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Molecular dynamics study on welding a defected graphene by a moving fullerene

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ABSTRACT

When a composite nanostructure is fabricated through van der Waals interaction only, the interaction among components may be sensitive to environmental conditions. To endow such a structure with relative stability, new covalent bonds should be applied. In this paper, a welding method for welding a circular graphene with a defect gap through a moving fullerene (C240 or C540 buckyball) is presented. When the buckyball moves above the gap, the two faces of the gap are attracted to each other and the distance between the two faces is shortened. When the dangling carbon atoms on both faces of the gap are excited to form new normal sp^2-sp^2 carbon bonds, the gap can be sewn up quickly. Molecular dynamics simulations are presented to demonstrate the welding process. When the gap is a sector, an ideal cone can be fabricated using the present method.

1. Introduction

Since graphene (GN) was discovered [1], it has attracted significant attention due to its outstanding properties described in [2]. For example, the sp^2 carbon atoms of a two-dimensional thin film are laid out in a honeycomb lattice that has an extremely large elastic modulus [3,4], perfectly controllable electronic properties [5], and thermal conductivity [6]. Due to the outstanding properties and geometric character of GN, many experimental approaches have been proposed during the last decade to fabricate a variety of patterns from GN [7–9] to meet specific application requirements. These approaches include a mechanical cleavage method [10], an electron irradiation method [11], a plasma etching method [12], a chemical etching method [8], a lithography method [13], high temperature [14], and so on. What is more, the size of the patterns can be controlled within 10 nm [10,13].

Besides the energy-based carving methods mentioned above, hydrogenation methods [15] are also popular for forming GN-based nanostructures. For instance, Liu et al. [16] used C4H to form various carbon nanoscrolls (CNS) by self-assembly or on a single-walled carbon nanotube (CNT). The mechanism is that each hydrogenated carbon atom (from sp^2 to sp^3 hybridization) leads to local bond distortion and further to bending deformation of the sheet. Reddy and Zhang [17] used a hydrogenation method to form a GN with quantized specified bending angles. They indicated that their method provided a controllable way to fabricate a complex nano electronic device without requiring a cutting or joining process. Similarly, Zhu and Li [18] used a hydrogenation method to fabricate nanobuilding blocks/nanocages with desired shapes. Such nanocages can be used to achieve molecular mass uptake, storage, and release.

The mechanism of the self-assembly of such nanostructures is that van der Waals (vdW) interaction [19] among the atoms in a GN leads to further deformation of the GN until the system reaches an equilibrium state at the desired ensemble. In fact, vdW interaction can also lead to other complex nanostructures, such as CNS [20–22], GN/(fullerene/)CNT-based composites [23,24], GN/metal (nanowire)-based nanostructures [25,26], GN/nanoparticle-based structures [27–29], and so on. It is obvious that the final nanostructures are developed with the components through vdW interaction. Given interactions between the components are easily produced in particular environments such as high temperature, certain liquid solutions, etc. On the other hand, sometimes there is no need for other elements such as hydrogen, iron, and so on to be involved in the fabrication of such structures. However, without extra excitation, the interaction among the components in a billet nanostructure is too weak to form the final stable structure. Hence we must use certain tools to trigger the initial deformation of the components.

In this paper, we suggest a method for welding the defect gap in a GN. The major idea is to use a fullerene with a relatively large radius (C240 or C540) [30] moving above the gap to attract the

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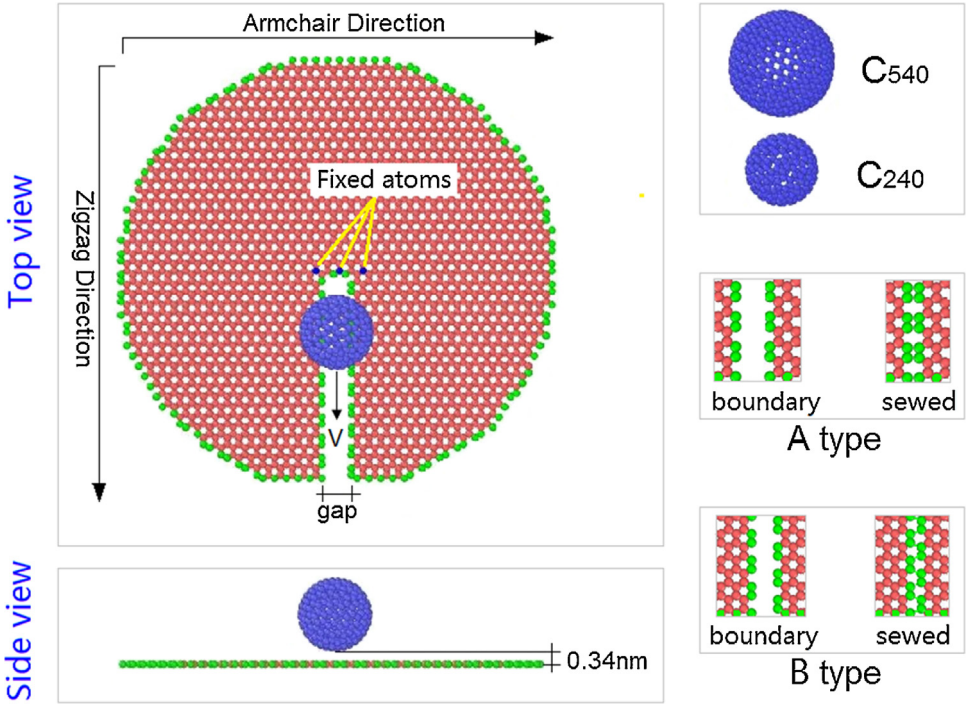
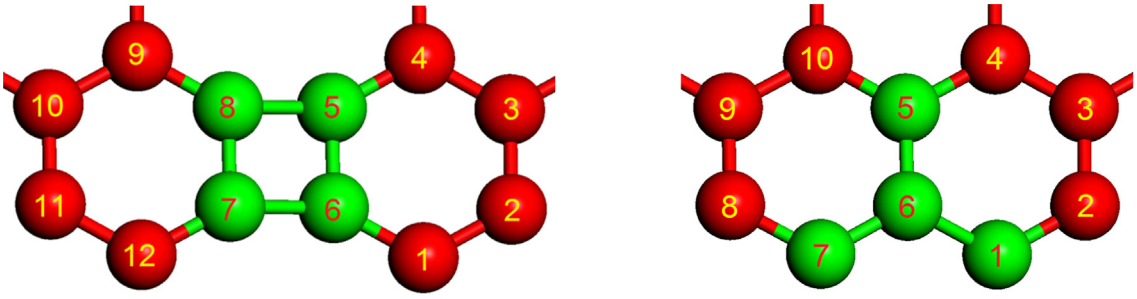


Fig. 1. The circular GN with radius of ~4.5 nm has a rectangular gap along the zigzag direction, and the inner side of the gap crosses the center of the sheet. A fullerene of either a C240 or a C540 buckyball is placed over the gap, the normal distance between the ball and the circular sheet being 0.34 nm. "v" is the fixed velocity of the buckyball along the radial direction (zigzag direction), the value of v is within [20,120] m/s. The route of buckball is fixed in motion. The gaps before and after being welded are classified into A-type and B-type. After minimization of the potential energy of the GN, the three dark blue atoms on the inner side of the gap are fixed during simulation. The green atoms are edge carbon atoms which are unsaturated. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article).



(a) A-type configuration with 12 carbon atoms (b) B-type configuration with 10 carbon atoms

Fig. 2. Carbon atom potentials in ideal configurations (with the same bond length of 0.142 nm) of a part of a sewn gap. (a) In the A-type configuration there are three different bond angles, 120°, 90°, and 150°. The potentials of the atoms are −5.251 eV of atom 1 or 12, −5.267 eV of atom 2 or 11, and −6.143 eV of atom 6 or 7 atom, respectively. (b) In the B-type configuration, all bond angles are 120°. The potentials of the atoms are −5.129 eV of atom 1 or 7, −5.267 eV of atom 2 or 8, and −7.587 eV of atom 6, respectively.

two faces of the gap. As the distance between the two faces sufficiently small, the dangling carbon atoms on the faces of the gap are excited to form new sp^2-sp^2 carbon (new C—C) bonds. From the point view of technology developed in nowadays, carbon nanotube probe is matured and popular in microscopes after over 15 years of development [31–34]. NASA [35] suggested a method for large-scale fabrication of carbon nanotube probe tips for application of space imaging and sensing. However, up to now, there is no simulation work which considered such welding problem. Hence, in the present study, we suggest to repair the defect gap on a graphene nanoribbon by a fullerene which can be considered as the tip of the carbon nanotube probe. In experimental research on fabrication of nanostructures, the size of a sample is commonly far greater than that (~1–3 nm) of the sample in the current simulation [36]. Hence, it is necessary to give a pre-investigation on the welding method by simulation.

2. Models and methods

Considering L = 0.12305 nm as the interlayer distance along the armchair direction of the sheet shown in Fig. 1, the width of the gap varies from 2L to 19L in the following simulations. It is known that a gap with the width of an odd number of L has an A-type boundary, on which the atoms are symmetrically laid out. For a gap with the width of an even number of L, the boundary is B-type. That does not mean that a gap with an A-type boundary will always have an A-type sewing result, and similarly with a B-type gap. Initially, the center of buckyball is over the middle dark blue atom in the sheet.

After building the model shown in Fig. 1, i.e., a circular grpahene with a rectangular gap and a fullerene over it with vertical distance of 0.334 nm, energy minimization on the whole model is carried out using steepest descending algorithm. The stopping tolerances of energy and force are 10-4 and 10-6, respectively. After poten-