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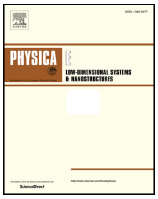

Dependence of wrinkling geometric patterns on the chirality of monolayer graphene under shear deformation

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ABSTRACT

Molecular dynamic simulations are performed to study the wrinkling behaviors of a rectangular graphene sheet with various chirality angles subject to in-plane shear displacements. The results indicate that the 1/4-power laws, which are for the average out-of-plane amplitude and half-wavelength of the wrinkles as functions of shear strain, are found to be valid for the graphene with all different chirality angles. Moreover, the dependence of wrinkling amplitude and half-wavelength of graphene on the applied shear strain is insensitive to the chirality. It is expected that the research could promote applications of graphene-based materials or nano-mechanical systems in engineering.

1. Introduction

Graphene is a classic two-dimensional material with a hexagonal monolayer network of carbon atoms. Owing to its extraordinary thermal, chemical, and mechanical properties, it has created considerable research interest during the past decade [1–4]. Its superlative physical properties make graphene an excellent candidate in a wide range of engineering fields [5–8] such as graphene-based mechanical sensors [9], switches [10], and resonators [11].

Due to the relatively small bending rigidity, wrinkles are often observed in graphene, especially under shear loadings. For instance, by using molecular dynamics (MD) simulations, Huang and Han [12,13] demonstrated the formation and development mechanisms of wrinkling in a single-layer graphene sheet subjected to in-plane shear displacements. Shen *et al.* [14] examined the formation of wrinkles and their effects on the corresponding Young's moduli of single-layer graphene sheets. Qin *et al.* [15] explored the changes of surface area resulting from wrinkling in loaded free-standing graphene sheets by using a combination of continuum mechanics-based and MD simulations. Xiang *et al.* [16] performed MD simulations to measure the shear wrinkling of rippled single-layer graphene in thermal environments.

The wrinkles of graphene sheet with thickness in the nanometer range are expected to strongly affect its physical properties. Shen [17,18] investigated wrinkling deformation and thermal conductivity of one graphene sheet at 300 K under shear. It was found that the thermal conductivity of single-layer graphene decreases when increasing the shear strain. By using scanning tunneling microscopy, Xu *et al.* [19] reported wrinkles with about 3 nm height for a graphene sheet, and they found the wrinkles have lower electrical conductance. Mei *et al.* [20] summarized a variety of wrinkle formation on nanoscale and revealed potential applications of these wrinkles, such as tunable fluidic nanochannels, nanofluidic templates and sieves, controllable transfer of colloidal patterns. Therefore, it is of critical importance to study the geometric pattern of wrinkles of graphene sheets under shear loading for developing patent graphene-based devices.

Due to its structural asymmetry, graphene exhibits distinct anisotropic shear behaviors. Zhao *et al.* [21] studied the effects of chirality on the shear properties of the monolayer graphene sheets. They found that the fracture strain of graphene in the armchair direction is less than that in the zigzag direction subjected to shear deformation. Yi *et al.* [22] investigated the chirality-dependent shearing behavior of graphene. Their results have shown that as the chirality angle of graphene increases, the shear strength and failure strain along the shearing direction first increase and then decrease. Zhao *et al.* [23] performed MD simulations to explore the loading-direction dependent shear behavior of graphene sheets at different temperatures. Their results show that due to the chirality of the hexagonal network structure, the shear properties, such as shear stress-strain curves and failure strains of graphene sheets depend strongly on the loading direction.

Despite the recent progress, little is known about the effects of

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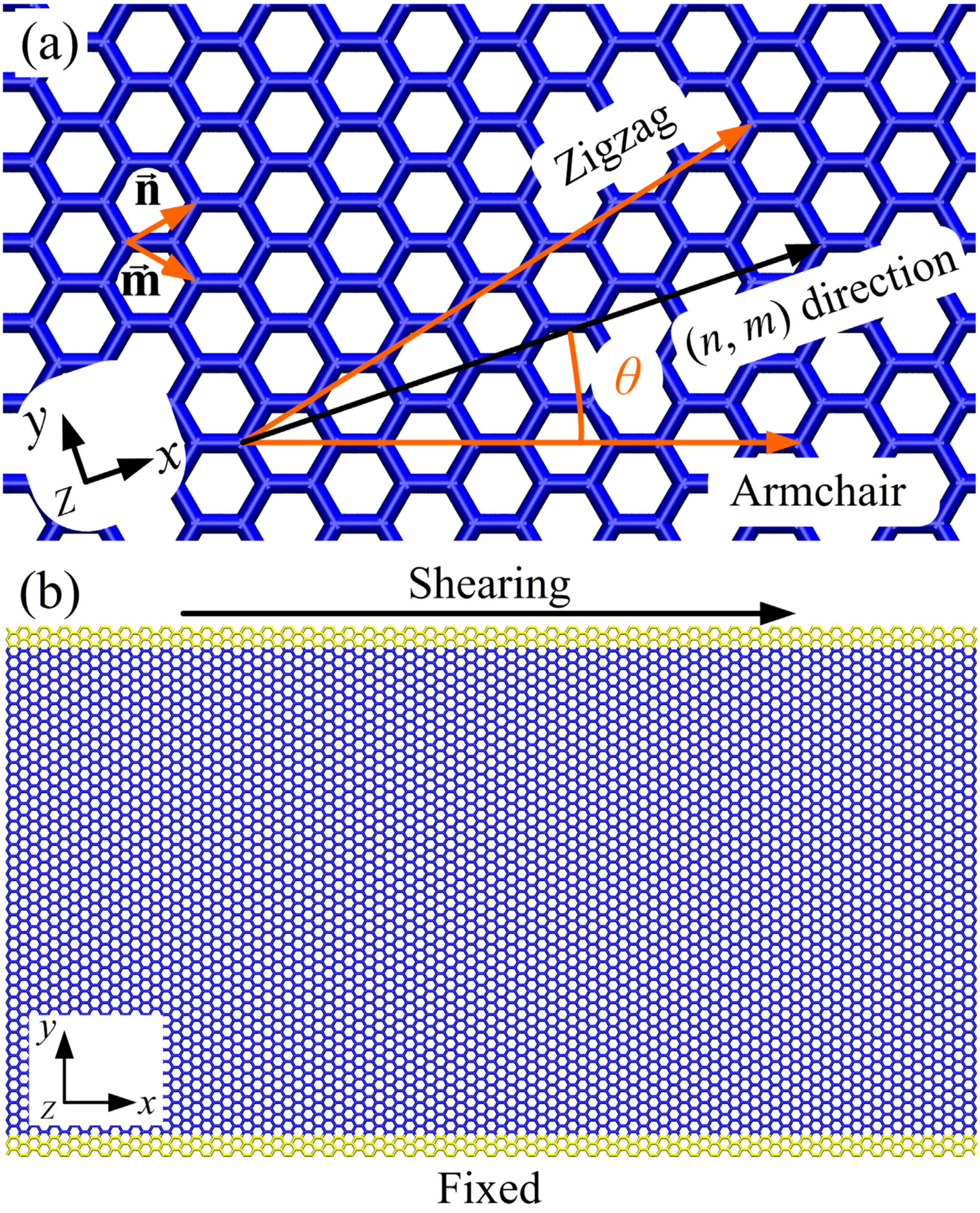

Fig. 1. Simulation model. (a) Illustration of graphene orientation. The chirality angle θ of an arbitrary direction is defined as the angle between this arbitrary direction (n, m) and the armchair direction (n, n) (b) MD model of graphene subject to in-plane shear displacements. The x-axis is set along the (n, m) direction, and the z-axis is normal to the graphene.

chirality on the geometric pattern of shear-induced wrinkles of a monolayer graphene sheet. In this work, we perform MD simulations to study wrinkles of graphene sheets with different chirality angles subjected to in-plane shear displacements. The average amplitude and half-wavelength of the wrinkles are considered to characterize the geometric pattern. An analytical theory is also used to analyze the sensitivity of the wrinkling behaviors for various chirality shear directions of graphene sheets.

2. Methods

Fig. 1(a) gives a schematic illustration of the honeycomb lattice of the carbon atoms in a graphene sheet. A chiral vector $\mathbf{D} = n\mathbf{n} + m\mathbf{m}$ can be used to describe the orientation of graphene, where n and m are two integers, $\mathbf{n}$ and $\mathbf{m}$ are unit vectors of the graphene lattice [24]. The chirality angle θ of an arbitrary direction is defined as the angle between this arbitrary direction (n, m) and the armchair direction (n, n) [25], i.e.,

$$\theta = \pi/6 - \arctan[3^{1/2}m/(2n + m)], \quad (1)$$

Due to the six-fold rotation symmetry of graphene, the chirality angle θ is in the range of $0° \le \theta \le 30°$.

The wrinkling behaviors of rectangular graphene sheets with various chirality angles subject to in-plane shear displacements are investigated. The simulation model used in this study is illustrated in Fig. 1(b). The x-axis is set along the (n, m) direction, and the z-axis is normal to the graphene. The (n, m) of (1, 1), (6, 5), (10, 7), (7, 4), (13, 6), (8, 3), (7, 2), (5, 1), (15, 2), (16, 1) and (1, 0) graphene sheets with