Mechanics of Materials 89 (2015) 151–158

Contents lists available at ScienceDirect

Mechanics of Materials

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

Elastic properties and sound velocities of silicane/graphane hybrids

L.B. Drissi [a,b,*], K. Sadki [a]

[a] LPHE, Modeling & Simulations, Faculty of Science, Mohammed V University, Rabat, Morocco
[b] CPM, Center of Physics and Mathematics, Faculty of Science, Mohammed V University, Rabat, Morocco

ARTICLE INFO

Article history:
Received 6 January 2015
Received in revised form 24 April 2015
Available online 18 June 2015

Keywords:
Silicene-graphene
Ab initio calculations
Elastic constants
Anisotropic honeycomb structures
Mechanical stability
Sound velocities

ABSTRACT

Using ab initio density functional theory, the effect of hydrogen arrangement on the elastic properties of silicene–graphene hybrid is studied. Mechanical stability, elastic constants and sound velocities of pure and five configurations of hydrogenated SiC sheet, namely, chair, table, boat, zigzag and armchair, are explicitly examined. To reveal the anisotropic properties of the six structures, the polar plots of Young's modulus, Poisson ratio and acoustic waves speed are given. Compared to graphene, it is shown that all the isotropic systems are less stiffer with lower in-plane Young's modulus and stronger with their larger Poisson ratio, moreover, their compressional and shear waves propagate faster. The analysis of linear elastic behavior shows that the armchair configuration has an auxetic structure. The result of this work could be used for the design of future silicane–graphane based nanodevices with potentially large technological impact in nanomechanics.

© 2015 Elsevier Ltd. All rights reserved.

1. Introduction

Two dimensional systems, like graphene and silicene, have attracted a lot of interest (Geim and Novoselov, 2007; Aufray et al., 2010; Drissi et al., 2010) and the references therein due to their peculiar properties such as; massless Dirac fermion character (Novoselov et al., 2005; Cahangirov et al., 2009), unusual mechanical properties (Georgantzinos et al., 2010; Liu et al., 2011) and their capacity to store molecules. Oxygen (Dikin et al., 2007; Wang and Ding, 2013), hydrogen (Leenaerts et al., 2010; Lew et al., 2010), fluorine (Nair et al., 2010; Ding and Wang, 2012), halogens (Şahin and Ciraci, 2012; Zheng and Zhang, 2012), and other radicals have been used to decorate graphene and silicene sheets. The surface modification process is very interesting as it changes/adjusts the intrinsic properties of the 2D materials with possibly large impact in nanotechnology.

Attaching hydrogen atoms to each site of the carbon or silicon 2D lattices, in a strictly periodic manner, generates a set of new materials. The hydrogenated form of graphene (silicene) is referred to as graphane (Boukhvalov et al., 2008; Pujari et al., 2011) (silicane) (Houssa, 2011; Wang et al., 2012). Graphane was theoretically predicted in Sofo et al. (2007). Geim's and co-workers confirmed experimentally its formation using cold hydrogen plasma process for 2 h (Elias et al., 2009). The reaction of graphene with hydrogen is reversible since annealing graphane at 450 °C in Ar atmosphere for 24 h (Srinivasan and Saraswathi, 2009) leads to restore all the original properties of pristine graphene. This result renders graphane strong candidates as a prospective hydrogen-storage in applications.

Chemical modification with H atoms in 2D-materials changes the sp^2 hybridization to the sp^3 one. For both graphene and silicene, hydrogenation is an efficient way to

* Corresponding author at: LPHE, Modeling & Simulations, Faculty of Science, Mohammed V University, Rabat, Morocco.
E-mail address: ldrissi@fsr.ac.ma (L.B. Drissi).

http://dx.doi.org/10.1016/j.mechmat.2015.06.011
0167-6636/© 2015 Elsevier Ltd. All rights reserved.

open and control the fundamental band gap (Lew et al., 2010). It also tunes the magnetic properties of these materials (Zhou et al., 2009; Zhang et al., 2012) and affects their elastic properties (Cadelano et al., 2010; Zhao, 2012). In terms of tensile strength and elastic modulus, graphane exhibits smaller elastic constants compared to graphene that is one of the strongest and stiffest materials yet discovered (Lee et al., 2008). The in-plane stiffness and Poisson ratio of graphane are reduced by a factor of 27% and 56% respectively, in reference to graphene. Moreover, the value of the yield strain in graphane varies upon temperature and stoichiometry (Topsakal et al., 2010). Hydrogenation has less effect on ultimate tensile strengths of silicane. Its Young modulus and Poisson ratio are reduced by a factor of 16% and 26%, respectively in reference to pure silicene (Peng and De, 2014).

All the studies on graphene and silicene generate, at nanoscale, significant interest on combining between atoms to create SiC based nanostructures. SiC one-dimensional materials, in the form of nanorods have been successfully prepared for the first time through a reaction between carbon nanotubes and SiO (Dai et al., 1995). Showing outstanding mechanical properties, SiC nanorods were considered as a candidate for the reinforcing element in ceramic-, metal-, and polymer-matrix composites (Wong et al., 1971). SiC nanotubes (Sun et al., 2002; Mavrandonakis et al., 2003) and SiC nanowires (Pan et al., 2000) have been investigated as promising candidates for hydrogen storage, nanoelectronic and microelectromechanical systems (Gori et al., 2012). Narrow SiC zigzag nanoribbons was shown to be half-metal without any chemical modification or applied external electric field (Sun et al., 2008; Lou and Lee, 2009).

Recently, SiC sheet, the analog of graphene, has been studied (Sahin et al., 2009; Bekaroglu et al., 2010; Drissi et al., 2012). It is shown that mixing silicon and carbon atoms in alternating arrangement generates silicene/-graphene monolayer that is a 2-dimensional planar sheet with a sp^2 hybridization, at the expense of the sp^3 hybridization that is classically favored in silicon (Drissi et al., 2012). Instead of being a semimetal, silicene/-graphene hybrid has a large band gap due to the sublattice asymmetry in its honeycomb lattices. The analysis of optical absorption spectra reveals that the excitonic effects in silicene–graphene hybrid are significant and lead to strong bound excitons (Drissi and Ramadan, 2015). Theoretically, the full hydrogenation of 2D silicene/graphene sheet in chair configuration yields to a buckled system with an insulating character. However, partial H coverage has a reverse effect on the electronic structure of SiC hybrid as the gap is reduced in favor of ferromagnetism (Drissi et al., 2012). It is found that the arrangement of the adsorbed hydrogen atoms influences significantly the structural and electronic properties of silicane–graphane configurations, namely chair, boat, zigzag, armchair and table (Drissi et al., 2015). For instance, conversely to graphane and silicane, complete hydrogenation increases slightly the initial gap of pure SiC sheet. In Drissi et al. (2015), it is also found that, except the table configuration, all the five configurations of full hydrogenated SiC are exothermic adsorptions.

So motivated by the existence of five configurations of hydrogenated SiC sheet as well as by the interest of the determination of the elastic constants in applications where mechanical strength and durability are important, there is a compelling necessity to investigate the effect of different arrangement of hydrogen adsorbents on the elastic properties of SiC hybrid. Especially, it is worthy to analyze the elastic behavior of isotropic and anisotropic hydrogenated SiC systems and to calculate their sound velocities.

In the frame of density functional theory, this work reports in details Young modulus, Poisson ratio, speed of shear and longitudinal waves characterizing the five different structures of the full hydrogenated SiC sheet. It is shown that all the configurations are mechanically stable and that the armchair structure exhibits an auxetic behavior. It is found that because all the configurations result from an equal combination of 50% of Si–H and 50% of C–H, their linear elastic modulus intermediate between the ones of silicene and graphene. The results of sound velocities reveal that shear waves propagate in all the structures faster along x-direction compared to graphene.

This paper is organized as follows. Section 2 outlines the general computational setup adopted in the calculations. The results and analysis are reported in Section 3 followed by a conclusion.

2. Computational details

All the calculations have been performed within Quantum espresso (QE) simulation package (Giannozzi et al., 2009) and density functional theory (DFT) formalism employing generalized gradient approximation GGA-DFT of Perdew–Burke–Ernzrhof (PBE) exchange–correlation functional (Perdew et al., 1996). An ultra-soft pseudo-potential description of the electron–electron is used with $2s^2 2p^2$, $3s^2 3p^2$ and $1s^1$ valence electron configurations for C, Si and H atoms respectively. We apply a plane-wave basis set for the electronic wave functions and the charge density, with a kinetic energy cutoff of 40 Ry and 400 Ry respectively. We run the calculations for large supercell (6×4) with a large space of 18 Å along the z-direction to avoid interactions between adjacent atomic sheets. For calculations of the elastic constants obtained from the energy-vs-strain curves, we apply sets of deformations to the (6×4) supercell. For any deformation, the magnitude of the scalar strain parameter ζ (introduced in Eq. (2)) is increased in steps of 0.001 up to a maximum strain of 0.05 to warrant that the linear elastic regime is carefully explored.

3. Elastic properties

Using DFT-based calculations, we are interested in the effect of full hydrogenation on the elastic properties of the one-atom thick material made of silicon and carbon atoms. In each hexagon of the honeycomb lattice of the pure silicene–graphene hybrid, the C atoms occupy the sites of the sub-lattice A remaining the B-sites to Si atoms

Download English Version:

https://daneshyari.com/en/article/800172

Download Persian Version:

https://daneshyari.com/article/800172

Daneshyari.com