Mechanics of Materials 120 (2018) 43–52

Contents lists available at ScienceDirect

Mechanics of Materials

journal homepage: www.elsevier.com/locate/mechmat

Strain induced anisotropic mechanical and electronic properties of 2D-SiC

Manju M.S.[a], Ajith K.M.[*,a], M.C. Valsakumar[b]

[a] Computational Physics Laboratory, Department of Physics, National Institute of Technology Karnataka (NITK), Surathkal, Mangaluru 575025, India
[b] Department of Physics, Indian Institute of Technology (IIT), Ahalia Campus, Kozhipara, Palghat 678557, India

ARTICLE INFO

Keywords:
2D-SiC
Density functional theory
Mechanical properties
Non-linear elastic constants
Electronic properties
Ionic nature

ABSTRACT

A silicene derivative of the form SiC was thoroughly investigated on its behaviour with changes in stress varying from around 140 N/m to around 20 N/m and strain from −0.2 to 0.3. Uniaxial stress (both zigzag and armchair) brought structural changes which reduced the symmetry of the system but biaxial stress brought no change in symmetry and shape of the material. Mechanical stability of the system was maintained upto a considerable stress in both uni- and biaxial cases and the system showed anisotropic behaviour with stress variations. Electronic structural variations showed strain engineering is a convenient method to tune the band gap very effectively causing semiconducting SiC to transform to metallic one at large stresses and direct to indirect bandgap in the semiconducting phase at lower stress. Charge density analysis showed a significant ionic nature of the material in the semiconducting phase.

1. Introduction

The past two decades have seen tremendous advancements in the prediction and synthesis of two dimensional materials having novel electronic, chemical, mechanical, optical and magnetic properties and their potential applications in various fields including mechanical engineering, electronics, information and energy technologies (Zhang et al., 2016). Graphene was the first of this kind which was extensively investigated theoretically prior to its experimental synthesis and its synthesis in 2004 opened a pathway for micro and nano device fabrications (Novoselov et al., 2004; Sahin and Peeters, 2013). Discovery of these two dimensional materials and their numerous applications have aroused interest in exploring new materials on the horizon of condensed matter physics and materials science (Lin and Ni, 2012; Wang et al., 2014). The advancement in practical synthesis of these materials will pave a way to the nanoelectronics. This generated interest in probing one and few atom thick materials for various practical applications. Most of the two dimensional materials tend to be anisotropic in nature. Anisotropic materials show different behaviour along different directions which could prove possibilities to design novel materials for sensors with anisotropic crystalline directions, electrical conductance, optical absorption and scattering etc. (Lang et al., 2016). Silicene, which was a monoatomic layer of silicon was another extensively explored candidate due to its potential application in silicon electronics (Kara et al., 2012).

Silicene is a monoatomic sheet with hexagonally arranged silicon atoms analogous to graphene buckled with sub-lattice displacement of 0.46 Å (Roman and Cranford, 2014; Kaloni and Schwingenschlögl, 2014). Graphene and silicene has zero band gap which reduces their functionality in electronic and optoelectronic applications which requires a sizeable and well defined band gap. Band gap in these materials can be tuned by introducing vacancies or by introducing foreign atoms or by applying external force or fields or by confining to 1D nanoribbons or by coupling with various other sheets (Kunstmann et al., 2017; Zhang et al., 2015; Tang et al., 2014; Ukpong, 2015). Graphene and also silicene were incorporated with various elements to verify if it could improve the properties of bare graphene and silicene (Ding and Wang, 2013). Among the various derivatives of silicene, SiC was found to be a promising candidate because of it's high mechanical strength, carrier mobility, thermal stability and thermal conductivity (Şahin et al., 2009).

SiC is a planar sheet akin to graphene with a lattice constant of 3.10 Å and Si−C bond length of 1.79 Å (Ding and Wang, 2013). SiC is a direct band gap semiconductor making it a futuristic material for electronic and optoelectronic applications (Shi et al., 2015). It is also assumed to play a major role as metal-free catalyst due to it's higher chemical reactivity towards foreign adsorbates (Wang et al., 2016). Kuzubov et al. (2013) claimed that they have been able to grow a monolayer of SiC on Mg(0001) and MgO(111) substrates, among which Mg tends to be the superior substrate over MgO, for growing 2D SiC. Chabi et al. (2016) also claimed that 2D SiC nanosheet was produced by carbothermal reaction and post sonication process. SiC nanowires and nanoribbons were also extensively studied and they were found to be a potential candidate for hydrogen storage, nanodevices and

* Corresponding author.
E-mail address: ajith@nitk.ac.in (A. K.M.).

https://doi.org/10.1016/j.mechmat.2018.02.005
Received 6 October 2017; Received in revised form 31 January 2018; Accepted 27 February 2018
Available online 07 March 2018

microelectrochemical systems (Gori et al., 2012; Bekaroglu et al., 2010). It is crucial to look into the stress dependent variation in properties of this material before deploying it for various applications.

The elastic constants of a material gives its response to external mechanical perturbation. Mechanical properties are divided into four strain domains based on loading : linear elastic, nonlinear elastic, plastic and fracture. Linear and nonlinear strain domains are reversible i.e., they are brought back to equilibrium after the removal of loads. Plastic and fracture domains are irreversible i.e., increase in strain nucleates and accumulates defects resulting in rupture (Peng et al., 2013b). Previous studies on various two dimensional materials have shown that they possess large non-linear elastic deformation in the tensile regime up to the intrinsic strength of the material and then strain softening until fracture (Peng et al., 2013a; Wang et al., 2010). Higher order elastic constants determine non-linear elastic response, anharmonic properties like phonon-phonon interactions, thermal expansion, Gruneisen parameter etc.

Stress or strain plays an important role in the physical properties of the materials. Application of stress or strain engineering is considered to be an efficient method to deform the material and determine the response of these materials looking into various behavioural changes occurring in the materials (Saxena and Tyson, 2008; Wang et al., 2012). Thorough understanding of the stress dependence of these materials is essential for their practical applications. Deformation brings changes in electronic as well as mechanical behaviours. Band gap tuning is essential for their potential applications in electromechanical devices, tunable photo detectors and lasers (Bhattacharyya and Singh, 2012). So, our efforts in this paper is to induce stress in SiC and understand the variation in properties with respect to variation in stress.

2. Computational methodology

Vienna Ab-Initio Simulation Package (VASP) was used to carry out the Density functional theory (DFT) calculations (Kresse and Hafner, 1993; 1994; Kresse and Furthmüller, 1996) which is based on Kohn–-Sham density functional theory approach (KS-DFT), to understand the changes in structural, mechanical and electronic properties of SiC. Generalized gradient approximation (GGA) (Perdew et al., 1996) parametrized by Perdew–Burke–Ernzerhof (PBE) was used for the calculation of exchange-correlation potential. The valence electrons were considered explicitly for the calculations and the core electrons are incorporated using projected augmented wave method based pseudopotential (Blöchl, 1994; Jones and Gunnarsson, 1989). The kinetic energy cutoff was maintained at 900 eV. Gamma-centered kpoint meshes were used to sample the Brillouin zone and it was found that a $20 \times 20 \times 1$ grid is sufficient to ensure convergence of energy and other physical properties. An interlayer spacing of 15 Å was found to be sufficient to make interlayer interactions, that arises because of the usage of periodic boundary conditions in VASP, to be negligible so that, for all practical purposes, the calculations being done pertain to a film of SiC. The energy was converged to 0.001 eV/atom between two ionic steps and a convergence of 10^{-8} eV was kept for each electronic self-consistency (SC) loop. Lattice parameters of the unitcell were changed corresponding to compression or elongation in both uni and biaxial directions and the stress required to equilibrate the system to a varied unit cell is considered as the applied stress. Stress was applied uniaxially both in zigzag and armchair directions and biaxially and the variation in structural, mechanical and electronic properties were noted for both compressive and tensile regimes. The structure with equilibrium lattice parameter is considered as the undeformed structure here, and the lattice parameters were varied, increased and decreased up to 20% from the undeformed lattice parameter.

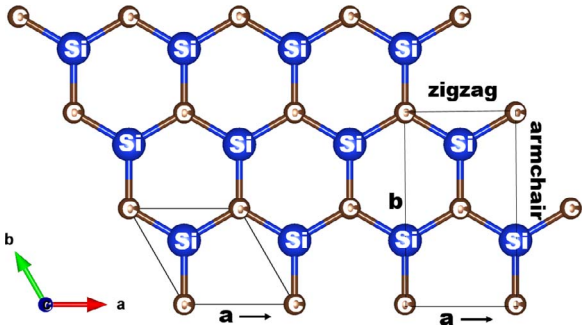

Fig. 1. Unitcell of SiC considered for Uniaxial and Biaxial stress. The cell in the form of a rhombus is used for biaxial stress and the cell in the form of rectangle for uniaxial application. The direction of zigzag and armchair is as marked.

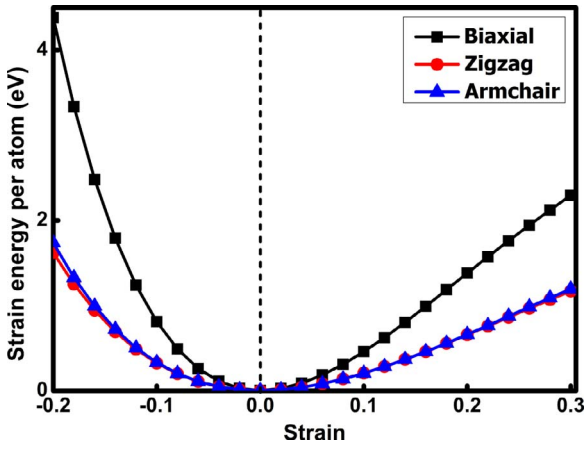

Fig. 2. Variation in strain energy per atom with strain for zigzag, armchair and biaxial cases. Strains are varied from −0.2 to 0.3 and all the three curves represents anharmonicity and anisotropy present in the material.

Table 1
Elastic constants of SiC along with graphene, silicene and bulk α-SiC. The values of C_{11} and C_{12} are in terms of N/m in the case of SiC, graphene, silicene and that of bulk α-SiC is represented in GPa.

	SiC*	Graphene**	Silicene†	α-SiC‡
C_{11}	179.2	358.1	71.3	397
C_{12}	54.5	60.4	23.2	136

* Present study, ** Shao et al. (2012), † (Ding and Wang, 2013) and ‡ (Malakkal et al., 2017).

3. Results and discussions

3.1. Structural properties

The structure of SiC is as shown in Fig. 1. It is planar in structure like graphene with Si and C atoms arranged alternatively in a hexagon. A system with hexagonal symmetry can be represented by an orthorhombic non-primitive unitcell which was considered for the application of uniaxial stress and the simulation cell was compressed and elongated along ‘a’ and ‘b’ thus obtaining zigzag direction along ‘a’ and armchair direction along ‘b’ and for biaxial the original unitcell with two atoms was considered as shown in Fig. 1. If a and b are equal, equal amount of stress is required to impart same amount of deformation along both directions. If a and b are terminated at 90° (non-primitive unitcell), the amount of stress required to deform would be different leading to different physics.