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Surface elasticity revisited in the context of second strain gradient theory

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ABSTRACT

Surface/interface stresses, when notable, are closely associated with a surface/interface layer in which the interatomic bond lengths and charge density distribution differ remarkably from those of the bulk. The presence of such topographical defects as edges and corners amplifies the noted phenomena by large amounts. If the principal features of interest are such studies as the physics and mechanics of evolving microscopic-/nanoscopic-interfaces and the behavior of nano-sized structures which have a very large surface-to-volume ratio, traditional continuum theories cease to hold. It is for the treatment of such problems that augmented continuum approaches like second strain gradient and surface elasticity theories have been developed by Mindlin (1965) and Gurtin and Murdoch (1975), respectively. In the mathematical framework of the former theory, the surface effect is explicitly revealed through surface characteristic length and modulus of cohesion, whereas within the latter theory, which views the bulk material and its complementary surface as separate interacting entities, the critical role of surfaces/interfaces is directly incorporated through the introduction of the notions of tangential surface strain tensor, surface stress tensor, and surface elastic modulus tensor into the formulation. In the realm of the experimentations, evaluation of the above-mentioned surface parameters poses serious difficulties. One of the objectives of the current study is to provide a remedy as how to calculate, not only these parameters, but also Mindlin's bulk characteristic lengths as well as Lame constants with the aids of first principles density functional theory (DFT). To this end, surface elasticity is reformulated by maintaining the first and second gradients of the strain tensor for the bulk; as a result two new key equations are obtained. One of these equations is an expression for the net surface stress, needed to relate the surface parameters in surface elasticity to the Mindlin's second gradient theory parameters. The other equation is for the total elastic energy which is utilized to find an analytical expression for the surface energy. The available data on surface relaxation obtained experimentally and computationally are in good correspondence with the results of the current theory. Moreover, employing the present theory, an estimate for the effective elastic constants of films with infinite extension is provided.

1. Introduction

Efforts towards the design and manufacturing of miniaturized devices in modern technologies as well as the description of the phenomena associated with the physics and mechanics of the evolving microscopic-/nanoscopic-interfaces have acquired a close examination of the

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The role of strain on the quantum spin hall effect and band inversion in stanene

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ABSTRACT

Examination of the role of strain on the quantum spin hall (QSH) effect and band inversion for the monolayer of tin, stanene, is of interest. To this end, several uniaxial and biaxial strain loadings along the armchair (AC)- and zigzag (ZZ)-directions are applied using first principles calculations based on density functional theory (DFT). We observe QSH insulator as well as semi-metallic property associated with the strained stanene.

1. Introduction

Topological insulators (TIs) are characterized by gapped band structures in the bulk configuration and conducting edge states lying inside the bulk insulating gap [11,26]. In fact, TIs behave as an ordinary insulator in the bulk, three-dimensional (3D) configuration with a gap separating valence and conduction energy bands. However, in the two-dimensional (2D) configuration, they have gapless surface (or edge) states due to time-reversal (TR) symmetry which lead to conducting states. Edge states are also called helical edge states since, at a given edge, two states with opposite spin polarization counterpropagate [13,30].

As stated in the preceding paragraph, conducting edge states lie inside the bulk gap region intersecting the Fermi energy level. The energy band corresponding to a right (left) moving chiral edge mode intersects the Fermi energy with a positive (negative) group velocity, which is calculated as the slope of the band structure curve. TR symmetry guarantees that the energy bands of edge states cross each other at special points in the Brillouin zone (BZ). It is worth mentioning that, in the special elements for which a large spin-orbit (SO) coupling exists, the usual band ordering is inverted and a topologically trivial insulator can be transformed into a quantum spin hall (QSH) insulator.

The QSH effect, a state of quantum matter, in particular, associated with monolayers has attracted great attention in condensed matter physics and materials science [11,31] due to its potential application in semiconductor spintronics [1]. QSH states are topologically different from all other known states of matter, including quantum hall (QH) states. The QH effect is the spatially separated counterflows of electrons which happens for a 2D gas of electrons in a semiconductor under a strong magnetic field [14]. In contrast, a QSH effect splits the spin-up forward movers and the spin-down backward movers in a TR-invariant fashion in the absence of any external magnetic field [1,13].

The energy gap in topological insulators can be tuned effectively by chemical functionalization like surface doping as well as applied external strain. In search of novel QSH insulators, extensive studies have been devoted to the 2D group IV honeycomb lattices. Ref. [36] studied stanene film functionalized with organic molecule ethynyl using first principles calculations and phonon modes. They found that organic molecule ethynyl enhances the thermostability of stanene film and leads to the achievement of QSH effect. Moreover, they noted a large-gap of about 0.22 *eV* under the applied external tensile strain of 3.0%. Later, [37] considered a class of large-gap QSH insulators in ethynyl-derivative functionalized stanene (SnC2X; X = H, F, Cl, Br, I). Ref. [38] disclosed a class of large-gap QSH

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Research paper

Elastic moduli tensors, ideal strength, and morphology of stanene based on an enhanced continuum model and first principles

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ABSTRACT

The present work aims to provide an accurate description of the tensile behavior of the planar as well as low-buckled stanene and to capture their ideal strength in armchair (AC)- and zigzag (ZZ)-directions. For an accurate description of anisotropic response of such hyperelastic materials as stanene, consideration of a highly nonlinear constitutive model in which up to the fourth power of strains is incorporated is inevitable. By utilizing first principles calculations based on density functional theory (DFT), the second, third, fourth, and fifth order elastic moduli tensors corresponding to both planar and low-buckled states are obtained. Moreover, the morphology of the free-standing stanene such as bond length and lattice parameter is determined; for low-buckled stanene two additional parameters, namely, buckling height and dihedral angle are computed. The effects of uniaxial and biaxial loadings germane to AC- and ZZ-directions on the buckling height and dihedral angle are also studied. Scrutinization of the electronic charge distribution reveals the phenomenon of the formation of necking in the Sn-Sn bonds under large uniaxial extension along the AC-direction. Moreover, the transformation of sp^3 hybridized orbitals to sp^2 hybridized orbitals is examined and confirmed through consideration of the structural geometries of the atomic bond angles.

1. Introduction

Ever since graphene has been introduced to the scientific world, it has attracted the attention of many researchers with diverse backgrounds. For the sake of achievable technological applications, abundant attention has been absorbed in graphene due to its unusual electronic properties arising from the sp^2 hybridized planar structure (Manjanath et al., 2014). Motivated by the intriguing electronic and optoelectronic properties of free-standing graphene, many researches have been made for probing alternative two-dimensional (2D) materials. Theorists predict that new monolayer materials with more better electronic properties than those of graphene can be fabricated being capable to be easily integrated with current generation of electronic technologies (Balendhran et al., 2015). Moreover, it is expected that advanced opportunities in nanoelectronic devices and energy technologies are triggered by these monolayer materials (Zhuang and Hennig, 2014). Recent studies show that more interesting phenomena are observed by proceeding down in group IV of the Periodic Table (Gross, 2014). In the hypothetical field of room-temperature superconductors, for example, monolayer stanene may act as zero-heat-loss interconnects in processor chips and hence may put an end to the one-century tantalization of engineers by physicists for superconductors (Webb, 2014).

In contrast to graphene which is stable in planar configuration, stanene is stable in low-buckled configuration. This is associated to the fairly weak strength of $\pi - \pi$ bonding between tin atoms. Buckling increases the overlap between π and σ bondings resulting in stability of low-buckled stanene (Xu et al., 2013). Similar to its 2D group-IV counterpart, silicene, the out-of-plane buckling of stanene makes it possible to be functionalized by an out-of-plane electric field. Since the buckling of stanene is larger than that of silicene, it is expected that a larger band gap is induced (Drummond et al., 2012; Van den Broek et al., 2014). Topological insulators (TIs) which behave as an ordinary insulator in three-dimensional (3D) configuration and have gapless surface (or edge) states in two-dimensional (2D) configuration have attracted great attention in condensed matter physics and materials science (Hasan and Kane, 2010; Xu et al., 2013). In special elements for which large spin-orbit (SO) coupling exists, the usual band ordering is inverted and a topologically trivial

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Research paper

Toupin–Mindlin first strain gradient theory revisited for cubic crystals of hexoctahedral class: Analytical expression of the material parameters in terms of the atomic force constants and evaluation via *ab initio* DFT

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ABSTRACT

Capture of the discrete nature of crystalline solids for the purpose of the determination of their mechanical behavior with high precision is of interest. To achieve this objective, two fundamental contributing factors are on top of the list: (1) formulation in the mathematical framework of an appropriate higher order continuum theory rather than using classical treatment, and (2) incorporation of the true anisotropy of the media. The present work revisits Toupin–Mindlin first strain gradient theory for media with general anisotropy, and then specialize it to cubic crystals of hexoctahedral class. This formulation in addition to 3 classical material constants encountered in classical theory of elasticity, gives rise to 11 additional material parameters peculiar to first strain gradient theory. To date, there is no experimental method in the literature for the measurement of these parameters. A methodology incorporating lattice dynamics is proposed, by which all the material parameters including the classic ones are analytically expressed in terms of the atomic force constants. Subsequently, the analytical expressions for the nonzero components of the 4th and 6th order elastic moduli tensors as well as 6 characteristic lengths are derived. Finally, with the aid of *ab initio* calculations all the material properties in Toupin–Mindlin first strain gradient theory are numerically obtained with high precision. In this work the transformation matrices of cubic crystals of diploidal class which also falls under centrosymmetric point groups are discussed as well.

1. Introduction

Design and fabrication of miniature structures, micro- and nano-objects with a desired precision require the incorporation of appropriate highly accurate analysis. It is well-known that, the accuracy of classical continuum theory of elasticity for describing the mechanical behavior of nano-sized structures is insufficient. Moreover, not only its accuracy in the vicinity of the nanoscopic defects deteriorates, but also it is incapable of capturing the size effect of such nono-sized embedded second phase as nano-inhomogeneities and nano-voids. The desire to increase the accuracy of solution through accounting for the discrete nature of matters, turned the attention of some prominent investigators, primarily in the period of about 1960–1975, towards the development of various higher order continuum theories. Despite the fact that such theories, due to their ability to remedy the aforementioned dilemmas, are nowadays in the spotlight, some serious challenges as how to obtain the associated material properties are posed. Herein, we mainly focus on first strain gradient theory for cubic crystals of hexoctahedral class and calculate, in this mathematical framework, all the pertinent material parameters and the components of the elastic moduli tensors.

The first generalization of the classical theory goes back to the nineteenth century. Voigt (1887, 1894) was the first to note that on each face of a differential volume element inside a body, in addition to the action of 3 stress components, there are also 3 moment vectors. Although Voigt's works being the pioneer of this theory, the first comprehensive theory was later presented by Cosserat and Cosserat (1909). In their proposed theory, they assumed that each point, in addition to the 3 translational degrees of freedom considered in classical theory of elasticity, possesses 3 rotational degrees of freedom as well. Appearance of couple stresses in the equations of motion within Cosserat media is a manifestation of consideration of the additional degrees of freedom. In contrast to classical theory of elasticity, it turns out that the pertinent stress tensor for Cosserat media is not symmetric. From a different point of view, each point of a Cosserat

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