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Stability and wrinkling of defective graphene sheets under shear deformation

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ABSTRACT

The molecular dynamic simulation is performed to study the wrinkling behavior of a graphene sheet with a hole subjected to a shear loading at different temperatures. Wrinkling is inevitable under pure shear loading. Four different hole diameters of 0, 0.8, 1.6, and 3.2 nm are chosen in this simulation. The results show that the number of ridges increases with an increase of the width of the graphene sheet. The shear stress induced in the defective graphene sheet increases with increasing temperature. In addition, the shear modulus of the defective graphene sheet also increases with an increase of temperature.

1. Introduction

In the recent years, graphene sheets have attracted great scientific interest due to their excellent physical and chemical properties, and potential applications in nanobiological devices and nano-electromechanical systems [1–3]. Because graphene is only one atom layer thick, it is easily amenable to external influences such as thermal loading and mechanical deformation [4]. Structure materials experience local buckling deformation which is often called wrinkling. The presence of wrinkles in graphene sheets may significantly influence their electronic structure and physical properties [5].

Nowadays, it is still a challenge to study the wrinkling and buckling behaviors of graphene sheets due to the difficulties encountered in the experimental measurements of nanoscale materials [6]. Therefore, the theoretical methods [7–14], including atomistic simulations and continuum mechanics, are often used. For example, Lu and Huang [11] studied the excess energy and deformation along free edges of graphene nanoribbons by atomistic simulations based on a reactive empirical bond-order potential. Duan et al. [12] investigated the initiation and development of wrinkles in a single layer graphene sheet by molecular mechanics simulations and a continuum model and found that the wrinkle wavelength decreased with an increase in shear loading. Zhang et al. [13] observed the wrinkle pattern of an annular graphene under circular shearing at the inner edge by performing molecular mechanics simulations.

In addition, some researchers investigated the defect effect on the physical properties of graphene sheets. Xiao et al. [15] carried out an atomistic based finite bond element model to study the effects of multiple Stone–Wales (5-7-7-5) defects on mechanical properties of graphene sheets. Sahin and Ciraci [16] studied the structural, mechanical, and electronic properties of defect-patterned graphene nanomeshes by means of first-principles calculations. In this article, the wrinkling behavior of a detective graphene sheet subjected to the shear deformation is investigated using the molecular dynamic simulation. Furthermore, the temperature effect on the shear stress induced in the detective graphene sheet is also studied.

2. Simulation method

The structure of the armchair graphene sheet has a length (L) of around 10 nm and different widths (W) of 2.397, 5, 5.781, 7.473, and 10 nm, containing a central defect hole with different diameters (d) of 0, 0.8, 1.6, and 3.2 nm, respectively, as shown in Fig. 1. Two layers of atoms on the left and right are fixed and four layers of thermostat atoms closed to the fixed layers are set to dissipate any excess heat generated during the shear loading. Constant-temperature molecular dynamics simulation at 300 K is performed using simple velocity scaling thermostat for temperature control. The simulation

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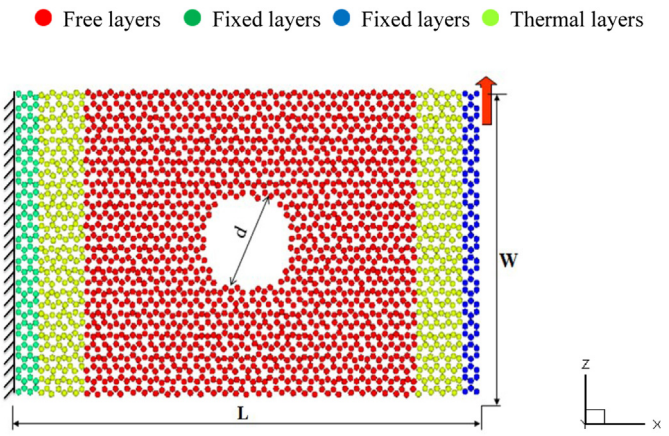

Fig. 1. Schematics of MD of a graphene sheet subjected to the shear loading.

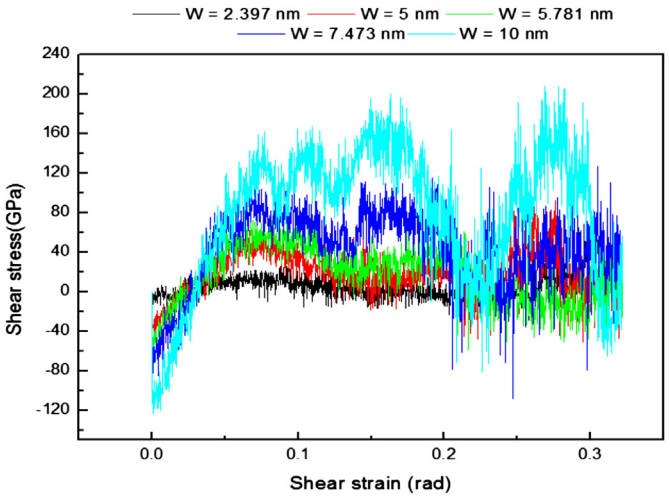

Fig. 3. The relationship between shear stress and shear strain of a graphene sheet with $L = 10$ nm and different graphene widths subjected to a shear loading with a velocity of 5 m/s at $t = 1200$ ps and $T = 300$ K.

is equilibrated for 5 ps in NVT ensemble (i.e., canonical ensemble). The simulation time step of 1 fs is employed and the total simulation time is 1600 ps.

To study the wrinkling phenomena of the graphene sheet subjected to shear deformation, a positive displacement Δw with a stretch rate of 5 m/s in the z direction is applied to the atoms on the top right edge. The total displacement is 8 nm for the shear test. The Tersoff potential [17] is used to model the interaction between the carbon atoms. Furthermore, the temperature effect on the shear properties of the defective graphene sheet at different temperatures of 300, 350, 400, 450, and 500 K is examined.

3. Results and discussion

3.1. Wrinkling phenomenon

Wrinkling is inevitable under pure shear. The more relevant aspect in the current geometry is probably wrinkling around the hole under external loading. In this article, we investigate the wrinkling behavior of a graphene sheet subjected to a shear

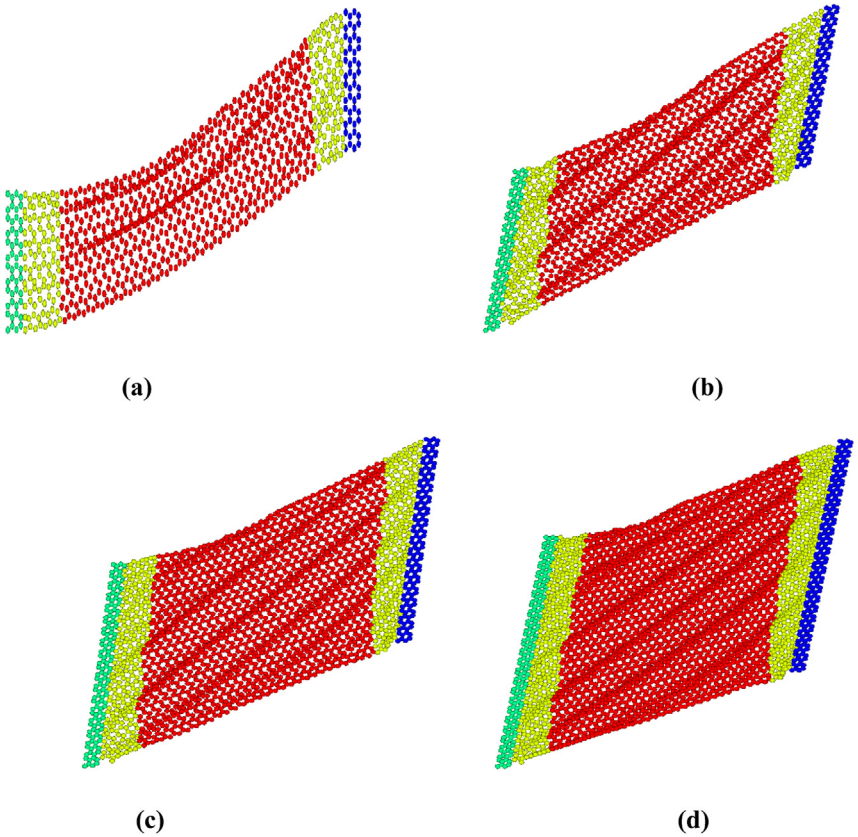

Fig. 2. Wrinkles in a perfect graphene sheet with $L = 10$ nm and (a) $W = 2.397$ nm, (b) $W = 5.781$ nm, (c) $W = 7.473$ nm, and (d) $W = 10$ nm subjected to a shear loading with a velocity of 5 m/s at $t = 1200$ ps and $T = 300$ K.