Physica E 61 (2014) 40–47

Contents lists available at ScienceDirect

Physica E

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

Electronic and optical properties of silicene under uni-axial and bi-axial mechanical strains: A first principle study

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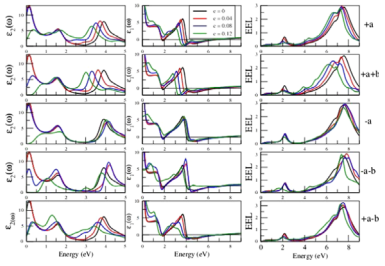
HIGHLIGHTS

- A direct band-gap of 389 meV is found for 6% of uni-axial compression.
- An indirect band-gap of 379 meV is found for 6% of bi-axial compression.
- The π plasmon in silicene disappeared with tensile and asymmetric strains.
- The $\pi+\sigma$ plasmons are red-shifted for tensile strains.
- The $\pi+\sigma$ plasmons are blue-shifted for compressive strains.

GRAPHICAL ABSTRACT

Dielectric response of uni-axial and bi-axial mechanically strained silicene with different types of strains at different magnitudes ($e=0$, 0.04, 0.08 and 0.12) is shown in figure.



ARTICLE INFO

Article history:
Received 21 August 2013
Received in revised form
14 January 2014
Accepted 11 March 2014
Available online 18 March 2014

Keywords:
DFT
Silicene
Electronic property
Dielectric property
Strain

ABSTRACT

The uni-axial and bi-axial mechanical strain mediated electronic band structures and dielectric properties of silicene have been investigated. It is found that on applying uni- and bi-axial strains, the band gap opens for smaller strain in silicene. However, on further increase of strain beyond 8% silicene changed into metal. The ultimate tensile strength estimated is 3.4 GPa. Imaginary part of dielectric function shows that the inter-band transitions are red-shifted for uni- and bi-axial tensile strains and are blue shifted for uni- and bi-axial compressive strains. Electron energy loss (EEL) function shows that the $\pi+\sigma$ plasmon energies are red-shifted for uni- and bi-axial strains and blue-shifted for compressive strains. The π plasmons disappears for tensile and asymmetric strains. Bi-axial asymmetric strain is found to have no influence on inter-band transitions and $\pi+\sigma$ plasmon energies.

1. Introduction

A two dimensional honeycomb lattice of carbon, graphene, has attracted researcher's attention due to its several exceptional properties. One of the graphene's standout properties is its inherent strength [1]. Due to the strength of its 1.42 Å long carbon bonds, graphene is the strongest material ever discovered, with an ultimate tensile strength of 130 GPa [2]. Graphene has been manipulated with strain [3,4] for its potential applications for nano-electronic devices. However, because of its incompatibility with silicon based nano-electronic industry, researchers proposed silicene [5–10], a two dimensional sheet of Si which is closely related to graphene. Theoretical studies [11–15] predict that the free standing silicene has a stable two dimensional buckled honeycomb structure. The buckling is due to the mixture of sp^2 and sp^3 hybridizations [7,10]. Silicene has also been experimentally realized on Ag(111) surface [16–19]. The band structure of buckled silicene has been theoretically found to be similar to that of graphene [20,21]. The absence of energy gap is the biggest obstacles for electronic applications.

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http://dx.doi.org/10.1016/j.physe.2014.03.013
1386-9477/

Therefore, the need for creating a band gap in silicene is the subject of intense investigations.

Previous studies have revealed that the mechanical strains effectively tune the band structure and optical properties of graphene and other two dimensional hexagonal structures [22–26]. The optical properties of silicene have been studied [21] since the realization of its two dimensional monolayer structure. A comprehensive study on the strain effects is promising which not only provides detailed information on the response of silicene to the strain but also helps explore their possible peculiar properties.

Although, electronic properties of silicene and its ribbons under strain have been studied recently by different researchers [27–32], but in this paper we have studied the silicene under both uni- and bi-axial tensile as well as compressive strains in systematic way to see their effect on electronic and dielectric properties. We have considered five different ways to apply the homogeneous strains namely uni-axial expansion $(+a)$, biaxial expansion $(+a+b)$, uni-axial compression $(-a)$, biaxial compression $(-a-b)$ and asymmetric biaxial $(+a-b)$ strain where 'a' is the magnitude of strain (e) along the direction of lattice parameter **a** while 'b' is the magnitude of strain (e) along the direction of lattice parameter **b**. However, in this study we have taken both a and b of equal magnitude. The strain dependent dielectric properties of silicene investigated here, to be best of our knowledge, have not been studied earlier.

2. Computational details

Calculations were performed by the SIESTA (Spanish Initiative for Electronic Simulation with Thousand of Atoms) code and method [33] by using an ab-initio pseudopotential based on density functional theory (DFT). We have used Troullier Martin, norm conserving relativistic pseudo-potential [34,35] in fully separable Kleinman and Bylander form. The exchange and correlation energies have been treated within the Local Density Approximation (LDA) according to the Ceperly and Alder (CA) parameterization. A sufficiently large 20 Å vacuum region was used to separate the two dimensional structures to rule out any interaction among the neighbouring layers along c-axis. Throughout geometry optimization, numerical atomic orbitals (NAOs) with double zeta polarization (DZP) basis set with confinement energy of 0.01 Ry were used. Minimization of energy was carried out using standard conjugate-gradients (CG) technique. Structures were relaxed until the forces on each atom were less than 0.01 eV/Å. A $10\times10\times1$ Monkhorst-Pack of k points was used for the Brillouin zone integration. The charge densities and the DFT potential were computed on the real space grid with equivalent plane-wave cutoff energy of 250 Ry.

SIESTA uses first order perturbation theory to calculate optical properties in which dipolar transition matrix elements between occupied and unoccupied single electron eigenstates were considered. Therefore, all the unoccupied states were used for the calculations of dielectric functions. The self-consistent ground state DFT energies and eigenfunctions were plugged into the dipolar transition matrix elements to introduce the exchange and correlation effects. The $90\times90\times3$ optical mesh points have been used for integration across Brillouin zone in the direction of reciprocal lattice vectors. Optical broadening of 0.2 eV was used for optical spectra. Although, including all the bands is computationally more expensive yet is the most accurate choice for optical calculations.

3. Results and discussions

The relaxed structure of silicene is shown in Fig. 1. The optimized lattice parameter $a=3.85$ Å and Si–Si bond length 2.28 Å with buckling parameter $\Delta=0.51$ Å have already been measured in our previous work [21]. These calculated lattice parameters have been used as a reference point for unstrained structure of silicene in this work for the electronic and dielectric property calculations of the strains. The strain is defined by $(e=\Delta a/a_0)$ as defined in previous paper [26]. The strained unit cell is modelled by applying tensile as well as compression strains by varying the lattice value 'a' with strain 'e' as $a\rightarrow ae$. The tensile strain was applied as uni-axial expansion in x direction $(+a)$ and biaxial expansion in x and y directions $(+a+b)$. Similarly, compression strains $(-a)$ and $(-a-b)$ were applied by uni-axial compression in x direction and biaxial compression in x and y directions respectively. These four configurations of strains are symmetric with same magnitude of the strain. Another configuration is also there, in which an asymmetric strain $(+a-b)$ is applied by expanding the lattice constant in x direction and compressing it in y direction by the same magnitude of the strains. The band structure has been calculated along $\Gamma-M-K-\Gamma$ high symmetric points of Brillouin zone for all configurations of strains.

3.1. Strain–stress relationship

The limit of strain to prevent breaking the sub-lattice symmetry has been obtained from the strain–stress relationship by calculating

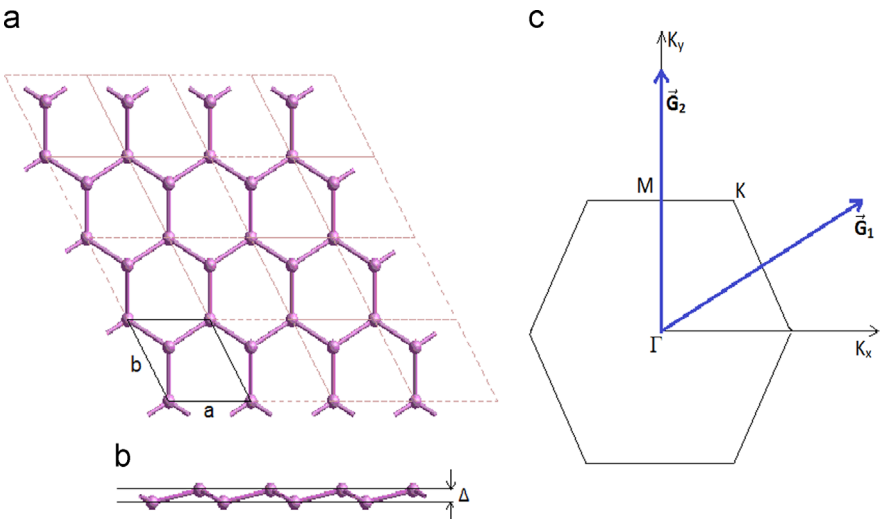

Fig. 1. (a) Top view and (b) side view of buckled silicene. (c) First Brillouin zone of silicene, where Γ, M and K are highly symmetric points.