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The temperature effect on mechanical properties of silicon carbide sheet based on density functional treatment

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ABSTRACT

In the current work, mechanical properties of SiC graphene sheet and influence of temperature on those properties are studied. The purpose of this work is to investigate the temperature dependency of the Young's modulus and Bulk's modulus of SiC graphene sheet. To reach these goals, density functional theory (DFT) and quasi-harmonic approximation (QHA) methods are used to calculate energies of electrons and phonons, and consequently to obtain total energy of system. Results have been compared with existing data from literature and good agreement has been found. It is found that the effect of temperature on the mechanical properties of the SiC graphene sheet is significant.

1. Introduction

Carbon nanomaterials such as fullerene, graphene and carbon nanotube (CNT) have been extensively studied and used as sensors, catalyst, biomaterials and biomedicine systems [1–4]. Amongst those materials, graphene has been of special interest recently. It was discovered in 2004 by Novoselov and Geim and colleagues [5], and has attracted attention as a zero band gap, sp^2 – hybridized carbon atoms in a honeycomb-like lattice material with high stability [6,7]. It is a two-dimensional form of carbon, including single layer of atoms in a hexagonal array. It is a promising candidate material to be used in variety of applications such as nanosensor [8], electronic application [9], lithium-ion batteries [10], light emitting devices [11] and mechanical resonators [12]. In comparison with CNT, much fewer studies have been carried out on graphene.

SiC graphene sheet is fascinating for its high thermal and mechanical properties, and also its chemical stability which makes it potentially can be used in harsh environments. Due to its excellent properties, the SiC sheet has been considered as chemical gas sensors [13,14]. Several works have been reported on the mechanical properties of Graphene sheet in the literature [15–26]. One of the most important types of mechanical properties is Young's modulus. Young's modulus and residual stress are key mechanical properties for the design of devices. The values of Young's modulus and residual stress for graphene are ranging between 100–400 GPa and 98–486 MPa, respectively. They mainly determine the stiffness of the material and show the ratio between the uniaxial stress and the uniaxial strain.

Jiang et al. used molecular dynamic (MD) simulation to investigate the Young's modulus of graphene [27]. Ansari et al. investigated the mechanical properties of graphene by using an ab initio treatment [28]. Frank et al. assigned the effective spring constants for stacks of Graphene sheet by using atomic force microscope (AFM) method and obtained a Young's modulus [19]. Li and Chou studied the elastic behavior of multilayered graphene sheet (MLGS) by using molecular mechanic method [29]. In general, computational simulation for predicting mechanical properties of SiC graphene sheets has been known as a powerful tool in comparison with the experimental techniques [30].

Andrew et al. studied the stability of crystalline silicon dicarbide based on density functional theory [31]. Ju Li et al. investigated transformation strain by chemical disordering in silicon carbide [32] and obtained the value of Bulk modules. On the other hand, jappor determined the value of bulk modules experimentally [33]. The values of bulk modulus of SiC are ranging between 200 and 250 GPa for both theoretical and experimental research.

In this work, the Young's and Bulk's modules of the SiC sheets, and their temperature dependency are studied using density functional theory (DFT) and quasi-harmonic

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approximation (QHA), and compared with the existing data in the literature. Bulk modulus is calculated as the second derivative of the total strain energy with respect to the area of SiC sheet graphene.

2. Computational details

Structure optimization and minimized energy were calculated by using density functional theory (DFT) method and phonons energies were determined by the QHA [34,35]. All calculations have been performed using PWscf code, distributed with the Quantum ESPRESSO package [36] which is implemented with plane-wave and pseudo-potential techniques [37]. Generalized gradient approximation (GGA) of the density functional theory is used to approximate exchange-correlation potential with Perdew–Burke–Ernzerhof (PBE) parametrization [38]. The utilization of GGA functionals are important, especially for successful description of physical properties of magnesium chalcogenides [39]. The phonon properties for optimized structure are studied by using density functional perturbation theory (DFPT) [40]. Monkhorst–Pack K point meshes of $20\times20\times1$ unit cell were used for Brillouin zone integration for optimized structure [41]. In the case of SiC sheet, a hexagonal unit cell with the optimized lattice constant $a=b=3.09$ and $c=20$ and Si–C bond length of 1.78 Å were used. In order to obtain complete phonon dispersions, dynamic matrices were calculated on a $4\times4\times1$ q-point mesh. Dynamic matrices are evaluated by means of a Fourier deconvolution at random wave vector checks. Cut-off energy for plane wave expansion was selected to be 60 Ry and the strained structure is optimized until the residual force is smaller than of 0.6 Ry/au.

3. Results and discussion

The aim of this paper is to focus on the mechanical properties (Young's and Bulk modulus) of SiC graphene sheet and their temperature dependency.

In order to do this, the total energy of SiC graphene is assumed as summation of the energies of the electrons and the phonons. The phonon energy is calculated by using the QHA code [35] which is based on the minimization of Helmholtz free energy with respect to the variations of all likely internal degrees of freedom [42]. Fig. 1 shows schematic of optimized SiC graphene sheet and its unit cell parameters. All atomic positions and lattice parameters are presented in Table 1. In Fig. 2, a schematic of relaxed graphene for calculation of the Young's and Bulk modulus is presented. Young's modulus is defined as the second derivate of the energy with respect to the applied strain [43].

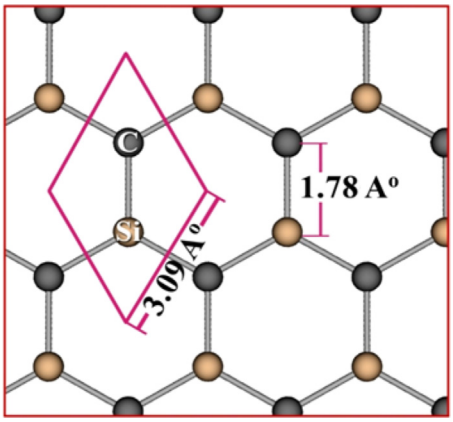

Fig. 1. Schematic representation of optimized SiC graphene sheet and unit cell parameters. (brown and gray atoms belong to Si and C atoms, respectively). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article).

$$Y_s=\left(\frac{1}{A_0}\right)\times\left(\frac{\partial {E_S}^2}{\partial \epsilon^2}\right) \tag{1}$$

where A_0 and E_S are equilibrium area and total energy (electronic and phonon energy) of the structure respectively, and ε is applied strain. The strain energy at each strain level is obtained by calculating the potential energy of the strained system minus the potential energy of the relaxed system. The Young's modulus could be extracted by calculating slope of linear part of engineering stress–true strain results. By fitting a parabola, $0.5\alpha x^2+\beta x+c$ to the strain energy at the low strain levels, the Young's modulus can be calculated as $Y_s=\left(\frac{1}{A_0}\right)\alpha$.

Poisson's ratio for SiC graphene sheet is explained as ratio of the transverse strain to the axial strain calculated from the following equation [44]:

$$\upsilon=\frac{-\epsilon_{\text{trans}}}{\epsilon_{\text{axial}}} \tag{2}$$

Results show that Poisson's ratio of a SiC graphene sheet is independent of the strain.

As shown in Fig. 3, to obtain the Young's modulus, structural relaxations for the SiC graphene sheet is performed with the applied strain in the harmonic region range is $-0.02<\varepsilon<+0.02$. Next, the Young's modulus is calculated with Eq. (1). According to these calculations, the value of Young's modulus and Poisson's ratio are measured as 185.435 Pa m (N/m) (550 GPa) and 0.317, respectively. The calculated value for the Young's modulus and Poisson's ratio of SiC graphene sheet was consistent with the values of 166 Pa m (N/m) and 0.29 reported in [44] which confirms the reliability of the current method. The high value of the Young's modulus, emphasizes that it could be a good candidate material for the design of future nanodevices.

According to Fig. 4, the maximum value of Young's modulus has a peak around 100 K, and then drop off slightly while the temperature increased additionally. At 800 K, it remains constant. By increasing the temperature around 500 K, the derivative of in-plane stiffness reaches a constant value. In higher temperatures, the variation between phonon energies of strained structures is disappearing and the phonon energy leans to a constant value.

Fig. 5 exhibits the variations of phonon energy versus temperature for the relaxed and strained SiC graphene sheet. In Fig. 5, the phonon energy is presented as a function of the temperature. It is calculated by the equation below:

$$E_{\text{Ph}}=\sum_q \hbar\omega_q\left[\exp\left(\frac{\hbar\omega_q}{k_BT}\right)-1\right]^{-1} \tag{3}$$

where k_BT is the Boltzmann's constant and ω_q is the vibrational frequency. It is observed that as the temperature increases, the phonon energy increases too. Therefore, in lower temperatures, the slope of the curve is more moderate than at higher temperatures. This means the phonon energy is more dependent on temperature at higher temperature than lower temperatures.

Results for the value of the Young's modulus indicate that the value is about 180 (N/m) (529 GPa) in the current work in the room temperature, which is around 23% higher than that value for graphene with the value 407 GPa reported in [45]. However,