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Elastic Constants and Elastic Moduli of Silicon Carbide Nanosheet

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Abstract

2-Dmensional silicon carbide (2D SiC) provides several advantages compared to the bulk silicon carbide, due to its two-dimensional structure. Elastic constants and elastic moduli of 2D carbide nanotubes were calculated employing density functional theory (DFT). There are six independent elastic constants for tetragonal lattice with (422, 4mm, -42/m, 4/mmm) point group. The calculated c_{11}, c_{12}, c_{13}, c_{33}, c_{44}, c_{66} of 2D SiC are reported in this work. The results suggest that the shear modulus of 2D SiC is 27.78 GPa, which is lower than that of the of single layered graphene sheet (=0.22 TPa). The bulk modulus of 2D SiC is 44.98 GPa as well. Moreover, Young's modulus of 2D SiC is lower than Young's modulus of single layered graphene sheet. Compared to Young's modulus of the amorphous phase of the SiC (=313.6 GPa), Young's modulus of 2D SiC (=156.19 GPa) is smaller. The main reason is that the stiffness of the 2D SiC in the x direction is smaller than the stiffness of the bulk SiC.

1. Introduction

Silicon carbide nanolayer (2D SiC) provides several advantages compared to the bulk silicon carbide, such as the capability of indirect-to-direct bandgap transition as the material changes from multilayer to monolayer, due to its two-dimensional structure. SiC is a promising nanomaterial in electronics, optics, optoelectronics, and the solar cell industry [1-3]. Cubic SiC is usually grown by the process of Chemical Vapor Deposition (CVD) of silicon hydride, nitrogen, and hydrogen [4]. Moreover, heteroepitaxial and homoepitaxial SiC layers can be grown using both liquid and gas phase approaches [5]. Silicon carbide can be exploited in the production of graphene due to their properties that promote the epitaxial production of graphene on the surface of SiC nanostructures.

2D silicon carbide may be a promising option in the semiconductor industry. The carbon and silicon atoms in 2D silicon carbide, just like these in graphene or silicene, are arranged in a 2D hexagonal lattice, with the difference being that 2D silicon carbide has a semiconducting behavior [6]. The effective elastic modulus of multiphase and multilayer silicon carbide ceramic matrix composite have been predicted by Xu, Zhang, and Wang [7]. In addition, the elastic constants of silicon carbide have been simulated by Kamitani et al. [8]. The elastic modulus of both vacancy defected 2D-SiC has been reported as well [9]. In this work, we intend to calculate the elastic constants of the infinite silicon carbide sheet (2D-SiC).

The ongoing study, including promising results, gives some hints to peruse the elastic and mechanical properties of 2D SiC.

2. Materials and Methods

2.1 *Computational details*

We have simulated the elastic and mechanical properties of 2D SiC by using the DFT method as implemented in the WIEN2k code. The calculation has been conducted via Generalized Gradient Approximation (PBE-GGA) to solving Kohn-Sham equations [10-12]. In order to reach energy eigenvalues convergence, the energy separating the valance state from the core state has been considered -9.0 Ry. The wave functions in the interstitial region were expanded in plane waves; therefore, the optimized cut-off K_{max} (the largest K vector in the plane wave expansion) was obtained for 5.5/RMT (RMT stands for the smallest atomic muffin-tin sphere radius).

The magnitude of largest vector in charge density Fourier expansion (G_{max}) and muffin-tin radius (R_{MT}) were optimized to 12 $a.u.^{-1}$ and 1.30 a.u., respectively. The k-point mesh of 20 × 20 × 1 was considered, tetragonal unit cell was chosen as a 2D SiC crystal lattice, and x-direction was selected as the normal vector of the plane; see Figure 1. The unite cell parameters are a=10 Å, b=10.8 Å, and c=3.11 Å.

3. Results and Discussion

Experiments suggest that the elastic constants in each class of solids, follow a simple inverse fourth power law with the lattice constants [13], so the simulated lattice constants of 2D SiC depend strongly on the artificial vacuum space volume. It is worth mentioning that the reduction of the vacuum space volume eventuates in increasing the interactions between the infinite nanolayers.

There are six independent elastic constants for tetragonal lattice with (422, 4mm, -42/m, 4/mmm) point group. The calculated c_{11}, c_{12}, c_{13}, c_{33}, c_{44}, c_{66} of 2D SiC are given in Table 1. In addition, the elastic constants of the bulk SiC are written in the table for comparison. Besides, these constants are not studied in reference [14] or other relevant reports.

There are no experimental and theoretical elastic constants of 2D SiC available to compare our data with. Using these constants, elastic moduli would be calculated in the present study.

From the data, it is clear that the quantum size effect in the nano dimension results in the difference between the elastic constants of the 2D SiC and bulk SiC.

The bulk modulus (B) of a substance describes the elastic properties of a solid or fluid when it is under pressure on all surfaces. It is defined as the ratio of the infinitesimal pressure increase to the resulting in the relative decrease of the volume [16]. The bulk modulus of 2D SiC is 44.98 GP (GP stands for Giga Pascal).

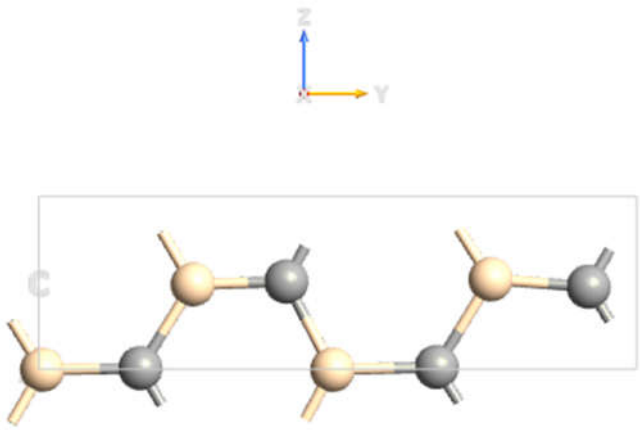

Figure 1: Artificial model of 2D SiC. The silicon and carbon elements are represented by yellow and gray spheres, respectively

Table 1: Elastic constants of 2D SiC. We have calculated these parameters after the optimization of the crystal lattice. These parameters are written from the output file of the simulation

Material	c_{11} (GPa)	c_{12} (GPa)	c_{13} (GPa)	c_{33} (GPa)	c_{44} (GPa)	c_{66} (GPa)
2D SiC	0.01	135.77	0.03	173.98	51.50	0.09
Bulk SiC [15]	4.79	0.98	0.55	5.21	1.48	1.90

The shear modulus (G) is a measure of the elastic shear stiffness of a material (τ) and is defined as the ratio of the shear stress (τ) to the shear strain (γ):

$$G = \frac{\tau_{xy}}{\gamma_{xy}} \quad (1)$$

Based on our simulation, the shear modulus of 2D SiC is 27.78 GPa. The shear modulus of a single layered graphene sheet is 0.22 TPa [17].

The Young's modulus (E) is a mechanical property that measures the tensile or compressive stiffness of a solid material when the force is applied lengthwise. It quantifies the relationship between tensile/compressive stress (σ) (force per unit area) and axial strain (ε) in the linear elastic region of a material and is determined using the formula [18-20]

$$E = \frac{\sigma}{\varepsilon} \quad (2)$$

We have calculated these elastic moduli after the optimization of the crystal lattice.

The calculated Young's modulus of 2D SiC is equal to 156.19 GPa. This output is lower than Young's modulus of single layered graphene sheet (=1.04 TPa) [17]. Moreover, compared to Young's modulus of the amorphous phase of the SiC (=313.6 GPa) [21], Young's modulus of 2D SiC (=156.19 GPa) is smaller. The main reason is that the stiffness of the 2D SiC in the x direction is smaller than the stiffness of the bulk SiC. Most importantly, the calculated Young's modulus and shear modulus are written from the output file of the simulation.

4. Conclusions

FP-LAPW calculation via GGA approach for the exchange-correlation potential has been used to calculate the elastic constants and mechanical properties of 2D SiC. Based on our simulation, the bulk modulus and shear modulus of 2D SiC are 44.98 GPa and 27.78 GPa, respectively. The shear modulus of a single layered graphene sheet is 0.22 TPa. The results predicted that Young's modulus of 2D SiC is 156.19 GPa as well. Moreover, compared to Young's modulus of the amorphous phase of the SiC (=313.6 GPa), Young's modulus of 2D SiC (=156.19 GPa) is smaller. The main reason is that the stiffness of the 2D SiC in the x direction is smaller than the stiffness of the bulk SiC. Most importantly, the calculated Young's modulus and shear modulus are written from the output file of the simulation.

Conflicts of Interest

The authors declare that they have no conflict of interest.

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