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Elastic and electronic properties of M585 carbon under pressure

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ABSTRACT

First-principles calculations were performed to study the elastic properties and electronic properties of M585 carbon under pressure. The obtained values are in accord with previous theoretical data. The calculated elastic constants indicate that M585 monoclinic carbon crystal is mechanically stable. Using the Voigte-Reusse-Hill method, elastic properties such as bulk modulus B, shear modulus G, Young's modulus E and Poisson's ratio σ under pressure have been investigated. It is observed that the M585 carbon should be classified as brittle material and possesses elastically anisotropic. The calculated Vicker's hardness of M585 carbon was 86.43 GPa, which indicates that it is a superhard material. The Debye temperature Θ_D calculated from elastic constants go up with the increasing pressure.

1. Introduction

Superhard materials are widely used in the modern industry as the cutting, polishing, drilling tools and surface protecting coatings due to their superior mechanical properties [1,2]. In recent years, it has attracted great interest to search for superhard carbon allotropes. Many superhard carbon phases have been proposed such as H-carbon [3], orthorhombic O-carbon [4], F-carbon [5–7], monoclinic M-carbon [8,9],C2/m-carbon [10], bct-C4 [11–13], W-carbon [14], Z-carbon [15–17], S-carbon [3,18], P222$_1$-carbon [19,20] and so on, and they possess significant stability. He et al. [3] proposed two new superhard carbon phases (H-carbon and S-carbon) in the process of cold compressing graphite. They are both more stable than M-carbon and W-carbon. The transition pressure of H-carbon and S-carbon from cold compressing graphite is 10.08 GPa and 5.93 GPa, respectively. An orthorhombic O-carbon via compressing graphite were investigated by Wang et al. [4]. It is dynamically stable and more favorable than other compressed graphite phases. F-carbon [5] has a gap of 4.55 eV at 15 GPa and its hardness is 93.9 GPa at zero pressure. It is a transparent superhard carbon. Oganov [8] firstly proposed M-carbon, and then Li et al. [9] reported it as a metastable low-energy polymorph. M-carbon can be synthesized by cold-compressing graphite above 13.4 GPa and its hardness is calculated to be 83.1 GPa. Xing et al. [10] calculated the structural, mechanical, and electronic properties of C2/m-carbon. They found that C2/m-carbon is an indirect band gap semiconductor with a gap of

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4.197 eV. Umemoto et al. [11] investigated the electronic, vibrational, and structural properties of bct-C4. This new carbon phase was found in molecular dynamics simulations of carbon nanotubes under pressure. It is transparent and dynamically stable at zero pressure. Above 18.6 GPa, bct-C4 is more stable than graphite. Orthorhombic W-carbon [14] was predicted in 2011, which possesses transparent and superhard properties as a potential product of cold-compressing graphite. Meanwhile, W-carbon is more stable than M-carbon and bct-C4 due to its lower enthalpy. Zhang et al. [19] report a new superhard carbon allotrope with orthorhombic $P222_1$ symmetry. Then Xing et al. [20] perform detailed first-principles calculations of the crystal structure, mechanical, elastic anisotropy, and electronic properties of $P222_1$-carbon. It is an indirect semiconductor with a band gap of 3.423 eV.

In addition to the above mentioned superhard carbon phases, a monoclinic carbon phase named M585 has been proposed in Ref [21], which consists of a 5–8–5 carbon rings linear boundary. Such a linear 5–8–5 carbon rings topology manner has never appeared in previous carbon phases. The structural, electronic and mechanical properties of M585 at ambient pressure have been investigated with first-principles calculations, but elastic and thermodynamic properties of M585 under pressure have never been investigated. In this work, we systematically investigate the stability, electronic structure, elastic modulus, hardness and thermodynamic properties of M585 under pressure.

2. Computational details and theory

The structural optimization and property predictions of the M585 polymorphs were performed using the plane-wave pseudopotential density functional theory (DFT) [22,23], with the generalized gradient approximation (GGA) parameterized by Perdew, Burke and Ernzerrof (PBE) [24] in the Cambridge Serial Total Energy Package (CASTEP) code [25]. Vanderbilt type non-local ultrasoft pseudopotentials [26] are employed to describe the electron–ion interactions. In the structure calculation, a plane-wave basis with energy cut-off 400 eV is used to consider convergence tests. Pseudo-atomic calculations are performed for C, where the $2s^2 2p^2$ are treated as valence electrons. The proper k-point grid ($4 \times 16 \times 9$) in the Brillouin zone is obtained with respect to the Monkhorst–Pack method [27]. The Broyden–Fletcher–Goldfarb–Shanno (BFGS) [28] minimization scheme was used in geometry optimization to find the lowest energy structure. All the structural optimizations and properties are under hydrostatic pressure which ranges from 0 to 100 GPa with a step of 10 GPa. The system reaches the ground state via self-consistent calculation when the total energy is stable less than 5×10^{-6} eV/atom, the maximum displacement of atoms during the geometry optimization is 0.01 eV/Å, the maximum ionic Hellmann-Feynman displacement within 5×10^{-4} Å and the maximum stress within 0.02 GPa.

3. Results and discussions

The M585 carbon (space group P21/m) has eighteen carbon atoms in the unit cell. The optimized structural and lattice parameters of M585 at 0 GPa are tabulated in Fig. 1 and Table 1, together with the previous theoretical results [21] for comparison. It is shown that our calculated results are consistent with previous theoretical values, which indicate that the proposed computational methodology in this work is available and the simulative results are reliable. In order to study the structural change under pressure, variations of the lattice parameters (a/a_0, b/b_0 and c/c_0) and unit cell volume (V/V_0) under pressure in the range of 0–100 GPa are calculated. The results are illustrated in Fig. 2. The ratio c/c_0 decreases more rapidly than a/a_0, b/b_0, which suggests that the c-axis is more compressible than a- and b-axes. Meanwhile, the unit cell volume V/V_0 of M585 changes between c-BN and diamond as the applied pressure increases, which predicts the incompressibility of M585 is slightly larger than c-BN and little smaller than diamond. It tends to be more difficult to further compression under pressure due to the distance between atoms reducing and the repulsive interaction between atoms strengthening.

The band structures of M585 carbon at 0 GPa and 100 GPa are shown in Fig. 3. The dashed line represents the Fermi level (E_F). The valence band maximum (VBM) and conduction band minimum (CBM) are at G point and D point, respectively. The Fermi level is 9.822 eV at 0 GPa and it increases to 12.640ev at 100 GPa. The value of VBM (CBM) is 9.881 eV (14.087 eV) at

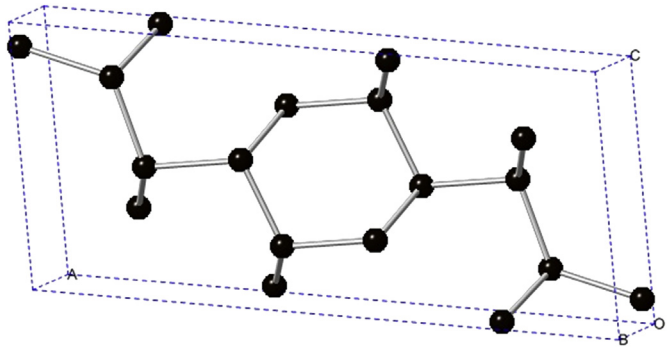

Fig. 1. Prespective view of M585 in its monoclinic crystalline cell.