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Defect-guided wrinkling in graphene

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ABSTRACT

This paper presents a design idea of defect-guided wrinkling controller of graphene based on the understanding of the defect-wrinkle interaction physics of graphene. Our results reveal that an extended one-dimensional Stone–Wales line defect has the potential to act as a controller embedded in another pristine graphene. The line defect has great effects on the graphene wrinkling. The wrinkling characteristics of graphene may be controlled by engineering the defect angle in graphene. This novel observation shows that it is a promising way to design and control graphene's properties and functionality by tuning the line defect. Our results and observations are significant to the development of the novel nano-mechanical systems and advanced graphene reinforced composite.

1. Introduction

Graphene has received a lot of attention in the past few years for its superior mechanical, electronic, optical, and thermal properties [1–4]. Many of these properties depend on the geometrical configuration of graphene membrane, and can be altered by deformation [5–10]. Deformations can be caused by various factors, including the thermal fluctuations [5], the chemical functionalization [6], the defects [7,8] as well as the wrinkles [9,10]. Defects and wrinkles are inevitable in graphene and have remarkably impact on the electronic conductivity [11,12], the magnetic states [13,14] and mechanical properties [15–17] of graphene. On the other hand, wrinkled graphene leads to new physical phenomena and is playing an increasingly important role in developing novel nano-electromechanical systems [18–23] and advanced graphene composite [24,25]. However, previous studies mainly focused on how to manipulate and control graphene defect and wrinkle, respectively. The effects of defects on wrinkling morphology have not been studied or understood clearly. It is the intent of this work to study the physics of the defect–wrinkle interaction of graphene and further to present an idea of the defect-guided wrinkling controller of graphene.

2. Model and method descriptions

The rectangular graphene (17.042 nm × 8.116 nm) is chosen as the example. The graphene is regarded as a system of micro-beams which properties are obtained using molecular mechanics method [26,27]. The elastic modulus and Poisson's ratio of micro-beams are 11.5 TPa and 0.37, respectively. The diameter of the micro-beam is 0.1 nm. In addition, the length of C—C bond is 0.142 nm [28]. The model of the micro-beam is shown in Fig. 1. There are 5530 C atoms in the model. The C atoms on bottom edge are fixed through the wrinkling analysis. The line defect which is an extended one-dimensional periodic Stone–Wales defect is introduced to the model. The rotated bond that creates the Stone–Wales defect makes an angle with the horizontal axis, named as the defect angle. Based on the feature of Stone–Wales defect, we classify the line defects as four angles, 30°, 90°, 150° and 180° (shown in Fig. 2).

A pseudo-relaxation progress is performed based on the optimized energy computation to obtain the stable equilibrium configuration. After this progress, the configurations of graphene with different defect angle are the V-shaped crest-like ripples, as shown in Fig. 3. The graphene with 150° defect angle has a similar crest-like ripple with the case of 30°. These defect-induced ripples are also observed in other studies [29,30]. These out-of-plane ripples are introduced into the model to be as the initial imperfections. A mandatory shearing displacement is then applied on the C atoms on upper edge of the model. The graphene wrinkling is then performed based on the modified displacement component method [31].

3. Results and discussion

The out-of-plane wrinkling deformation and the wrinkling waves of graphene with different defect angle under 0.5 nm shearing displacement are shown in Fig. 4. Compared with the pristine

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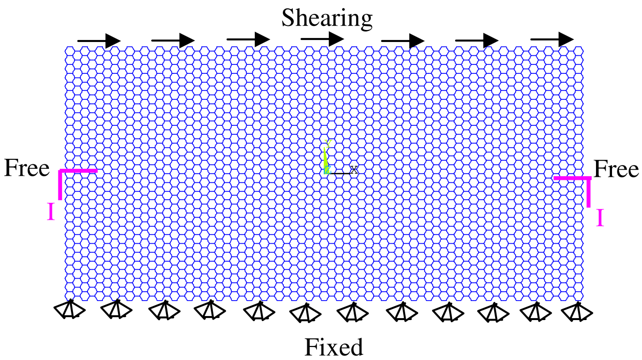

Fig. 1. Rectangular garphene under shearing.

graphene (shown in Fig. 5), the defect angle has great effects on the wrinkling characteristics of defected graphene.

The out-of-plane displacements of graphene with different defect angle are compared in Fig. 6. The detailed comparisons of wrinkling characteristics are listed in Table 1. The wrinkling wavelength, wrinkling amplitude and wrinkling angle decrease as the defect angle increases. While the percentage of wrinkling area and the wrinkling number increase as the defect angle increases. Both the wrinkling extent and magnitude are reduced when the defect angle is increased. It reveals that the defect angle may be tuned to control the graphene wrinkling. This novel observation should support us to control graphene's properties and functionality by designing the defect angle in graphene. In other words, it is a promising way to design a high-conducted graphene with slightly

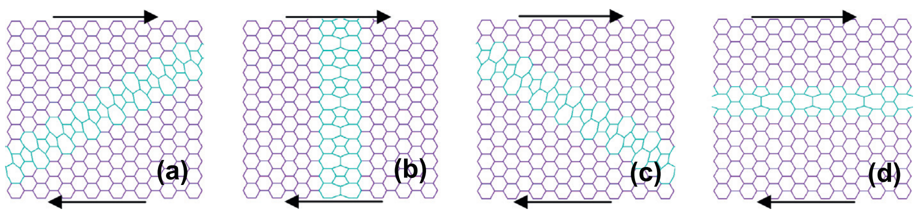

Fig. 2. The defect angle (a) 30°; (b) 90°; (c) 150° and (d) 180°.

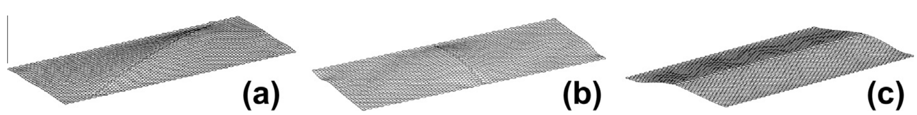

Fig. 3. The crest-like ripple of graphene after pseudo-relaxation (a) 30° defect angle; (b) 90° defect angle and (c) 180° defect angle.

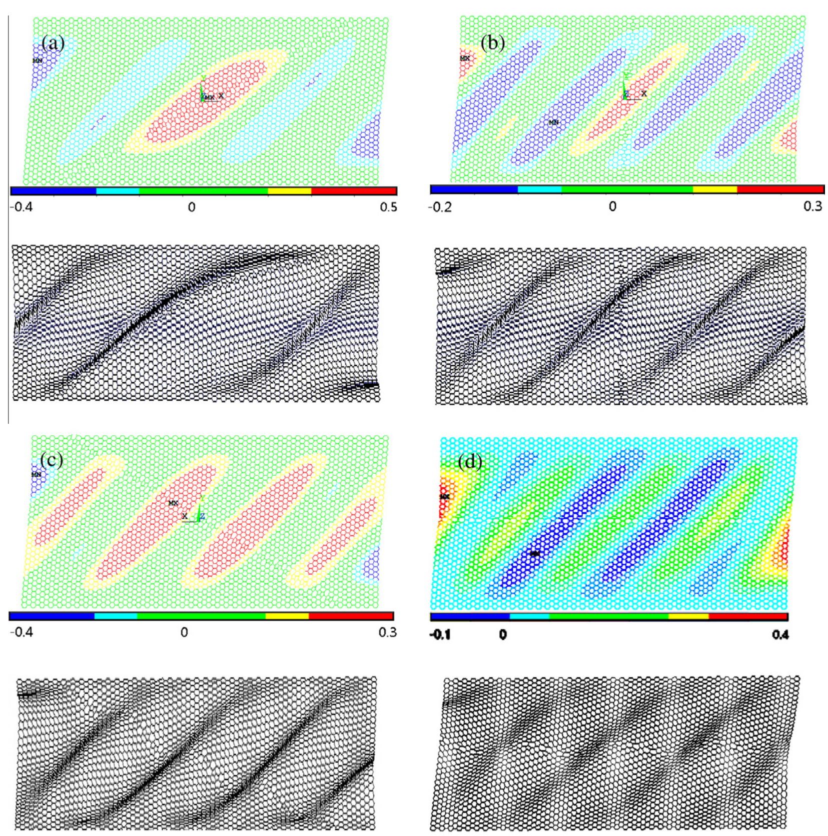

Fig. 4. Wrinkling characteristics of graphene with different defect angle under 0.5 nm shearing displacement, (a) 30° defect angle; (b) 90° defect angle; (c) 150° defect angle and (d) 180° defect angle.