



## Research paper

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

Hossein M. Shodja<sup>a,b,\*</sup>, Farzaneh Ojaghnezhad<sup>c</sup>, Azadeh Etehadieh<sup>a</sup>, Maryam Tabatabaei<sup>a</sup><sup>a</sup> Department of Civil Engineering, Sharif University of Technology, P.O. Box 11155-4313, Tehran, Iran<sup>b</sup> Institute for Nanoscience and Nanotechnology, Sharif University of Technology, P.O. Box 11155-9161, Tehran, Iran<sup>c</sup> School of Engineering, Alzahra University, Vanak St., 1993891176, Tehran, Iran

## ARTICLE INFO

## Article history:

Received 12 March 2017

Available online 8 April 2017

## Keywords:

Stanene

Nonlinear continuum

Morphology

Elastic moduli tensors

Ideal strength

Ab-initio

## 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.

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## 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 Henig, 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).

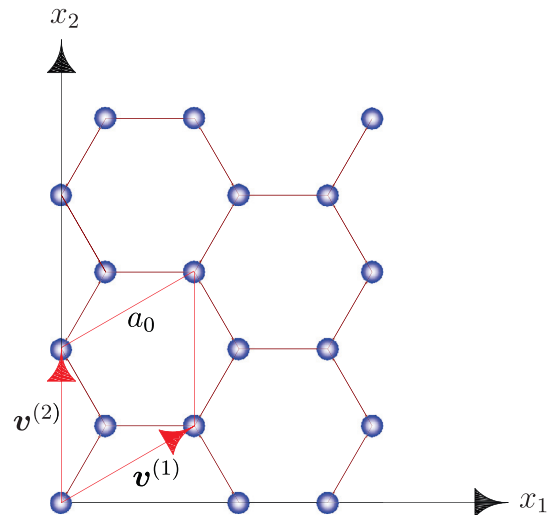
In contrast to graphene which is stable in planar configuration, stanene is stable in low-buckled configuration. This is associated to the fairly weak strength of  $\pi - \pi$  bonding between tin atoms. Buckling increases the overlap between  $\pi$  and  $\sigma$  bondings resulting in stability of 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

\* Corresponding author.

E-mail addresses: [shodja@sharif.edu](mailto:shodja@sharif.edu), [shodja.hossein@gmail.com](mailto:shodja.hossein@gmail.com) (H.M. Shodja).

insulator can be converted into a quantum spin hall (QSH) insulator. Xu et al. (2013) and Liu et al. (2011) have observed that the presence of SO interaction results in QSH state in stanene. Recently, we have also obtained the phenomenon of band inversion in both strained and unstrained states of stanene due to SO coupling. Moreover, we found that lattice distortion at special strain level of 0.4 along armchair direction can play the key role in the transformation of a 2D semi-metallic state to nontrivial QSH insulator for stanene (Tabatabaei et al., 2017). In comparison to graphene with extremely small opened gap (Min et al., 2006; Yao et al., 2007), the unstrained stanene has a band gap of about 0.115 eV which is tunable using strain loading (Tabatabaei et al., 2017). In addition to the application of strain loading to modulate the band gap of stanene, Zhang et al. (2015; 2016) showed that it can also be tuned by functionalization. Stanene as a large-gap quantum spin Hall insulator is expected to find a wide range of applications in development of room-temperature dissipationless conduction, spintronic devices, and highly miniaturized electronics (Xu et al., 2013; Zhu et al., 2015; Song et al., 2014). It is notable to mention that incorporation of the room-temperature dissipationless conductors in appropriate sections of integrated circuits and microprocessors would significantly cut down on the power consumption and heat production. The hope for practicability of these intriguing applications has enormously increased after the successful fabrication of stanene on  $\text{Bi}_2\text{Te}_3(111)$  substrates by molecular beam epitaxy as recently reported by Zhu et al. (2015). They have determined the atomic and electronic structures of epitaxial stanene by scanning tunneling microscopy and angle-resolved photoemission spectroscopy in combination with first principles calculations. Their experimental observations are in a reasonable agreement with the previous theoretical predictions. More interestingly, Saxena et al. (2016) have recently synthesized one-atom thick free-standing layer of stanene.

Determination of the mechanical properties of novel materials, due to its fundamental importance, has been the subject of numerous works in the literature. Regarding the possible vast applications, the mechanical properties of such a novel material as stanene are critical in designing the associated structures. Surprisingly, a brief surveying the publications on stanene shows that neither the nonlinear elastic behavior of stanene nor its intrinsic stress is addressed in the literature. Owing to the computationally power-intensive feature of simulation methods as well as the reasonable mechanical predictions of the continuum approaches in nanoscale problems (Delfani et al., 2013), the development of the continuum framework for stanene would be of great benefit to predict its in-plane elastic response in nano-devices. The nonlinear elastic behavior of some monolayer materials up to the ultimate stress followed by a strain softening until fracture are previously studied by some researchers (Topsakal et al., 2010; Peng et al., 2012; 2013; Wei et al., 2009; Delfani et al., 2013). To develop the continuum framework, the higher order series expansion of the strain energy density function of 2D stanene with respect to the Lagrangian strain is considered. Subsequently, the enhanced continuum constitutive relations are written in terms of the higher order elastic moduli tensors. The higher order elastic constants are evaluated by fitting the nonlinear stress-strain analytical expressions to the corresponding ab-initio data for appropriate number of loading modes. Ab-initio simulations are carried out employing Vienna Ab-initio Simulation Package (VASP) based on pseudopotential density functional theory (DFT). The most mentionable advantages of the first principles calculations are their high transferability and quantitative reliability. The total energies of the system, forces on each atom, and stresses on the simulation box can be directly obtained from DFT calculations. By numerical values of the higher order elastic constants on hand, one can study the nonlinear elastic response of the material in uniaxial tensile



**Fig. 1.** The atomic structure of stanene and the corresponding in-plane lattice vectors,  $\mathbf{v}_1$  and  $\mathbf{v}_2$  and lattice parameter,  $a_0$ . AC- and ZZ-directions of the monolayer coincide with  $x_1$  and  $x_2$  axes, respectively. The two-atomic rhomboid unit cell formed by the lattice vectors  $\mathbf{v}_1$  and  $\mathbf{v}_2$  is shown.

stress up to some point beyond its intrinsic stress. In this way, the ideal strength of stanene can be determined in zigzag (ZZ)- and armchair (AC)-directions. DFT calculations can be employed to assess the ideal strengths for validation of the continuum model, as well. Moreover, the in-plane Young's modulus and Poisson's ratio can be calculated via the second order elastic constants of the material. In this work, stanene is considered as a continuous lamina with non-zero thickness. We assume that the deformed state of stanene is such that the contribution of bending to the strain energy density is negligible as compared to the in-plane strain contribution. This requires that the radius of curvature of any out-of-plane deformation be significantly larger than the in-plane interatomic distance. The stress state of stanene under these assumptions can be assumed to be in-plane (Fumi, 1952).

The paper is organized as follows. Details of the atomic structure of stanene is presented in Section 2. Section 3 is devoted to illustrate the nonlinear elastic continuum description and the fifth order series expansion of the strain energy density function. In Section 4, the details of employed methodologies for determination of the higher order elastic constants are presented. The detailed explanations are given for both analytical exploited approaches such as stress-strain and energy-strain methods and the ab initio computational simulations. In Section 5, the methods for calculation of ideal tensile strength are described in detail. The first method is based on an analytical model in the nonlinear continuum framework (Section 5.1) and the next one is a computational approach including uniaxial tension simulation in VASP (Section 5.2). The numerical results and pertinent discussions are reported in Section 6. In Section 6.1, the morphological properties are given and compared with the existing data in the literature. The values of the higher order elastic constants for planar stanene, buckled stanene, and graphene are tabulated in Section 6.2. Section 6.3 represents the numerical values for ideal strength of the considered materials, and in Section 6.4 the values for Young's modulus and Poisson's ratio are given.

## 2. Atomic structure of stanene

The geometry of the monolayer tin film called stanene is depicted in Fig. 1. It is well known that stanene is a 2D hexagonal lattice of the crystal class,  $D_{6h}$  possessing a six-fold rotation axis and six mirror planes perpendicular to its plane. Assume that the

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