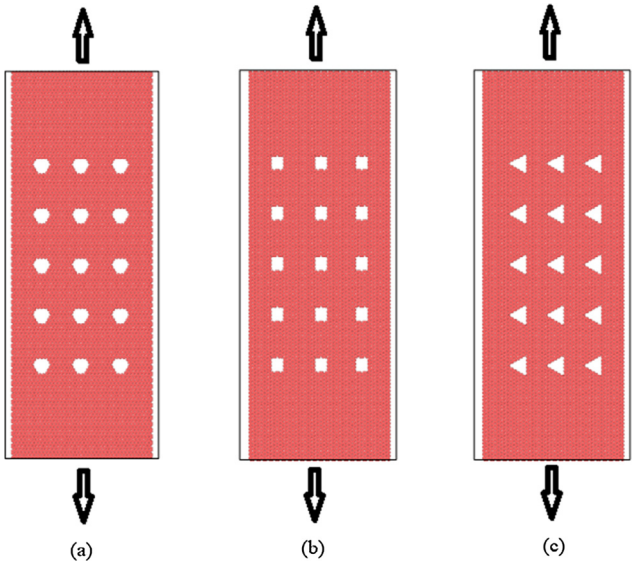

Fig. 1. Simulated GNM with (a) circular holes, (b) square holes, and (c) triangular holes.

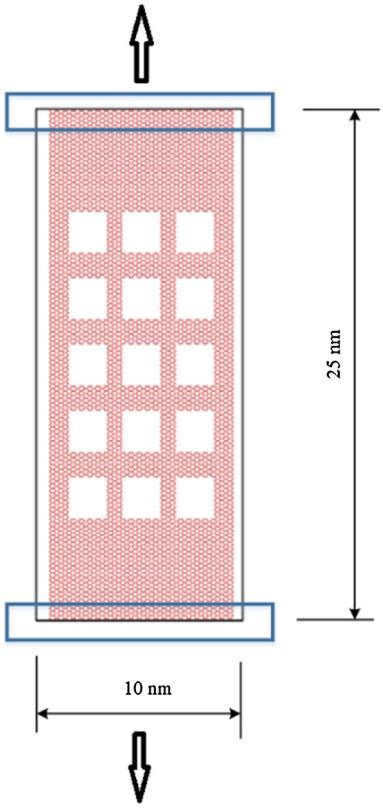

Fig. 2. GNM under uniaxial tension.

introduced in the semiconducting region are summarized in Table 1 as multiples of the graphene lattice constant a which is 2.46 Å.

Strain rate and loading scheme may have an influence on the stress-strain behavior [68–71]. To consider this factor, two types of loading schemes are applied with the same average speed which is compatible with previously recommended values in the literature [72]. In the first one, GNM was first subjected to one displacement increment of 0.0125 Å and then fully relaxed for 50 time steps until thermodynamic equilibrium is reached before the next displacement increment. In the second loading scheme, GNM was subjected to a uniaxial tension with

[1] For interpretation of color in Fig. 2, the reader is referred to the web version of this article.