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Small size effect on the wrinkling hierarchy in constrained monolayer graphene

Jianzhong Zhao, Xingming Guo*, Lu Lu

Shanghai Institute of Applied Mathematics and Mechanics, Shanghai Key Laboratory of Mechanics in Energy Engineering, Shanghai University, Shanghai 200072, PR China

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ABSTRACT

The present paper investigates the small size effect on a localized transition zone in the merging of two wrinkles in constrained suspended graphene under in-plane shear. It is found the classical elasticity theory overestimates the wrinkle amplitude and wavelength in contrast with the results of atomistic simulation. The analytic formulations for the wrinkling hierarchy are obtained by using nonlocal plate theory. Here, this small size effect can be estimated by correct value of nonlocal parameter e0a = 1.9 nm. Besides, the orientation of graphene slightly influences the wrinkling hierarchy of graphene. The temperature effect is significant under small shear strain, while this effect is significant in the constrained edges and insignificant in the middle region under large strain. The occurrence of cracking is always in constrained edges, where the stress concentration releases in the wrinkling hierarchy. This work is expected to provide a better understanding of the mechanism of nanometer scale wrinkles.

1. Introduction

Graphene, as the thinnest material ever found, has received significant interest since it was conclusively isolated via the Scotch tape method (Novoselov et al., 2004). Distinctive from 3D nanomaterials, graphene exhibits unstable corrugations such as wrinkles, ripples and crumples due to very small bending stiffness and thermal fluctuations (Deng & Berry, 2016). Hence, the tunable wrinkle-patterns, wavelength and amplitude are very important in flexible electronics, microelectromechanical systems and device fabrication (Akinwande et al., 2017; Bunch et al., 2007; Ghorbanpour-Arani, Kolahdouzan, & Abdollahian, 2018; Prasai, Tuberquia, Harl, Jennings, & Bolotin, 2012; Zhang, Huang, & Rogers, 2015b). To figure out the interplay between mechanical activities and wrinkle parameters, the wrinkles of graphene have been extensively investigated experimentally and theoretically. Bao et al. reported that controlled and organized microscale wrinkles can be produced for the suspended graphene on a trench by using both spontaneously and thermally generated strains (Bao et al., 2009). Bai et al. showed that one-dimensional periodic graphene wrinkles of nanoscale dimensions (2 nm to 10s of nm) can be implemented on pre-trenched copper foils via thermal strain engineering and the observed wrinkles modes are beyond the descriptions of continuum mechanics (Bai et al., 2014). From classical elasticity theory, the amplitude and wavelength for wrinkles produced spontaneously on suspended few layers graphene was described by $A^2 \sim lh\gamma^{1/2}$ and $\lambda^2 \sim lh\gamma^{-1/2}$, respectively. h and γ donate the thickness and longitudinal tensile strain in the graphene of length l(Cerda & Mahadevan, 2003). The classical elasticity theory has been successfully applied to describe the wrinkles of graphene with large wavelength

* Corresponding author.
E-mail address: xmguo@shu.edu.au (X. Guo).

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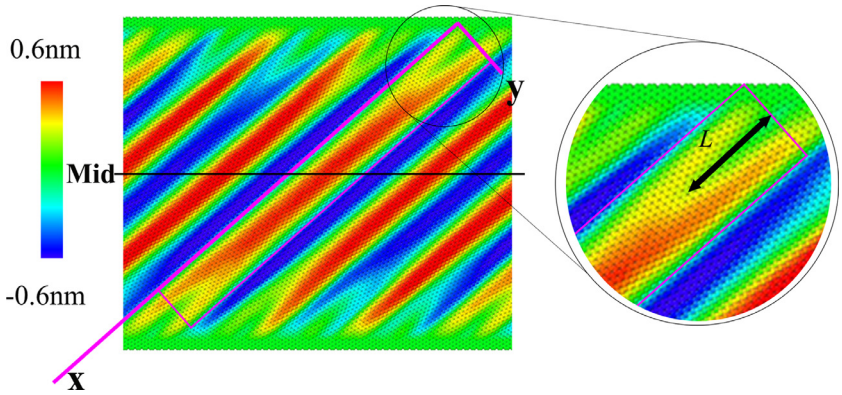

Fig. 1. Illustration of a rectangular graphene subjected to in-plane shear with the wrinkling hierarchy in the vicinity of top and bottom ends.

($\lambda > 300$nm), however, it was proven to be invalid for nanometer scale wrinkles (Tapasztó et al., 2012) (even for thickness of monolayer graphene from 0.08 to 0.35 nm). Vandeparre et al. showed that thin sheets under boundary confinement spontaneously generate a universal self-similar hierarchy of wrinkles from strained suspended graphene (the wavelength is beyond 0.15 nm) to ordinary hanging curtains (Vandeparre et al., 2011). This transition zone where two or more wrinkles merge into one can be also found in graphene nanoribbons or step-like changes in the Young's modulus of elastomeric substrates supporting stiff layers (Glatz et al., 2015; Meng et al., 2013; Zhou, Liu, Dmitirev, Korznikova, & Baimova, 2016). The breakdown of continuum mechanics for nanometer wavelength wrinkling of graphene is because the wrinkles are influenced by the atomic structure of graphene much more than by continuum mechanics rules (Lambin, 2014). Hence, the small-scale effect must be taken into consideration.

Atomistic simulation is another powerful tool in studying the wrinkle behaviors of larger systems for graphene. Duan et al. used molecular mechanics (MM) simulations to predict the wrinkles of graphene sheet subjected to in-plane shear displacements (Duan, Gong, & Wang, 2011), which the error of the prediction is less than 20% in contrast with the theoretical results by effectively using $h \approx 0.1$nm from the bending stiffness (Wang, 2010). The shear buckling mode of rectangular graphene sheets obtained from the molecular dynamic (MD) simulations is different from the one as predicted by continuum mechanics models (Xiang & Shen, 2015). In particular, the MD simulation results revealed that the graphene wrinkling strongly depends on the size of graphene (Los, Fasolino, & Katsnelson, 2016; Wang, Liu, Lan, & Tan, 2013).

In this work, we report on the wrinkling hierarchy in constrained suspended graphene under in-plane shear deformation. The evolution of wrinkle amplitude and potential energy are discussed first. We then demonstrate a comparative study between the simulation and nonlocal plate theory, which have helped in understanding the size effects on a localized transition zone in the merging of two wrinkles. Furthermore, the orientation and temperature effect on the wrinkle of graphene sheets under shear are discussed.

2. Methodology

The constrained graphene is adopted to study the wrinkling behaviors when subjected to in-plane shear. We consider a rectangular graphene fixed on its bottom end, with an in-plane shear imposed on its top end, while periodic boundary condition is applied in the left and right ends. The x and y-axes are aligned with the tangent and transverse directions to the wrinkles. Fig. 1 shows clearly that the graphene subjected to in-plane shear generates the wrinkling hierarchy in the vicinity of top and bottom ends. This localized transition distance in the merging two wrinkles is characterized by L. The interactions between carbon atoms are described by the adaptive intermolecular reactive empirical bond-order (AIREBO) potential function (Donald et al., 2002). To facilitate the simulation of graphene wrinkle, we adopt a general switch function parameter 2.0 Å and add longer-ranged interactions using a form similar to the standard Lennard Jones potential in the range of 2.0 Å–10.2 Å. The equations of motion are integrated by the Verlet algorithm with a time step of 1 fs. The Nose-Hoover thermostat (Hoover, 1985; Nosé, 1984) is employed to maintain constant temperature and volume. The MD simulations are performed using the publicly available simulation code LAMMPS (Plimpton, 1995). The OVITO package (Stukowski, 2010) is used for visualization. In order to have a deep insight into the evolutions of the wrinkle amplitude and wavelength in the wrinkling hierarchy, various MD simulations are performed.

3. Results and discussion

3.1. Wrinkling progress

Fig. 2 shows the evolution of amplitude and potential energy with shear strain in the graphene of dimension 20 nm × 20 nm. The corresponding surface patterns are shown by the top configurations in Fig. 2(b). Referenced Wang's