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Mechanical and electronic properties of Si–Ge alloy in *Cmmm* structure

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ABSTRACT

Using the density functional theory, a first-principles calculation for a novel orthorhombic structure (z-phase) property of silicon, germanium and their alloy $Si_{0.5}Ge_{0.5}$ is carried out in this work. The crystal structure is optimized to be in agreement with existing results, and based on this, the elastic properties including elastic constants and moduli are calculated, satisfying the elastic stability criteria. The anisotropic properties are represented by multiple anisotropic factors and linear bulk moduli, and the results indicate z-phase $Si_{0.5}Ge_{0.5}$ performs slight anisotropy in the *c*-axis direction. Besides, solid sound velocities in different propagation orientations and modes as well as Debye temperature are predicted using elastic moduli. At last, the band structure and density of states of z-phase $Si_{0.5}Ge_{0.5}$ are calculated, and comes out z-phase $Si_{0.5}Ge_{0.5}$ is indirect band semiconductor with a narrow band gap.

1. Introduction

In recent decades, germanium-silicon alloy is widely used in a variety of areas due to its unique properties differ from simple silicon and germanium. For instance, the lattice mismatch resulting from the crystal constant discrepancy between silicon and germanium lead to lattice strain, stress and in turn deformation, which is applied to enhance carriers' mobility in complementary metal oxide semiconductor process [1]. The band width of SiGe is adjustable exactly by changing the composition of Si and Ge, therefore the band can be bended properly, and it is beneficial in heterojunction bipolar transistor manufacture [2]. In addition, silicon germanium is also adopted in photoelectron field especially for solar cell, due to smaller band width and higher mobility, so that a higher coefficient of light absorption and photoelectric conversion efficiency are obtained, and performs better in short wave utilization comparing with traditional monocrystalline silicon battery [3]. Since the extensive application of Si–Ge alloy, more and more theoretically investigations on its properties are carried out. Karl Brunner [4] reviewed the formation mechanism, heterostructure band structure, quantum well structure and their properties of Si–Ge alloy. Zhu et al. [5] discussed the heat capacity, Debye temperature and thermal expansion coefficient of ordered and disordered structures SiGe using density functional theory. Hao et al. [6] calculated the electronic and elastic properties of

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SiGe under high pressure, and come up with a pressure-induced structure transition to explain the available experimental results and the previous theoretical data.

On the other hand, the exploration for new structural SiGematerial has gotten much attention in these years. Iori et al. [7] presented a first principle prediction aiming at SiGe nanowire, and the discovered calculated structural properties along with band gap, to some extent, satisfying with Vegard's law accurately. Zhou et al. [8] investigated the role of vacancies in four distinct SiGe nanowire. Zhang et al. [9] explored the structural, electronic and magnetic properties of low-dimensional zigzag SiGenanoribbon material with different edge modifications. Zhou et al. [10] proposed a new kind of Dirac-fermion monolayer SiGe material analog of silicene, and proved the kinetic stability and energetic stability. Zhang et al. [11] calculated the structural stability, elastic properties, dynamical and thermodynamic properties for Si–Ge, Si–Sn and Ge–Sn zinc-blende structure alloy. Amsler et al. [12] came up with a new carbon allotrope structure (z-phase) to explain experimental x-ray diffraction and Raman spectra of graphite under pressure, while Bautista-Hernández et al. [13] calculated the structural properties, vibrational properties, elastic properties and electronic properties of z-phase Si and Ge, and demonstrated the probability of existing.

In the present work the structure of z-phase $Si_{0.5}Ge_{0.5}$ is built up at first, and based on this, the elastic constants, elastic moduli, Poisson ratios and Vickers hardnesses are calculated. The anisotropic properties are investigated by means of elastic anisotropy index, and the solid sound velocities along different crystal orientation and Debye temperatures are obtained within elastic constants and moduli. At last, the electronic properties including band structure and density of states of $Si_{0.5}Ge_{0.5}$ are calculated and discussed.

2. Computational method

In the study of the properties of Si–Ge alloys, a first principle calculation was adopted using the density functional theory (DFT) [14,15], integrated in Cambridge sequential total energy package [16]. The structure optimization and the theoretical modeling were carried out with exchange-correlation functional described by the Local Density Approximation (LDA) based on the Ceperley and Alder data as parameterized by Perdew and Zunger(CA-PZ) [17,18] and the generalized gradient approximation (GGA) proposed by Perdew, Burke and Ernzerhof (PBE) [19], Wu and Cohen (WC) [20], and PBE for solid (PBEsol) [21] to compare the deviation resulted from different functionals [22]. Besides, diamond-Si and Ge are also calculated with comparison to experimental data to ensure the reliability in this work. In order to approximate the interaction between atomic core with inner electrons and valence electrons, ultrasoft pseudo potentials were adopted. The cut-off energy for plane wave was set to be 340 eV and 260 eV for Si ($Si_{0.5}Ge_{0.5}$) and Ge after convergence test, and the first irreducible Brillouin zones [23] were meshed into 0.025 1/Åby $3 \times 6 \times 10$ and $8 \times 8 \times 8$ Monkhorst-Pack [24] grid k-points for orthorhombic structure and diamond-like silicon (germanium), respectively. The Broyden-Fletcher-Goldfarb-Shanno algorithm [25] was used in structure optimization. The convergence tolerance and SCF (self-consistent field) tolerance were set as 5×10^{-6} eV/atom and 5×10^{-7} eV/atom, respectively. The maximum force, the maximum stress and the maximum displacement on atom were restricted to be 0.01 eV/Å, 0.02 GPa and 5×10^{-4} Å, respectively.

3. Results and discussion

The crystal structural diagrams of $Si_{0.5}Ge_{0.5}$ are depicted in Fig. 1. The z-phase $Si_{1-x}Ge_x$ belong to orthorhombic symmetry, with the space group of *Cmmm*, and have 16 atoms in a conventional cell, while each atom forms sp^3 bonds with adjacent 4 atoms. The optimized lattice parameters calculated by method PBE, PBEsol, WC, and CA-PZ with reference data are shown in Table 1, and the calculated parameters are in good agreement with other results, while the lattice parameters increase with the composition *x*'s increasing as Fig. 2 shows. We also calculated diamond-Si and Ge, and the lattice constants are consistent with experimental data [26,27] with a maximum errors in 1.5%. Besides, an obvious bias occurs between GGA and LDA method, due to the underestimation of lattice parameters in LDA method compared with GGA, generally.

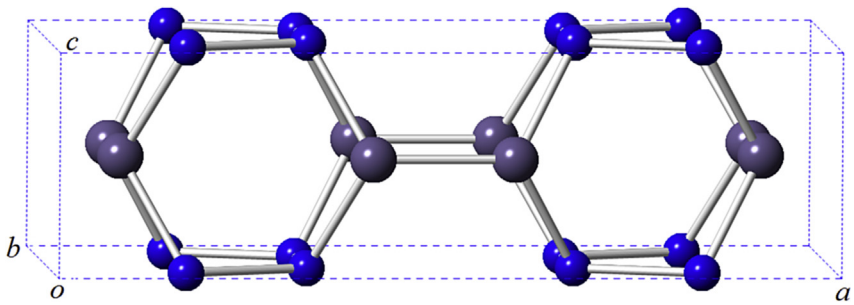

Fig. 1. Conventional cell structure of z-phase $Si_{0.5}Ge_{0.5}$, blue and grey spheres represent Si and Ge atoms, respectively.