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Defects controlled wrinkling and topological design in graphene

Teng Zhang [a,1], Xiaoyan Li [b,c,1], Huajian Gao [a,*]

[a] School of Engineering, Brown University, Providence, RI 02912, USA
[b] Centre of Advanced Mechanics and Materials, Tsinghua University, Beijing 100084, People's Republic of China
[c] Applied Mechanics Laboratory, Department of Engineering Mechanics, Tsinghua University, Beijing 100084, People's Republic of China

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ABSTRACT

Due to its atomic scale thickness, the deformation energy in a free standing graphene sheet can be easily released through out-of-plane wrinkles which, if controllable, may be used to tune the electrical and mechanical properties of graphene. Here we adopt a generalized von Karman equation for a flexible solid membrane to describe graphene wrinkling induced by a prescribed distribution of topological defects such as disclinations (heptagons or pentagons) and dislocations (heptagon–pentagon dipoles). In this framework, a given distribution of topological defects in a graphene sheet is represented as an eigenstrain field which is determined from a Poisson equation and can be conveniently implemented in finite element (FEM) simulations. Comparison with atomistic simulations indicates that the proposed model, with only three parameters (i.e., bond length, stretching modulus and bending stiffness), is capable of accurately predicting the atomic scale wrinkles near disclination/dislocation cores while also capturing the large scale graphene configurations under specific defect distributions such as those leading to a sinusoidal surface ruga[2] or a catenoid funnel.

1. Introduction

Topological defects including disclinations (heptagons or pentagons) and dislocations (heptagon–pentagon dipoles) have been found to exist in large-area polycrystalline graphene (Li et al., 2009; Kim et al., 2009, 2011; Huang et al., 2011), and thought to play crucial roles in tailoring mechanical and physical properties of graphene (Lusk and Carr, 2008; Yazyev and Louie, 2010a, 2010b; Grantab et al., 2010; Huang et al., 2011; Wei et al., 2012a; Zhang et al., 2012; Ovid'ko, 2012; Wu and Wei, 2013; Yi et al., 2013; Rasool et al., 2013). As a special class of solid membrane with two-dimensional (2D) crystalline structure, free standing graphene undergoes fully three-dimensional (3D) deformation to minimize its energy in the presence of topological defects (Nelson and Peliti, 1987; Seung and Nelson, 1988), as verified by recent high-resolution transmission electron microscopy (HRTEM) experiments (Lehtinen et al., 2013; Warner et al., 2013), density functional theory (DFT) calculations (Yazyev and Louie, 2010b) and atomistic simulations (Liu and Yakobson, 2010; Liu et al., 2011, Pao et al., 2012). As illustrated in Fig. 1a, a dislocation dipole in graphene can induce large wrinkles near the dislocation core,

* Corresponding author.
E-mail address: Huajian_Gao@brown.edu (H. Gao).
[1] These authors contributed equally to this work.
[2] The Latin word ruga is used to refer a large-amplitude state of a wrinkle, crease, ridge or fold (Diab et al., 2013).

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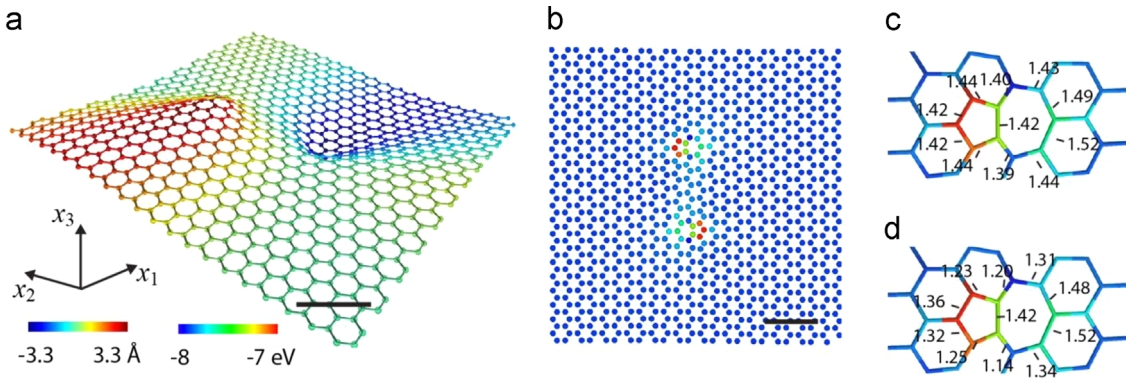

Fig. 1. Atomic configuration of a dislocation dipole in a graphene sheet of dimension 20×20 nm^2 (only a part of the region around the dislocation dipole is shown here). (a) A perspective view of deformation around the dislocation dipole. (b) Top view of the dislocation dipole. (c) Bond structures around the dislocation core in 3D. (d) Bond structures around the dislocation core in 2D projection. The color represents the scale of the out-of-plane displacement in (a) and potential energy in (b–d), respectively (scale bar: 1 nm). (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this paper.)

with out-of-plane displacement amplitude up to 3.3 Å. Fig. 1b shows the potential energy of carbon atoms around the dislocation dipole, where atoms in the dislocation cores exhibit higher energy than those in the far field. In particular, three atoms on the heptagon side have the highest energy. The 3D distributions of bond lengths around a dislocation and the corresponding 2D projection are presented in Fig. 1c and d, respectively. It can be clearly observed that the 2D projection significantly underestimates the length of covalent bonds around the dislocation core (Lehtinen et al., 2013). Interestingly, it has also been shown that the out-of-plane displacement in graphene can be used to tune the electrical (Levy et al., 2010; Pereira et al., 2010; Klimov et al., 2012) and mechanical properties of graphene, such as anisotropic friction (Choi et al., 2011) and tunable wettability through controllable crumpling (Zang et al., 2013) of graphene on substrate. These recent studies are calling for systematic investigations of topological defects induced wrinkling in graphene.

From a continuum perspective, topological defects in flexible membrane and shell structures have been investigated during the past several decades. Nelson and collaborators (Nelson and Peliti, 1987; Seung and Nelson, 1988) derived a generalized von Karman equation to describe coupling between topological defects, in-plane stress and out-of-plane deformation in a 2D crystalline membrane; they showed that the out-of-plane deformation can significantly reduce the magnitude of in-plane stresses generated by the defects. Zubov (1997, 2007, 2010) investigated topological defects in plates and shells, and proposed a geometrical analogy to transform the problem of a thin shell with defects into its dual problem of a thin shell with external loading (Zubov, 2010). Chen and Chrzan (2011) calculated the self-energy of a periodical array of dislocation dipoles in a graphene sheet with and without out-of-plane deformation by modeling dislocations as topological constraints and performing energy minimization in the Fourier space. In spite of these impressive progresses on dislocations/disclinations in solid membranes, it remains a challenge to develop an efficient continuum model that can accurately capture both the atomic-scale rippling near the defect core and large-scale wrinkles in the membrane.

In linear elastic solids, dislocations can be treated as an eigenstrain field that can be analytically or numerically treated using Green's function method (Mura, 1982). In comparison, topological defects in graphene present a greater challenge due to the complex nonlinear coupling between in-plane and out-of-plane deformations. It has been difficult to obtain analytical solutions even for a single, isolated dislocation in a membrane. Similar problems with incompatible deformation significantly influencing the final morphology of the structures occur in the growth of biological tissue (Dervaux and Ben Amar, 2008; Liang and Mahadevan, 2009; Li et al., 2011a, 2011b) and the swelling of a soft membranes (Klein et al., 2007; Kim et al., 2012). A number of theoretical frameworks have been proposed to treat incompatible deformation in these phenomena, such as non-Euclidean plate theory (Efrati et al., 2009) and multiplicative decomposition of deformation gradient (Dervaux et al., 2008; Lewicka et al., 2011; Li et al., 2012). A comparison between the governing equations for defects and growth in thin plates would suggest that the defects can be represented as an equivalent eigenstrain field, an idea that has been widely used in micromechanics (Eshelby, 1957; Mura, 1982).

The nonlinear coupling between topological defects and curvature in a 2D crystalline membrane can induce a variety of interesting phenomena. It has been shown that lattice defects tend to adopt specific patterns on curved surfaces (Bausch et al., 2003; Vitelli et al., 2006; Hexemer et al., 2007; Bowick and Giomi, 2009; Irvine et al., 2010, 2012; Kusumaatmaja and Wales, 2013) and can trigger different buckling modes in a spherical elastic shell, which has been used to shed light on the understanding of virus shape (Lidmar et al., 2003) and morphological changes between smooth and faceted structures (Funkhouser et al., 2013; Yong et al., 2013). Reversible transformation between flat sheets and surfaces with non-zero Gaussian curvature in nematic glass sheet has been studied by combining the effects of disclinations with thermal/optical stimuli (Modes et al., 2010, 2011). In parallel with recent attempts to design 3D surface profiles of inhomogeneous gel composites with controllable swelling ratio (Klein et al., 2007; Kim et al., 2012), it will also be challenging and exciting to explore the possibility of designing curved structures with distributed topological defects in graphene and other 2D crystalline materials. The rapid developments in new experimental techniques