Physica E 68 (2015) 102–106

Contents lists available at ScienceDirect

Physica E

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

Influence of line defects on relaxation properties of graphene: A molecular dynamics study

Jiu-Ren Yin*, Wen-Hu Wu, Wei Xie, Yan-Huai Ding, Ping Zhang

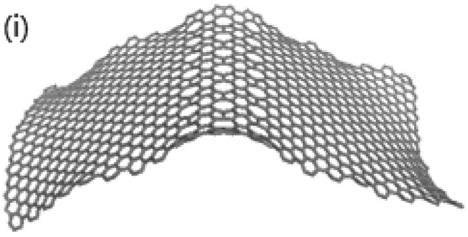
Institute of Rheology Mechanics, Xiangtan University, Hunan 411105, China

HIGHLIGHTS

- Relaxation properties of single layer graphene sheets containing line defects were investigated.
- Graphene sheet is bent with the line defects at the end of the sheet.
- Extent of the bend increases with the increase of the defect number.
- Graphene sheet transforms into a paraboloid with the line defects at the middle of the sheet.

GRAPHICAL ABSTRACT

The surface morphology of graphene changes into a paraboloid with the line defects at the middle of the sheet.



ARTICLE INFO

Article history:
Received 7 October 2014
Received in revised form
3 December 2014
Accepted 9 December 2014
Available online 11 December 2014

Keywords:
Graphene
Relaxation properties
Line defect
Molecular dynamics simulation

ABSTRACT

The relaxation properties of single layer graphene sheets containing line defects were investigated using molecular dynamics simulation with AIROBE bond-order interatomic potential. The dynamic evolution of graphene sheets during relaxation condition was analyzed. The simulation results show that the single layer graphene sheets are not perfectly flat in an ideal state, and the graphene sheet shows a significant corrugations at the verge of sheet. The graphene sheet is bent with the line defects at the end of the sheet, and the extent of this bend also increases with the increase of the defect number. Furthemore, the graphene sheet transforms into a paraboloid with the line defects at the middle of the sheet.

1. Introduction

Graphene, also known as two-dimensional graphite, is another new low-dimensional material following the discovery of fullerenes and carbon nanotubes. Graphene have attracted considerable interest over the last few years on account of its extraordinary electrical, thermal, and mechanical properties arising from its unique structure [1, 2]. However, a variety of defects, such as topological defects [3, 4], vacancy [5–10], adatom [11–14], were inevitably produced during the preparation of graphene. Line defects in the graphene lattice can significantly change its physical and chemical properties, such as bandgap opening and carrier mobility. However, only a few papers discussed the effect of line defects on the properties of graphene [20, 21]. It was difficult to characterize the physical properties of single layered graphene sheets because the propeties were effected dramatically by the substrates. Molecular simulation is a very powerful tool, and enables us to follow and understand structure and dynamics with extreme detail where motion of individual atoms can be tracked [18, 19]. In recent years, molecular dynamics simulation has been used to study the mechanical and relaxation properties of graphene nanoribbons in different directions and temperatures [15–17]. The simulation results showed that the single layer graphene nanoribbon is not of a perfect planar structure and that a certain degree

* Corresponding author. Fax: +86 731 58293240
E-mail address: yhding@xtu.edu.cn (Y.-H. Ding).

http://dx.doi.org/10.1016/j.physe.2014.12.015
1386-9477/

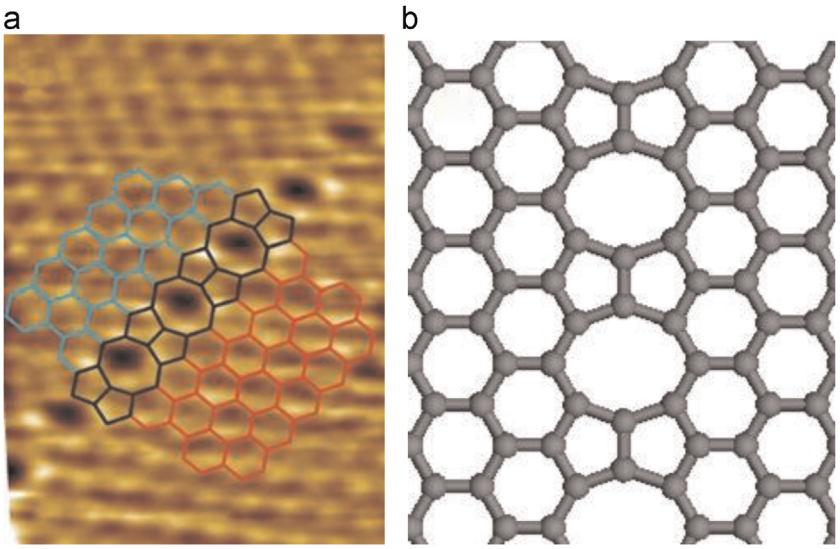


Fig. 1. STM image of graphene with line defect (a) and structure diagram with a line defect (b).

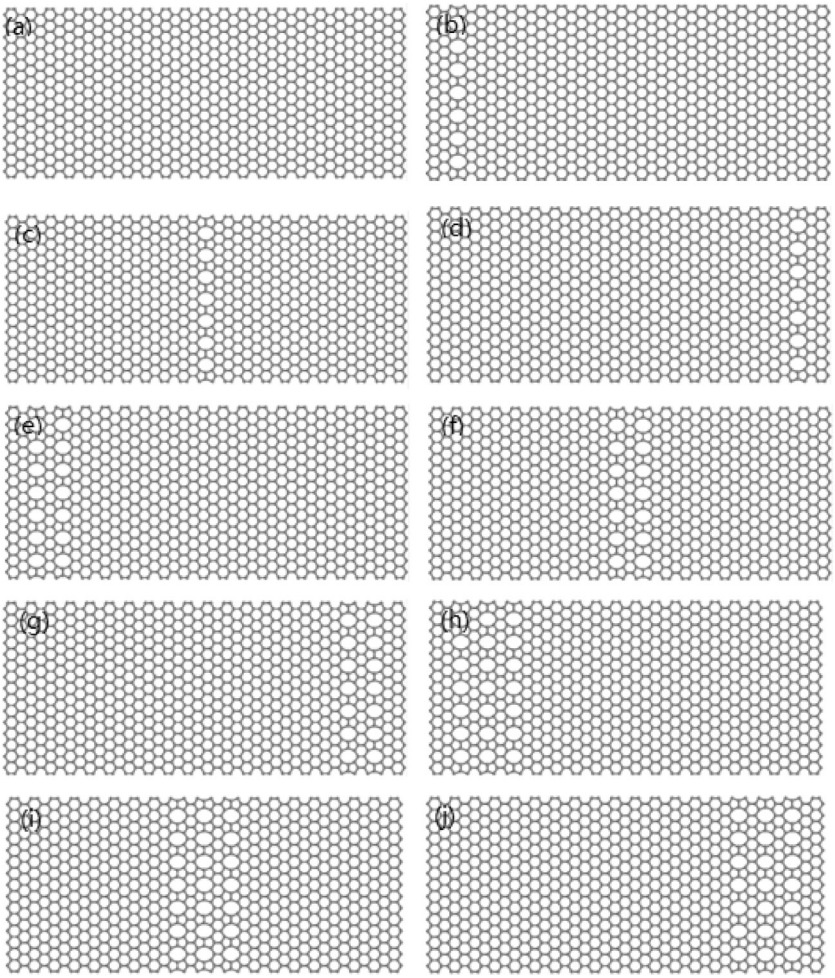


Fig. 2. Schematic showing the defects locations and numbers. The model of perfect graphene sheet (a). The model of graphene with a line defect in the right (b), middle (c) and left (d). The model of graphene with two line defects in the right (e), middle (f) and left (g). The model of graphene with three line defects in the right (h), middle (i) and left (j).

of fluctuations and folds occur at the edges and inside of nanoribbons.

In this paper, molecular dynamics method was used to simulate the homeostasis evolution of graphene with line defects in the relaxation process. The paper is organized as follows. In the following section, we introduce the numerical model, defining first the microstructure of graphene and the defect location in graphene. In Section 3, we present the results of our numerical