Theoretical Investigations of Si-Ge Alloys in $P4_2/ncm$ Phase: First-Principles Calculations

Zhenyang Ma *, Xuhong Liu, Xinhai Yu, Chunlei Shi and Fang Yan

Tianjin Key Laboratory for Civil Aircraft Airworthiness and Maintenance, Civil Aviation University of China, Tianjin 300300, China; hxliu@126.com (X.L.); xhyucauc@126.com (X.Y.); clshi01@126.com (C.S.); fyancauc@126.com (F.Y.)
* Correspondence: zyma@cauc.edu.cn; Tel.: +86-22-2409-2287

Abstract: The structural, mechanical, anisotropic, electronic and thermal properties of Si, $Si_{0.667}Ge_{0.333}$, $Si_{0.333}Ge_{0.667}$ and Ge in $P4_2/ncm$ phase are investigated in this work. The calculations have been performed with an ultra-soft pseudopotential by using the generalized gradient approximation and local density approximation in the framework of density functional theory. The achieved results for the lattice constants and band gaps of $P4_2/ncm$-Si and $P4_2/ncm$-Ge in this research have good accordance with other results. The calculated elastic constants and elastic moduli of the Si, $Si_{0.667}Ge_{0.333}$, $Si_{0.333}Ge_{0.667}$ and Ge in $P4_2/ncm$ phase are better than that of the Si, $Si_{0.667}Ge_{0.333}$, $Si_{0.333}Ge_{0.667}$ and Ge in $P4_2/mnm$ phase. The Si, $Si_{0.667}Ge_{0.333}$, $Si_{0.333}Ge_{0.667}$ and Ge in $P4_2/ncm$ phase exhibit varying degrees of mechanical anisotropic properties in Poisson’s ratio, shear modulus, Young’s modulus, and universal anisotropic index. The band structures of the Si, $Si_{0.667}Ge_{0.333}$, $Si_{0.333}Ge_{0.667}$ and Ge in $P4_2/ncm$ phase show that they are all indirect band gap semiconductors with band gap of 1.46 eV, 1.25 eV, 1.36 eV and 1.00 eV, respectively. In addition, we also found that the minimum thermal conductivity $\kappa_{\text{min}}$ of the Si, $Si_{0.667}Ge_{0.333}$, $Si_{0.333}Ge_{0.667}$ and Ge in $P4_2/ncm$ phase exhibit different degrees of anisotropic properties in (001), (010), (100) and (010) planes.

Keywords: Si-Ge alloys; mechanical properties; anisotropic properties; electronic properties

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1. Introduction

As the most widely used semiconductor material, diamond silicon has many advantages: silicon is abundant in the earth, so the manufacturing cost is lower than that of other semiconductor materials; the diamond silicon purification process has been developed for several decades and has reached the highest level of human beings; there is extensive research on the doping and diffusion of silicon, and much experience has been gained. However, the electron and the hole mobility of diamond silicon is lower than that of other semiconductor materials, so it is difficult to meet the demand of higher performance semiconductor devices in the future. Diamond silicon belongs to indirect band-gap semiconductor materials, as light emission efficiency is not high enough. The inventions of the first transistor and the first IC (integrated circuit) based on the diamond germanium brung us two Nobel Prizes. The hole mobility of diamond germanium is four times that of diamond silicon and the electron mobility is about two times that of diamond silicon; the band gap of diamond germanium is relatively small, which is beneficial to the development of low voltage devices and the reduction of current leakage. However, diamond germanium belongs to active material. The defect of GeO is generated because redox reaction occurs easily on the dielectric material interface, along with other defects, so the performance of diamond germanium is significantly affected. In addition,
the GeOI (germanium-on-insulator) technology is necessary for the development of future devices because diamond germanium cannot be directly used as substrate. Though this technology has some difficulties, it is generally believed that these difficulties will be overcome by researching diamond silicon material in the near future. With the goal of improving the performance of semiconductor devices, reducing power consumption and designing advanced microelectronic applications, diamond silicon is no longer able to meet the demand.

In order to solve this problem, more and more new phases of silicon and germanium with direct band gaps and better light absorption are studied [1–10]. In addition, the theme of new phases of Si-Ge alloys research [11–15] is of significant importance since new types of Si-Ge crystals are keys to the next generation devices. Si$_1$Ge$_x$ alloys have been studied a lot in recent years due to their applications in both the optoelectronics and microelectronics industry. Zhang et al. [12] investigated the structural stability, dynamical, elastic and thermodynamic properties of Si–Ge, Si–Sn and Ge–Sn alloys in zinc blende structure by using first-principles calculations. The calculated cohesive energies and formation energies indicate that Si–Ge has the highest structural stability and Ge–Sn has the strongest alloying ability. Zhu et al. [13] investigated the structure, formation energy, and thermodynamic properties of Si$_{0.5}$Ge$_{0.5}$ alloys in zinc blende phase and rhombohedra phase through first-principles calculations. Bautista-Hernandez et al. [16] found a stable structure of silicon and germanium in the monoclinic (M phase) and orthorhombic structures (Z phase), respectively. From these works, both the M and Z phases happen to be mechanically and dynamically stable and the energy of these two phases for Si and Ge are slightly larger than that of Si and Ge in diamond structure. Therefore, these phases can be synthetized at room temperature. Using first-principles calculations, a new orthorhombic structure (Z-phase) property of Si$_{0.5}$Ge$_{0.5}$ alloy is carried out by Zhang et al. [17]. However, the Si$_{0.5}$Ge$_{0.5}$ alloy in the Z-phase is also an indirect semiconductor. A systematic density functional theory calculation has been performed on Si$_{12}$Ge$_{12}$ and Si–Ge alloys in P4$_2$/mma phase by Fan et al. [18], including the stability, mechanical properties, anisotropic properties and electronic properties. The electronic structure calculations using the alloys are calculated by Heyd–Scuseria–Ernzerhof (HSE06) hybrid functionals, and reveal that Si$_{12}$ in P4$_2$/mma phase is a semiconductor with an indirect band gap of 1.24 eV, Ge$_{12}$ in P4$_2$/mma structure is a direct band gap semiconductor with the band gap of 0.71 eV, and Si$_{9}$Ge$_{4}$ and Si$_{4}$Ge$_{8}$ are indirect band gap semiconductors with the band gap of 1.25 and 1.03 eV, respectively.

This paper presents two new Si-Ge alloys in P4$_2$/ncm phase; their physical properties, such as structural, mechanical, elastic, electronic and thermal properties are investigated by using first-principles calculations. The original structures of silicon and germanium in P4$_2$/ncm phase were reported in Ref. [19].

2. Materials and Methods

The computational investigations were performed under the framework of density functional theory (DFT) [20,21] as implemented in the Cambridge Serial Total Energy Package (CASTEP) code [22]. The Kohn–Sham equations are solved within the framework of DFT by expanding the wave functions of valence electrons in a basis set of plane waves with kinetic energy smaller than a specified cut-off energy, $E_{\text{cut}}$. Plane wave cut-off energy $E_{\text{cut}}$ of 340 eV and $2\pi \times 0.025$ Å$^{-1}$ ($8 \times 8 \times 4/8 \times 8 \times 4/7 \times 7 \times 4$) grid of Monkhorst–Pack [23] points have been employed for Si, Si$_{0.667}$Ge$_{0.333}$, Si$_{0.333}$Ge$_{0.667}$ alloys in P4$_2$/ncm phase and $E_{\text{cut}} = 300$ eV and high Monkhorst–Pack points $2\pi \times 0.025$ Å$^{-1}$ ($7 \times 7 \times 4$) have been employed for Ge in P4$_2$/ncm phase to ensure well convergence of the computed structures and energies in this work. The presence of tightly-bound core electrons was represented by ultra-soft pseudo-potentials [24]. The exchange-correlation potential is treated within the local density approximation (LDA), developed by Ceperly and Alder, and parameterized by Perdew and Zunger (CA-PZ) [25,26] and Perdew–Burke–Ernzerhof (PBE) [27], developed by generalized gradient approximation (GGA). The structural parameters were determined using the Broyden–Fletcher–Goldfarb–Shanno (BFGS) algorithm [28], with the flowing thresholds for converged structures: energy change less than $5 \times 10^{-6}$ eV per atom, residual force below 0.01 eV/Å, stress less than 0.02 GPa and the displacement of atoms during the geometry optimization less than 0.0005 Å.
The phonon frequencies were calculated using linear response theory [29]. Other works [30,31] also give more credibility of the whole concept applied to diversified binary systems. The electronic band structures of the Si, Si$_{0.667}$Ge$_{0.333}$, Si$_{0.333}$Ge$_{0.667}$ and Ge in P4$_2$/nmc phase were calculated utilizing the Heyd–Scuseria–Ernzerhof (HSE06) [32,33] hybrid functional.

3. Results and Discussion

3.1. Structural Properties

The crystal structures of Si$_{0.667}$Ge$_{0.333}$ and Si$_{0.333}$Ge$_{0.667}$ alloys, together with the Si (Ge) in P4$_2$/nmc space group are displayed in Figure 1a–c. The structures of the silicon germanium alloys can be obtained with the lowest energy structure when the position of the silicon atom is replaced by the germanium atom. The optimal lattice parameters of Si (Ge), Si$_{0.667}$Ge$_{0.333}$, and Si$_{0.333}$Ge$_{0.667}$ alloys in P4$_2$/nmc phase are listed in Table 1; in addition, the optimized lattice parameters and experiment values of diamond Si and diamond Ge are also listed in Table 1. From Table 1, it is clear that the lattice parameters of P4$_2$/nmc-Si and P4$_2$/nmc-Ge in this work are in excellent agreement with the previous report [19], and the optimized results of diamond Si and diamond Ge in this work are also in excellent agreement with experiment values [34,35]. At zero pressure, within P4$_2$/nmc structure, two inequivalent atoms occupy the crystallographic 4b and 8i sites in the conventional cell, which are 4b Ge (0.0000, 1.0000, 0.5000), Si 8i (−0.1624, 0.3376, 0.3551) for Si$_{0.667}$Ge$_{0.333}$. For P4$_2$/nmc-Si$_{0.333}$Ge$_{0.667}$, Si occupy the crystallographic 4b sites (0.0000, 1.0000, 0.5000), Ge occupy the crystallographic 4b sites (−0.1622, 0.3338, 0.3607). The energies of Si$_{0.667}$Ge$_{0.333}$ and Si$_{0.333}$Ge$_{0.667}$ alloys are the lowest when the silicon atoms and germanium atoms occupy these positions, respectively. The silicon atoms occupy the 4b sites and the silicon atoms occupy the 8i crystallographic sites consisting of five-membered, six-membered, and seven-membered silicon rings for P4$_2$/nmc-Si. The position of five-membered, six-membered, and seven-membered silicon rings for P4$_2$/nmc-Si are shown in Figure 1d. The angles of five-membered, six-membered, and seven-membered silicon rings are shown in Figure 1e–g. In this article, we used the six-membered silicon rings as an example. The distribution of angle for the six-membered silicon rings are in a symmetric fashion. From P4$_2$/nmc-Si to P4$_2$/nmc-Ge, with the composition of the Ge atom increasing, the change of the angle has no rule to be found. The top angle is 109.0° for P4$_2$/nmc-Si, 108.6° for P4$_2$/nmc-Si$_{0.667}$Ge$_{0.333}$, and it is changed to 110.0° for P4$_2$/nmc-Si$_{0.333}$Ge$_{0.667}$, while the top angle is 109.5° for P4$_2$/nmc-Ge. Just like the top angle, the middle angles are 112.2°, 111.2°, 112.4° and 111.4° for P4$_2$/nmc-Si, P4$_2$/nmc-Si$_{0.667}$Ge$_{0.333}$, P4$_2$/nmc-Si$_{0.333}$Ge$_{0.667}$, and P4$_2$/nmc-Ge, respectively. There is no law to follow, either. The lattice parameters of P4$_2$/nmc-Si, P4$_2$/nmc-Si$_{0.667}$Ge$_{0.333}$, P4$_2$/nmc-Si$_{0.333}$Ge$_{0.667}$, and P4$_2$/nmc-Ge as a function of the percentage of the Ge composition are shown in Figure 2a. From Figure 2a, it is obvious that the lattice parameters of Si-Ge alloys in P4$_2$/nmc phase increases with the increasing percentage of the Ge composition. The larger the atomic radius of germanium is, the larger the chemical bond length between germanium and silicon atoms is. This is the reason why the lattice parameters increase.

Table 1. The lattice parameters (in Å) of Si, Si$_{0.667}$Ge$_{0.333}$, Si$_{0.333}$Ge$_{0.667}$ and Ge alloys in P4$_2$/nmc phase.

| Materials         | PBE          | CA-PZ         | Experimental |
|-------------------|--------------|---------------|--------------|
|                   | a  | c  | a  | c  | a  |
| Si                | 5.237 | 9.274 | 5.132 | 9.125 | - |
| Si$_{0.667}$Ge$_{0.333}$ | - | - | 5.135 | 9.167 | - |
| Si$_{0.333}$Ge$_{0.667}$ | 5.306 | 9.397 | 5.185 | 9.163 | - |
| Ge                | 5.380 | 9.635 | 5.222 | 9.361 | - |
| Diamond-Si        | 5.462 | 9.779 | 5.281 | 9.396 | - |
| Diamond-Ge        | 5.441 | - | 5.419 | - | 5.431 |
|                   | 5.699 | - | 5.580 | - | 5.660 |

1 Ref [19], 2 Ref [34,35].
3.2. Mechanical and Anisotropic Properties

According to the mechanical stability criteria of tetragonal symmetry [36,37], the Si$_{0.667}$Ge$_{0.333}$ and Si$_{0.333}$Ge$_{0.667}$ alloys belong to the tetragonal symmetry, we mainly discussed the different mechanical properties between Si$_{0.333}$Ge$_{0.667}$ alloys in the $P4_2/mnm$ phase both satisfy it. Since the [18] phases both belong to the tetragonal symmetry, we mainly discussed the different mechanical properties between Si$_{0.333}$Ge$_{0.667}$ alloys in the $P4_2/mnm$ phase.

The calculated elastic constants and elastic moduli of Si, Si$_{0.667}$Ge$_{0.333}$, Si$_{0.333}$Ge$_{0.667}$, Ge in $P4_2/mnm$ and $P4_2/mmm$ phases, together with diamond Si and diamond Ge are listed in Table 2. From Table 2,

**Figure 1.** The crystal structures of Si (a), Si$_{0.667}$Ge$_{0.333}$ (b), Si$_{0.333}$Ge$_{0.667}$ (c) alloys in $P4_2/mnm$ phase. The blue and red spheres represent the Si atoms and Ge atoms. Si$_5$, Si$_6$ and Si$_7$ rings in the $2 \times 2 \times 2$ supercell (d). Si$_5$ (e), Si$_6$ (f) and Si$_7$ (g) rings in the $P4_2/mnm$ phase.

**Figure 2.** Lattice parameters (a) and elastic modulus (b) as a function of germanium concentration for Si–Ge alloys in $P4_2/mnm$ phase.

3.2. Mechanical and Anisotropic Properties

The calculated elastic constants and elastic moduli of Si, Si$_{0.667}$Ge$_{0.333}$, Si$_{0.333}$Ge$_{0.667}$, Ge in $P4_2/mnm$ and $P4_2/mmm$ phases, together with diamond Si and diamond Ge are listed in Table 2. From Table 2,
according to the mechanical stability criteria of tetragonal symmetry [36,37], the Si$_{0.667}$Ge$_{0.333}$ and Si$_{0.333}$Ge$_{0.667}$ alloys in the P4$_2$/nmc phase both satisfy it. Since the P4$_2$/ncm and P4$_2$/mnm [18] phases both belong to the tetragonal symmetry, we mainly discussed the different mechanical properties between these two silicon allotropes. In addition, the elastic moduli of Si, Si$_{0.667}$Ge$_{0.333}$, Si$_{0.333}$Ge$_{0.667}$, Ge in P4$_2$/nmc phase as a function of the percentage of the Ge composition are shown in Figure 2b. Obviously, the elastic moduli of P4$_2$/nmc-Si are larger than that of P4$_2$/nmc-Ge; in other words, the elastic moduli of Si-Ge alloys in P4$_2$/nmc phase decreases with the increasing percentage of the Ge composition. The calculated elastic constants of P4$_2$/nmc phase are almost smaller than those of P4$_2$/nmc phase (see Table 2). In addition, Young’s modulus E and Poisson’s ratio $\nu$ of P4$_2$/nmc and P4$_2$/mnm phases are also listed in Table 2. Young’s modulus and Poisson’s ratio are estimated by the following two formulas: $E = 9BG/(3B + G)$, $\nu = (3B - 2G)/(2(3B + G))$. The calculated Young’s modulus of P4$_2$/nmc-Si is 135 GPa, which is slightly smaller than that of diamond Si (155 GPa), but the Young’s modulus of P4$_2$/nmc-Ge is about two times than that of Si$_{0.667}$ (69 GPa [8]) and slightly greater than that of P4$_2$/mnm Si, while the calculated Young’s modulus of P4$_2$/nmc-Ge is 105 GPa, which is also slightly smaller than that of diamond Ge (122 GPa) and slightly greater than that of P4$_2$/mnm Ge (83 GPa [18]). Compared with P4$_2$/mnm phase, the elastic constants and bulk modulus, shear modulus and Young’s modulus of Si$_{0.667}$Ge$_{0.333}$, Si$_{0.333}$Ge$_{0.667}$ alloys in the P4$_2$/nmc phase are all slightly greater.

| Materials          | C$_{11}$ | C$_{12}$ | C$_{13}$ | C$_{33}$ | C$_{44}$ | C$_{66}$ | B    | G    | E    | $\nu$ | A$^1$  |
|--------------------|----------|----------|----------|----------|----------|----------|------|------|------|------|--------|
| P4$_2$/nmc-Si      | 141      | 61       | 49       | 138      | 61       | 73       | 82   | 55   | 135  | 0.226| 0.237  |
| Si$_{0.667}$Ge$_{0.333}$ | 130      | 56       | 43       | 130      | 56       | 68       | 75   | 51   | 125  | 0.220| 0.225  |
| Si$_{0.333}$Ge$_{0.667}$ | 122      | 45       | 38       | 115      | 53       | 61       | 66   | 48   | 117  | 0.207| 0.156  |
| P4$_2$/nmc-Ge      | 108      | 41       | 33       | 106      | 47       | 56       | 59   | 44   | 105  | 0.205| 0.158  |
| P4$_2$/mnm-Si$^1$  | 123      | 47       | 48       | 146      | 49       | 61       | 75   | 48   | 119  | 0.236| 0.134  |
| Si$_{0.667}$Ge$_{0.333}$ | 111      | 36       | 42       | 130      | 43       | 38       | 66   | 40   | 100  | 0.252| 0.035  |
| Si$_{0.333}$Ge$_{0.667}$ | 100      | 32       | 37       | 110      | 39       | 44       | 58   | 38   | 94   | 0.231| 0.056  |
| P4$_2$/mnm-Ge$^1$  | 88       | 26       | 32       | 100      | 35       | 40       | 50   | 34   | 83   | 0.223| 0.054  |
| Diamond-Si         | 160      | 62       | -        | -        | 79       | -        | 95   | 65   | 159  | 0.221| 0.279  |
| Diamond-Ge         | 123      | 47       | -        | -        | 62       | -        | 72   | 51   | 124  | 0.213| 0.293  |

$^1$Ref [18]. $^2$Ref [38]-experiment.

The anisotropy is an important characteristic for materials. This work mainly discusses the mechanical anisotropy of Si, Ge and their Si$_{0.667}$Ge$_{0.333}$, Si$_{0.333}$Ge$_{0.667}$ alloys in the P4$_2$/nmc phase. In our previous work [39], the methods we discussed are used to investigate the mechanical anisotropy. Based on the fundamental elastic constants, a useful visualization of the elastic anisotropy can be obtained by plotting a three-dimensional figure which shows the dependence of the Poisson’s ratio $\nu$, shear modulus G, and Young’s modulus E on a direction in a crystal. The three-dimensional surface representation of Poisson’s ratio $\nu$ and shear modulus G for Si, Ge and their Si$_{0.667}$Ge$_{0.333}$, Si$_{0.333}$Ge$_{0.667}$ alloys in the P4$_2$/nmc phase are illustrated in Figure 3a–h, respectively. The green and purple surface representation denotes the minimum and the maximum values of Poisson’s ratio $\nu$ and shear modulus G along different directions, respectively. For an isotropic system, the three-dimensional directional dependence would exhibit a spherical shape, while the deviation degree from the spherical shape reflects the content of anisotropy [40]. From Figure 3a–h, it is clear that the shape of the three-dimensional directional dependence do not all exhibit a spherical shape, and the shape of the three-dimensional directional dependence for Si, Ge and their Si$_{0.667}$Ge$_{0.333}$, Si$_{0.333}$Ge$_{0.667}$ alloys in the P4$_2$/nmc phase all exhibit mechanical anisotropy in Poisson’s ratio and shear modulus. Also, because the shape of the three-dimensional directional dependence of Si, Ge and their Si$_{0.667}$Ge$_{0.333}$, Si$_{0.333}$Ge$_{0.667}$ alloys in the P4$_2$/nmc phase are not changed much, it follows that the mechanical
properties in Poisson’s ratio and shear modulus should have little changes. The details of Poisson’s ratio (001), (100) and (010) planes for Si, Ge and their Si0.667Ge0.333, Si0.333Ge0.667 alloys in the P42/n cm phase are shown in Figure 4a–c, respectively. The black line, blue line, green line and red line represent the Poisson’s ratio of Si, Si0.667Ge0.333, Si0.333Ge0.667 and Ge in the P42/n cm phase, respectively, and the solid line and dotted line denote the minimum and the maximum values of Poisson’s ratio \( \nu \) for Si, Si0.667Ge0.333, Si0.333Ge0.667 and Ge in the P42/n cm phase, respectively. From Figure 4, the shape of the two-dimensional representation of Poisson’s ratio for Si, Si0.667Ge0.333, Si0.333Ge0.667 and Ge in the P42/n cm phase has few changes. Moreover, for the same direction, the lines in different colors and types are very close to each other, which indicates that the Poisson’s ratio of Si, Si0.667Ge0.333, Si0.333Ge0.667 and Ge in the P42/n cm phase in this direction does not increase or decrease too much with the increasing percentage of the Ge composition. While along x-axis ([100] direction), y-axis ([010] direction) and other unusual directions, the Poisson’s ratio of Si0.667Ge0.333 is slightly larger than that of Si in P42/n cm phase; but in (1–10) plane, the Poisson’s ratio of Si0.667Ge0.333 in P42/n cm phase along [001] direction is not larger than that of P42/n cm-Si. The maximum value of Si, Si0.667Ge0.333 in P42/n cm phase are both 0.37, and the Si0.333Ge0.667 and Ge in P42/n cm phase are both 0.32, but they do not have the same location of the maximum values. The positions of the maximum values are located at \( \theta = 1.00, \phi = 0.00 \) (more details in the Refs. [39,41]); \( \theta = 1.13, \phi = 0.00; \theta = 2.16, \phi = 0.00 \) and \( \theta = 1.08, \phi = 0.00 \) for Si, Si0.667Ge0.333, Si0.333Ge0.667 and Ge in P42/n cm phase, respectively; all angles are measured in radians. The maximum value of Si, Si0.667Ge0.333 Si0.333Ge0.667 and Ge in P42/n cm phase all occupy the position \( \theta = 1.57, \phi = 3.93 \).

**Figure 3.** The surface constructions of Poisson’s ratio \( \nu \) (a–d) and shear modulus \( G \) (e–h) for Si, Ge and their Si0.667Ge0.333, Si0.333Ge0.667 alloys in the P42/n cm phase. For all graphs, the units are in GPa.
Figure 4. The two-dimensional representation of Poisson’s ratio in the (001) plane (a), (100) plane (b) and (010) plane (c) for Si–Ge alloys in $P4_2/ncm$ structure.

To understand plastic deformations in Si, $\text{Si}_{0.667}\text{Ge}_{0.333} \text{Si}_{0.333}\text{Ge}_{0.667}$ and Ge in $P4_2/ncm$ phase, the variations of the shear modulus on stress direction are plotted in Figure 5. In Figure 5, in all the shear planes, the variation tendencies of shear moduli of Si, $\text{Si}_{0.667}\text{Ge}_{0.333} \text{Si}_{0.333}\text{Ge}_{0.667}$ and Ge in $P4_2/ncm$ phase with the increasing percentage of the Ge composition are similar. In addition, the variation tendencies of shear moduli of Si, $\text{Si}_{0.667}\text{Ge}_{0.333} \text{Si}_{0.333}\text{Ge}_{0.667}$ and Ge in $P4_2/ncm$ phase with the angle $\gamma$ that is between the [100] and shear stress direction are also similar. For (001) shear plane, with the shear stress direction rotated from [100] direction to [010] direction, the shear moduli of $P4_2/ncm$-Si are equal to each other when the angle $\gamma$ is from 13° to 75°. The range of the same shear moduli of $\text{Si}_{0.667}\text{Ge}_{0.333} \text{Si}_{0.333}\text{Ge}_{0.667}$ and Ge in $P4_2/ncm$ phase decreases with the increasing percentage of the Ge composition. Unlike (001) shear plane, with the shear stress direction rotated from [100] direction to [010] direction, there is no region with the same shear moduli in the (100) shear plane with the shear stress direction rotated from [001] direction to [010] direction and (010) shear plane with the shear stress direction rotated from [001] direction to [110] direction. From Figure 5, the ordering of the shear modulus when the tensile axis is along a specific direction is: $G_{[100]} \approx G_{[010]} > G_{[001]} \approx G_{[110]}$. 
Young’s modulus is a measure of the stiffness of an isotropic elastic objective, which is a physical quantity that represents the nature of the material, and only depends on the physical properties of the material itself. The Young’s modulus indicates the rigidity of the material, and the bigger the Young’s modulus is, the less likely it is to deform. The three-dimensional surface representation of Young’s modulus for Si, Ge and their Si0.667Ge0.333, Si0.333Ge0.667 alloys in the P42/ncm phase are illustrated in Figure 6a–d, respectively. Compared with Poisson’s ratio and shear modulus, Young’s modulus does not change too much with the increasing percentage of the Ge composition; Figure 6a–d are almost identical, except for the size of Young’s modulus. In addition, the Si, Si0.667Ge0.333, Si0.333Ge0.667 and Ge in P42/ncm phase exhibit mechanical anisotropic properties in Young’s modulus. Figure 7 shows the variation of Young’s modulus in the (001) plane for the quadrant of directions [uvw] between [100] and [010], (001) plane for the quadrant of directions [uvw] between [001] and [010], and (0T0) plane for the quadrant of directions [uvw] between [001] and [110], respectively. One can see that the largest Young’s modulus of P42/ncm-Si0.667Ge0.333 is 146.1 GPa in (001) plane, and the E_{[001]} ≈ E_{[010]} = 100.3 GPa of Young’s modulus of P42/ncm-Si0.667Ge0.333, the E_{[100]} ≈ E_{[010]} is also the smallest value of P42/ncm-Si0.667Ge0.333 in (001) plane. In addition, E_{[001]} = 110.4 GPa in (100) plane for P42/ncm-Si0.667Ge0.333, the smallest value of P42/ncm-Si0.667Ge0.333 in (100) plane is 100.3 GPa in [010] direction. Also, in (0T0) plane, the largest Young’s modulus of P42/ncm-Si0.667Ge0.333 is 146.1 GPa, and the smallest value of P42/ncm-Si0.667Ge0.333 in (1–10) plane is 110.4 GPa in [001] direction. It is worth noting that the Young’s modulus of P42/ncm-Si0.667Ge0.333 and P42/ncm-Ge increases with the increasing angle between the [100] and Young’s modulus stress direction, but for P42/ncm-Si and P42/ncm Si0.333Ge0.667, it increases first and then decreases with the increase of the angle. So, the (001) plane exhibits the largest mechanical anisotropic properties (in Young’s modulus) of the Si, Si0.667Ge0.333 Si0.333Ge0.667 and Ge in P42/ncm phase, and the (100) plane exhibits the smallest mechanical anisotropic properties in Young’s modulus.
Figure 6. The surface constructions of Young's modulus $E$ for Si (a), $Si_{0.667}Ge_{0.333}$ (b), $Si_{0.333}Ge_{0.667}$ (c) and Ge (d) in the $P4_2/ncm$ phase. For all graphs, the units are in GPa.

Figure 7. Orientation dependence of Young's modulus in (001) plane (a), (100) plane (b) and (010) plane (c) for Si, $Si_{0.667}Ge_{0.333}$, $Si_{0.333}Ge_{0.667}$ alloys and Ge in the $P4_2/ncm$ phase.
In addition, except for Poisson’s ratio, shear modulus and Young’s modulus, there is another physical quantity to characterize the mechanical anisotropy of a material: the universal anisotropic index $A^U$ [42], which is defined as $A^U = 5G_V/G_R + B_V/B_R - 6$, where $G$ and $B$ represent shear modulus and bulk modulus, respectively, and the subscripts $V$ and $R$ denote the Voigt and Reuss approximations, respectively. The calculated universal anisotropic index of the Si, Si$_{0.667}$Ge$_{0.333}$, Si$_{0.333}$Ge$_{0.667}$ and Ge in $P4_2/ncm$ phase are also listed in Table 2. Compared with the Si, Si$_{0.667}$Ge$_{0.333}$, Si$_{0.333}$Ge$_{0.667}$ and Ge in $P4_2/mnm$ phase, the universal anisotropic index of the Si, Si$_{0.667}$Ge$_{0.333}$, Si$_{0.333}$Ge$_{0.667}$ and Ge in $P4_2/ncm$ phase is two times, or even almost three times that of the Si, Si$_{0.667}$Ge$_{0.333}$, Si$_{0.333}$Ge$_{0.667}$ and Ge in $P4_2/mnm$ phase, respectively. Among the Si, Si$_{0.667}$Ge$_{0.333}$, Si$_{0.333}$Ge$_{0.667}$ and Ge in $P4_2/ncm$ phase, $P4_2/ncm$-Si exhibits the largest mechanical anisotropic properties in the universal anisotropic index than that of $P4_2/mnm$-Ge, Si$_{0.667}$Ge$_{0.333}$ and Si$_{0.333}$Ge$_{0.667}$. Moreover, the universal anisotropic index of the $P4_2/ncm$-Si is slightly larger than that of Si in $Amn2$, $C2/m$-16, $C2/m$-20 phases, much larger than that of Si in $I-4$ phase, while it is slightly smaller than that of diamond silicon ($Fd-3m$ phase).

3.3. Electronic Properties

In solid state physics, the energy band structure of a solid, also known as the electron band structure, describes the energy that is forbidden or permitted by electrons. The band structure of a material determines a variety of properties, especially its electronic and optical properties. The band structures of Si, Si$_{0.667}$Ge$_{0.333}$, Si$_{0.333}$Ge$_{0.667}$ and Ge in $P4_2/ncm$ phase calculated utilizing the Heyd–Scuseria–Ernzerhof (HSE06) [32,33] hybrid functional are shown in Figure 8a–d, respectively. The calculated band gaps of Si, Si$_{0.667}$Ge$_{0.333}$, Si$_{0.333}$Ge$_{0.667}$ and Ge in $P4_2/ncm$ phase are 0.63 eV, 0.58 eV, 0.55 eV and 0.39 eV utilizing the CA-PZ function, respectively; the calculated universal anisotropic index of the Si, Si$_{0.333}$Ge$_{0.667}$, Si$_{0.667}$Ge$_{0.333}$, and Ge in $P4_2/ncm$ phase are in excellent agreement with the previous report [19]. In Figure 8, one can see that the band gaps of the Si, Si$_{0.667}$Ge$_{0.333}$, Si$_{0.333}$Ge$_{0.667}$ and Ge in $P4_2/ncm$ phase are all much larger than those of the CA-PZ function. From Figure 8, the $P4_2/ncm$-Si, $P4_2/ncm$-Ge and their alloys Si$_{0.667}$Ge$_{0.333}$, Si$_{0.333}$Ge$_{0.667}$ in $P4_2/ncm$ phase are all indirect band gaps with band gaps of 1.46 eV, 1.00 eV, 1.25 eV and 1.36 eV, respectively. The valence band maximum (VBM) of the $P4_2/ncm$-Si, $P4_2/ncm$-Ge and their alloys Si$_{0.667}$Ge$_{0.333}$, Si$_{0.333}$Ge$_{0.667}$ are all located at M point, while the conduction band maximum (VBM) of the $P4_2/ncm$-Si, $P4_2/ncm$-Ge and their alloys Si$_{0.667}$Ge$_{0.333}$, Si$_{0.333}$Ge$_{0.667}$ in $P4_2/ncm$ phase are all located at the point (0.196 0.196 0.5) along the Z-A direction. In addition, the Fermi level of Si, Ge and their alloys Si$_{0.667}$Ge$_{0.333}$, Si$_{0.333}$Ge$_{0.667}$ in $P4_2/ncm$ phase decreases with the increasing percentage of the Ge composition.

![Figure 8. Cont.](image-url)
The thermal conductivity $\kappa$ is the property of a material that conducts heat in physics. The minimum thermal conductivity $\kappa_{\text{min}}$ can be calculated using the following theoretical method, namely, Clarke’s model [43], expressed as follows: $\kappa_{\text{min}} = 0.87k_\text{B}m^{-2/3}(E/\rho)^{1/2}$, where $m$ is the number of atoms in unit volume, and $m = (M/n_\rho N_A)$, $M$ is the molecular weight; $n$ is the number of atoms in the unit cell, $k_\text{B}$ is Boltzmann’s constant, $N_A$ is Avogadro’s number, $\rho$ is the density of the P4$_2$/ncm-Si, P4$_2$/ncm-Ge and their alloys Si$_{0.667}$Ge$_{0.333}$, Si$_{0.333}$Ge$_{0.667}$. The calculated minimum thermal conductivity $\kappa_{\text{min}}$ of the P4$_2$/ncm-Si, P4$_2$/ncm-Ge and their alloys Si$_{0.667}$Ge$_{0.333}$, Si$_{0.333}$Ge$_{0.667}$ in different planes are plotted in Figure 9. The black, red, green and blue line representations denote the minimum thermal conductivity of the Si, Si$_{0.667}$Ge$_{0.333}$, Si$_{0.333}$Ge$_{0.667}$ and Ge in P4$_2$/ncm phase, respectively. From Figure 9, the minimum thermal conductivity of the Si, Si$_{0.667}$Ge$_{0.333}$, Si$_{0.333}$Ge$_{0.667}$ and Ge in P4$_2$/ncm phase exhibits varying degrees of anisotropic properties in different planes. In (001), (010) and (100) planes, the values of the minimum thermal conductivity $\kappa_{\text{min}}$ is almost a square with four rounded vertex angles, while the minimum thermal conductivity $\kappa_{\text{min}}$ in (010) plane is like an inverted ellipse. The minimum thermal conductivity $\kappa_{\text{min}}$ of the Si, Si$_{0.667}$Ge$_{0.333}$, Si$_{0.333}$Ge$_{0.667}$ and Ge in P4$_2$/ncm phase decreases with the increasing percentage of the Ge composition, as will be readily seen. Also, the minimum thermal conductivity $\kappa_{\text{min}}$ decreases more and more slowly with the increasing percentage of the Ge composition.
In summary, we have predicted the structural, mechanical, anisotropic and thermal properties of two silicon germanium alloys with space group P42/ncm using the density functional theory. The calculated lattice parameters of the P42/ncm-Si, P42/ncm-Ge are in excellent agreement with the previous report. The elastic constants and elastic moduli of the Si, Si0.667Ge0.333, Si0.333Ge0.667 and Ge in P42/ncm phase are calculated using strain-stress method. Compared with P42/mmm phase, the elastic constants and bulk modulus, shear modulus and Young’s modulus of Si0.667Ge0.333, Si0.333Ge0.667 alloys in P42/ncm phase are all slightly greater. The Si, Si0.667Ge0.333, Si0.333Ge0.667 and Ge in P42/ncm phase exhibit different degrees of mechanical anisotropic properties in Poisson’s ratio, shear modulus, Young’s modulus, and universal anisotropic index. From the band structures of Si, Si0.667Ge0.333, Si0.333Ge0.667 and Ge in P42/ncm phase, we can conclude that the Si, Si0.667Ge0.333, Si0.333Ge0.667 and Ge in P42/ncm phase are all indirect band gap semiconductors. By adjusting the composition of germanium atoms, Si, Si0.667Ge0.333, Si0.333Ge0.667 and Ge in P42/ncm phase can be used to make different semiconductor devices. In addition, the minimum thermal conductivity κmin of Si, Si0.667Ge0.333, Si0.333Ge0.667 and Ge in P42/ncm phase in different planes are also investigated in this work; the results show that the minimum thermal conductivity κmin of the Si, Si0.667Ge0.333, Si0.333Ge0.667 and Ge in P42/ncm phase has the largest anisotropy properties in (010) plane.

4. Conclusions

In summary, we have predicted the structural, mechanical, anisotropic and thermal properties of two silicon germanium alloys with space group P42/ncm using the density functional theory. The calculated lattice parameters of the P42/ncm-Si, P42/ncm-Ge are in excellent agreement with the previous report. The elastic constants and elastic moduli of the Si, Si0.667Ge0.333, Si0.333Ge0.667 and Ge in P42/ncm phase are calculated using strain-stress method. Compared with P42/mmm phase, the elastic constants and bulk modulus, shear modulus and Young’s modulus of Si0.667Ge0.333, Si0.333Ge0.667 alloys in P42/ncm phase are all slightly greater. The Si, Si0.667Ge0.333, Si0.333Ge0.667 and Ge in P42/ncm phase exhibit different degrees of mechanical anisotropic properties in Poisson’s ratio, shear modulus, Young’s modulus, and universal anisotropic index. From the band structures of Si, Si0.667Ge0.333, Si0.333Ge0.667 and Ge in P42/ncm phase, we can conclude that the Si, Si0.667Ge0.333, Si0.333Ge0.667 and Ge in P42/ncm phase are all indirect band gap semiconductors. By adjusting the composition of germanium atoms, Si, Si0.667Ge0.333, Si0.333Ge0.667 and Ge in P42/ncm phase can be used to make different semiconductor devices. In addition, the minimum thermal conductivity κmin of Si, Si0.667Ge0.333, Si0.333Ge0.667 and Ge in P42/ncm phase in different planes are also investigated in this work; the results show that the minimum thermal conductivity κmin of the Si, Si0.667Ge0.333, Si0.333Ge0.667 and Ge in P42/ncm phase has the largest anisotropy properties in (010) plane.

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