Two novel SiC phases: structure, mechanical, and transport properties

Linchun Kong, Changchun Chai, Yanxing Song, Wei Zhang, Zheren Zhang and Yintang Yang
School of Microelectronics, Xidian University, Xi'an 710071, People's Republic of China
1 Author to whom any correspondence should be addressed.
E-mail: syx73986768@163.com

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Abstract
Two novel phases of SiC are put forward in this paper, in which the crystal structural, mechanical, and electronic properties, as well as effective mass and carrier mobility of SiC in the Pnmm phase (Pnmm-SiC) and Pm phase (Pm-SiC) are researched utilizing first principles calculations. Both of the novel SiC phases are certificated to have good mechanical and dynamic stability. Through analysis of the three-dimensional perspective of Young’s modulus, shear modulus and Poisson’s ratio, visible anisotropies of mechanical properties are found. The band structure calculations predict two wide bandgap semiconductors, that the Pnmm-SiC is an indirect with a bandgap value of 3.12 eV, While the Pm-SiC is a quasi-direct with a bandgap value of 2.64 eV, which indicates the Pm-SiC has a higher application potential in the optoelectronic device area. An extremely large electronic mobility (7200 cm² V⁻¹ s⁻¹) is found in the Pnmm-SiC. Based on the wide band gap, large carrier mobility, good mechanical and dynamic stability, the Pnmm-SiC is a promising material in the field of high performance electronic device in harsh environment.

1. Introduction

With the continuous progress of the semiconductor material industry, increasing number of researchers are attempting to seek out semiconductors with an enhanced performance analogue to that of IV alloys. SiC is considered as a quite promising technical material owing to its outstanding properties, such as chemical inertness, high hardness and melting temperature, and prominent semiconductor properties [1–20]. The most of polytypes being under ambient conditions are constituted of Si₄C tetrahedral units with cubic (3C–SiC), hexagonal (2H-, 4H-, and 6H-SiC), or rhombohedral (15R-, 21R-, and 33R-SiC) structures relying on the stacking sequence [2–8]. The cubic structure is also called beta-SiC (β-SiC), as well as the structures of hexagonal and rhombohedral are all sort out under the general term alpha-SiC (α-SiC) [9–12]. Daviau et al [13] made a comprehensive review, under different conditions, the phase of SiC changes one polytype to another polytype. They explore high-pressure SiC with experiment and computation, and the effect of measuring pressure on SiC vibration and material properties. In addition, high temperature studies, including thermal expansion and the equation of thermal state of SiC, and the melting behavior at high temperature and pressure have probed. SiC has been observed over 250 polytypes under ambient conditions [14], in order to know the formation of specific polytypes, the transformation conditions, transformation mechanisms, and high temperature between different polytypes much work has been done [15, 16].

Over the past decades, many researches have paid much effort on carbon materials or carbon-based materials that emerge hardness and stiffness approach that of diamond. Xing et al [17] put forward C2/m-20 carbon and made a comparison that other monoclinic symmetry was investigated. Moreover, they discovered that C2/m-20 carbon displays the largest elastic modulus, and anisotropy of Young’s modulus. In addition, many researchers predicted other carbon allotropes, such as lonsdaleite [18, 19], TAL-carbon [20], W-carbon [21], PBCF-graphene [22], C-carbon [23], Z-carbon [24], H-carbon, S-carbon [25], T-carbon [26], and so on. Fan et al [27] came up with four new silicon allotropes, including Armm2, C2/m-16, C2/m-20, and I-4, and
confirmed that all structures are mechanically and dynamically stable, and C2/m-20 phase shows the higher anisotropy compared with other structures. Bai et al. [28] proposed a novel silicon allotrope which is in the P2/m space group, and discovered that P2/m-Si is brittle. The results also show along different directions the difference of elastic anisotropy is larger than other phases (P2221, Fd-3m, C2/m-16, C2/m-20, Amm2). With the continuous deep research of carbon and silicon allotropes by researchers, the development of C–Si alloys has been promoted, and C–Si alloys are fascinating more attention in academic and electronic industry owing to their potential outstanding properties unlike elemental silicon and carbon. Recently, researchers are engaged in finding new kinds of C–Si alloys with fabulous physical properties. Many the three-dimensional silicon carbide materials are found by researchers, Zhang et al. [29] put forward two novel phases of P42/mnm symmetry of Si6C6 and Si8C6 and systematically researched their structural, electronic, and elastic properties, and both of them are confirmed to have mechanical and dynamical stability, and the calculations of electronic structure present that Si6C6 and Si8C6 are indirect materials with the band gap values of 0.74 and 0.15 eV. The mechanical, electronic and anisotropic properties of SiC2 and SiC4 were investigated by Fan et al. [30], and the results indicated that those structures all have anisotropy and that SiC2 is an indirect material with a band gap value of 2.28 eV, but for SiC4 is a quasi-direct material with a band gap value of 0.91 eV. Tan, and Zhang et al. [31, 32] put forward C–Si alloys in the orthorhombic structure of P2221 space group, and confirmed that all structures have mechanical stability and elastic anisotropy, and the results of band structure display that the put forward structures are all indirect band gap material. Wang et al. [33] put forward C–Si alloys (C16, C12Si4, C8Si6, Si16, and C3Si12) in C2/m structure, and shown that their alloys are mechanically stable, meanwhile their C–Si alloys are brittle. The results of band structure display that C16 and Si16 are indirect material, but for C12Si4, C8Si6 and C3Si12 are semi-metallic alloys. In addition, theoretical prediction of new SiC allotropes in C2/m-20 structure were proposed by Xu et al. [34], and confirmed that all structures have mechanical and dynamic stability. The calculations of the band structures indicate that C12Si6 is a direct bandgap, C3Si12 and C4Si16 are semi-metallic alloys, but for C16Si6 is indirect. It should be noted that dope two indirect band gap semiconductors (C20, Si20), and a direct band gap semiconductor (C12Si6) is attained.

Based on the previous work, two novel phases of SiC (Pnmm-SiC, and Pm-SiC) are put forward. The structural, mechanical, electronic, anisotropic, and transport properties of SiC in different phases are calculated applying first principles calculations. The Pnmm-SiC is an indirect semiconductor while Pm-SiC is a quasi-direct semiconductor, but all SiC structures have mechanical and dynamic stability. The mechanical anisotropy is analyzed utilizing elastic modulus from the three-dimensional perspectives. What’s more, the anisotropy of the carrier mobility is analyzed using the phonon-limited model, and an exceedingly high electron mobility (7200 cm² V⁻¹ s⁻¹) and hole mobility (170 cm² V⁻¹ s⁻¹) are found in the Pnmm-SiC.

2. Computational methods

The theoretical calculations are executed with the Vienna ab initio simulation package (VASP) in view of density functional theory (DFT) [35–37]. The projector augmented wave (PAW) method is applied to rewrite the electron-ion interaction, and the Perdew-Burke-Ernzerh (PBE) exchange-correlation functional of the generational gradient approximation (GGA) is taken [38]. In all calculations, k-point samplings with 0.04 Å⁻¹ is adopted to Pnmm- and Pm- SiC, and the value of energy cutoff of the plane wave is set to 500 eV. The geometry optimization parameters are determined using the Broyden-Fletcher-Shanno (BFGS), with the following convergence tolerance: the self-consistent convergence of the energy is 5 × 10⁻⁷ eV Å⁻¹, the maximum force on the atom is 0.02 eV Å⁻¹, and stress is less than 0.02 GPa. The phonon frequencies are computed utilizing linear response theory (DFPT) [39]. DFT-D3(BJ) method is adopted in the structural, elastic properties, and carrier mobility (effective elastic constant) calculations [40, 41]. Moreover, on account of the DFT usually underrates the band energy of solid materials, the electronic band structures of Pnmm- and Pm- SiC are calculated applying a hybrid functional (HESO6) [42–44].

3. Results and discussions

3.1. Structural and mechanical properties

The crystal structures perspective view of Pnmm-SiC and Pm-SiC in the [100] direction, [010] direction, and [001] direction are shown in figures 1(a)–(f). Their number of atoms of Pnmm-SiC and Pm-SiC in conventional cell are 24 and 16, respectively. As for the Pnmm-SiC, which contains sp³-bonded rings, including 4- and 8-membered rings (4 + 8) and six-atom hexagonal C–Si rings. Figures (d)–(f) are Pm-SiC, which contains 5- and 7-membered rings (5 + 7) and six-atom hexagonal C–Si rings. After the geometry optimization using PBE, PBE-D3, and LDA method, the calculated lattice parameters of β-SiC, Pnmm-SiC, and Pm-SiC are enumerated in table 1. According to table 1, the computed lattice parameter of β-SiC using PBE-D3 method is in fabulous
accordance with experimental results [45] in that its minute difference 0.016 Å between this calculation work and experimental lattice parameters. So the lattice parameter computed by PBE-D3 method is more consistent with previous experiment value relative to PBE method and LDA method.

Figure 1. The crystal structures perspective view of the Pnmm-SiC in the [100] direction (a), [010] direction (b) and [001] direction (c), and Pm-SiC in the [100] direction (d), [010] direction (e) and [001] direction (f). The purple and green colors deputy C atoms and Si atoms.

Table 1. The lattice parameters a, b and c; \( \alpha \), \( \beta \), and \( \gamma \) (in°); cell volume; and cell density of \( \beta \)-SiC, Pnmm-SiC, and Pm-SiC, respectively.

| Material  | Method | \( a / \AA \) | \( b / \AA \) | \( c / \AA \) | \( \alpha /^\circ \) | \( \beta /^\circ \) | \( \gamma /^\circ \) | \( V / (\AA^3) \) | \( \rho / (g \ cm^{-3}) \) |
|-----------|--------|-------------|-------------|-------------|----------------|----------------|----------------|----------------|----------------|
| \( \beta \)-SiC | PBE   | 4.385       | 4.385       | 4.385       | 90             | 90             | 90             | 84.501         | 3.152          |
|           | PBE-D3 | 4.343       | 4.343       | 4.343       | 90             | 90             | 90             | 81.897         | 3.251          |
|           | LDA   | 4.323       | 4.323       | 4.323       | 90             | 90             | 90             | 80.774         | 3.297          |
|           | EXP.a | 4.359       |             |             |                |                |                |                |                |
| Pnmm-SiC  | PBE   | 16.048      | 5.104       | 3.087       | 90             | 90             | 90             | 256.199        | 3.119          |
|           | PBE-D3| 15.968      | 5.097       | 3.066       | 90             | 90             | 90             | 249.543        | 3.202          |
|           | LDA   | 15.897      | 5.052       | 3.036       | 90             | 90             | 90             | 245.460        | 3.255          |
| Pm-SiC    | PBE   | 10.802      | 3.096       | 5.214       | 90             | 98.9           | 90             | 172.242        | 3.092          |
|           | PBE-D3| 10.765      | 3.077       | 5.192       | 90             | 98.802         | 90             | 169.944        | 3.134          |
|           | LDA   | 10.707      | 3.061       | 5.159       | 90             | 98.8           | 90             | 167.086        | 3.188          |

* Reference [43].
The enthalpy of SiC in different phases can be utilized as a significant norm to consider whether the semiconductor materials can be synthesized. Enthalpy of formation is the energy absorbed or released by various atoms from simple compounds \[^4\text{6}\] which expresses the difficulty level of the formation of compounds. The formation enthalpy \(\Delta H\) is computed using the following expression:

\[
\Delta H = \left( E_{\text{total}} - n_{\text{Si}}E_{\text{Si}^{\text{solid}}}^{E_{\text{Si}^{\text{solid}}}} - n_{\text{C}}E_{\text{C}^{\text{solid}}}^{E_{\text{C}^{\text{solid}}}} \right) / \left( n_{\text{Si}} + n_{\text{C}} \right)
\]  

Where the \(E_{\text{total}}\) is the entire energy of \(Pnmm\)-SiC or \(Pm\)-SiC; the \(n_{\text{Si}}\) is the number of Si atoms in the cell; \(n_{\text{C}}\) is the number of C atoms in the cell; \(E_{\text{Si}^{\text{solid}}}^{E_{\text{Si}^{\text{solid}}}}\) is the energy of a silicon atom in elemental silicon; and \(E_{\text{C}^{\text{solid}}}^{E_{\text{C}^{\text{solid}}}}\) is the energy of a carbon atom in elemental carbon. According to the expression, the formation enthalpies of \(Pnmm\)-SiC and \(Pm\)-SiC are calculated, and their formation enthalpies are \(-0.373\) eV and \(-0.261\) eV, respectively. It is noteworthy that formation enthalpies of SiC in different phases are negative, it can be seen that both of SiC have relative stability.

The phonon spectrum of SiC in the two different phases are computed to certify its dynamic stability, and the spectrum of SiC in different phases are displayed in figure 2. From figure 2, the SiC of these different phases all have dynamical stability because there are no imaginary frequencies throughout the entire Brillouin zone for the \(Pnmm\)-SiC and \(Pm\)-SiC.

On the other hand, the material’s mechanical properties determine whether its mechanical stability and it can exist in the nature. The elastic constant and modulus of \(\beta\)-SiC, \(Pnmm\)-SiC and \(Pm\)-SiC are calculated in this work. There are nine independent elastic constants \(C_{ij}\) in the orthorhombic symmetry of the space group of \(Pnmm\). But for the monoclinic symmetry of the space group of \(Pm\), besides the nine independent elastic constants are the same as the orthorhombic symmetry, which also contains other four independent elastic constants \((C_{15}, C_{25}, C_{35}, C_{46})\). The values of the main elastic constant of SiC in the different phases are computed utilizing the strain-stress method are displayed in table 2. In addition, the values of elastic constants \(C_{15}, C_{25}, C_{35}\), and \(C_{46}\) of the \(Pm\)-SiC are 7, 11, \(-15\), and 8 GPa, respectively.

Both of the independent elastic constants of \(Pnmm\)-SiC and \(Pm\)-SiC accord with the mechanical stability criteria \([48, 49]\). That is to say, both of different phases of SiC have mechanical stability under ambient condition. Moreover, bulk modulus \((B)\) and shear modulus \((G)\) are fracture and plastic deformation resistance. The Voigt-Reuss-Hill approximation \([50-52]\) is taken to compute \(B\) and \(G\), and they are defined in the following

### Table 2. The elastic constant (in GPa) and the elastic moduli (in GPa) of \(Pnmm\)-SiC, \(Pm\)-SiC, and \(\beta\)-SiC.

| Materials | Method | \(C_{11}\) | \(C_{22}\) | \(C_{33}\) | \(C_{44}\) | \(C_{55}\) | \(C_{66}\) | \(C_{12}\) | \(C_{13}\) | \(C_{23}\) | \(B\) | \(G\) | \(E\) | \(\nu\) |
|-----------|--------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|------|------|------|------|
| \(Pnmm\)-SiC | PBE    | 473 | 463 | 502 | 152 | 186 | 145 | 146 | 85 | 36 | 197 | 179 | 412 | 0.151 |
|            | PBE-D3 | 469 | 455 | 494 | 152 | 186 | 145 | 139 | 79 | 33 | 191 | 179 | 409 | 0.143 |
| \(Pm\)-SiC | PBE    | 454 | 454 | 443 | 191 | 153 | 126 | 29 | 54 | 82 | 187 | 170 | 391 | 0.151 |
|            | PBE-D3 | 448 | 449 | 437 | 191 | 153 | 126 | 23 | 47 | 75 | 180 | 170 | 388 | 0.141 |
| \(\beta\)-SiC | PBE | 400 | 400 | 400 | 255 | 255 | 255 | 137 | 137 | 137 | 125 | 195 | 454 | 0.164 |
|            | PBE-D3 | 390 | 390 | 390 | 255 | 255 | 255 | 130 | 130 | 130 | 120 | 195 | 450 | 0.153 |

\(^a\) Reference \([47]\)
equation:

\[ B = (B_V + B_R)/2 \]  \hspace{1cm} (2) 

\[ G = (G_V + G_R)/2 \]  \hspace{1cm} (3) 

Where \( B_V \) means the Voigt approximation of \( B \); \( B_R \) is the Reuss approximation of \( B \); \( G_V \) is the Voigt approximation of \( G \); and \( G_R \) is the Reuss approximation of \( G \).

The Young’s modulus \( E \) is applied to measure the solid’s stiffness, and we find that the higher the value of \( E \) is, the stiffer the material is [55]. Meanwhile, the \( E \) can be computed by the equation, and the equation is as follows [52]:

\[ E = 9BG/(3B + G) \]  \hspace{1cm} (4) 

The ratio of \( B \) to \( G \) is an identifier that can determine a solid is brittle or not according to the Pugh’s theory [47]. Poisson’s ratio \( \nu \) is accord with \( B/G \), which indicates the brittle compounds with a small value of \( \nu (<0.26) \), and ductile compounds with a large value of \( \nu (>0.26) \) [54]. \( \nu \) can be attained from the formula, and the formula is as follows:

\[ \nu = (3B - 2G)/[2(3B + G)] \]  \hspace{1cm} (5) 

All of the elastic moduli, including \( B, G, E \) and \( \nu \) of \( Pnnm-\text{SiC} \) and \( Pm-\text{SiC} \) are enumerated in table 2. From the table, the elastic constants of \( \beta \)-SiC in this work using PBE-D3 method is in fabulous accordance with the results of previous results [55], which proves our work is accurate and faithful. Besides, on the basis of the above criteria mentioned, both of the elastic constants of \( Pnnm-\text{SiC} \) and \( Pm-\text{SiC} \) at ambient condition are positive and meet the mechanical stability standard, demonstrating that both of SiC are mechanically stable. The \( E \) can be applied to depict the relevant tensile strain, and according to the above discovery of \( E \) we find that \( Pnnm-\text{SiC} \) is stiffer than \( Pm-\text{SiC} \). The \( B \) of \( Pnnm-\text{SiC} \) is slightly larger than that of \( Pm-\text{SiC} \), while both of SiC in different phases are slightly smaller than \( \beta \)-SiC. For \( \nu \) of SiC in different phases, as proposed by Pugh [47], \( \beta \)-SiC, \( Pm-\text{SiC} \) and \( Pnnm-\text{SiC} \) are brittle materials because they have small values of \( \nu (<0.26) \). Moreover, the \( B, G \) and \( E \) of \( Pnnm-\text{SiC} \) and \( Pm-\text{SiC} \) are possible to reach that of the \( \beta \)-SiC, which indicates both of SiC in different phases have good mechanical stability.

3.2. Anisotropic properties

As we all know, the elastic anisotropy is a significant implication in crystallophysics. Moreover, the three-dimensional (3D) surface construction is an effective method to depict the elastic anisotropy [36], and the spatial distribution of elastic modulus has been researched. The directional dependence of Young’s modulus, the maximum of shear modulus (shear modulus MAX), the minimum of shear modulus (shear modulus MIN), the maximum of Poisson’s ratio (Poisson’s ratio MAX), and the minimum of Poisson’s ratio (Poisson’s ratio MIN) for \( Pnnm-\text{SiC} \) and \( Pm-\text{SiC} \) at zero pressure are shown in figures 3(a)–(e), and 4(a)–(e), respectively. Moreover, the three-dimensional directional dependence of isotropic material will present a spherical shape; and the higher the spherical shape deviation is, the higher the mechanical anisotropy is [57]. Different from \( E \), the magnitude of \( \nu \) and \( G \) in the two directions, including direction \( a \) and direction \( b \), and demands three angles to be described [58]. The \( G \) is defined as the ratio of shear stress to linear shear strain, and \( \nu \) is defined as the ratio of transverse strain to axial strain [59]. The shear modulus MAX is the set of maximum values of all shear moduli in direction \( b \), and the shear modulus MIN is the set of minimum values of all shear moduli in direction \( b \). The description of Poisson’s ratio MAX and MIN is analogue to that of shear modulus. The values of maximum and minimum of Young’s modulus, shear modulus MAX and MIN, and Poisson’s ratio MAX and MIN of SiC in different phases are listed in table 3.

From figures 3 and 4, these structures all have mechanical anisotropy, and there are two Young’s moduli peaks of \( Pnnm-\text{SiC} \) in the YZ-plane and four Young’s moduli peaks of \( Pm-\text{SiC} \) in the x-axis and YZ-plane that can be discovered in the 3D perspective, which indicates the structures in different phases of SiC have a higher resistance to deformation in these directions of peaks. In addition, all directional dependence of \( \nu \) and \( G \) of \( Pnnm-\text{SiC} \) and \( Pm-\text{SiC} \) are different spherical shapes, indicating that both of these elastic modulus appear mechanical anisotropy to varying degrees.

Moreover, according to table 3, both of SiC in different phases have anisotropy, with a minimum value of \( E_{\text{min}} = 364.08 \text{ GPa} \) and a maximum value of \( E_{\text{max}} = 479.54 \text{ GPa} \) of the \( Pnnm-\text{SiC} \), and it \( (E_{\text{max}}/E_{\text{min}} = 1.317) \) shows smaller mechanical anisotropy than \( Pm-\text{SiC} \) \( (E_{\text{max}}/E_{\text{min}} = 1.394) \). As for the shear modulus \( G \), \( Pm-\text{SiC} \) \( (G_{\text{MAX}/G_{\text{MIN}}} = 1.476, G_{\text{MIN}/G_{\text{MAX}}} = 1.473) \) has larger mechanical anisotropy than \( Pnnm-\text{SiC} \) \( (G_{\text{MAX}/G_{\text{MIN}}} = 1.443, G_{\text{MIN}/G_{\text{MAX}}} = 1.279) \). Meanwhile the Poisson’s ratio of SiC in different phases also show same result as the shear modulus that \( Pm-\text{SiC} \) has larger mechanical anisotropy than \( Pnnm-\text{SiC} \). In general, the \( Pm-\text{SiC} \) has larger mechanical anisotropy than \( Pnnm-\text{SiC} \).
Figure 3. The directional dependence of Young’s modulus (a), shear modulus MAX (b), shear modulus MIN (c), Poisson’s ratio MAX (d), and Poisson’s ratio MIN (e) for the Pnnm-SiC.

Figure 4. The directional dependence of Young’s modulus (a), shear modulus MAX (b), shear modulus MIN (c), Poisson’s ratio MAX (d), and Poisson’s ratio MIN (e) for the Pm-3c-SiC.
3.3. Electronic properties and carrier effective mass

The band structures of Pnnm-SiC and Pm-SiC are calculated in figure 5 so as to analyze the band gap, orbital distribution and carrier effective mass. These calculations of band structures in different phases of SiC are used to the HSE06, and the integral path of the band structures of SiC in different phases are given by the Medea-VASP. The calculated results are shown in figure 5. And from figure 5, the values of band gap of Pnnm-SiC and Pm-SiC are 3.12 eV and 2.57 eV. The Pnnm-SiC is an indirect semiconductor material, and Pm-SiC is also an indirect semiconductor, but for the Pm-SiC can be called quasi-direct band gap at the \( \Gamma \) point because the difference 0.07 eV between the conduction band at \( \Gamma \) point and minimum point of conduction band.

In addition, the carrier effective mass has the greatest influence on the carrier transport properties, such as the larger the effective mass but the smaller carriers mobility, So there is no doubt for us to calculate effective mass. As for the solution of carrier effective mass, which is related to the band dispersion as:

\[
E(\vec{k}) = E(\vec{k}_0) \pm \left( \hbar^2 / 2 \right) \left[ \vec{k} - \vec{k}_0 \left[ m^{-1}_{ij} \right] \vec{k} - \vec{k}_0 \right] \]

Where \( E(\vec{k}_0) \) indicates the energy eigenvalues at the band extreme of energy band; \( \vec{k}_0 \) is the value in the Brillouin zone; and the matrix \( [m^{-1}_{ij}] \) \( (i, j = 1, 2, 3) \) is the inverse effective mass tensor. What is more, the band structure effective mass in the certain orientation is defined as the following equation:

\[
\frac{1}{m^*} = \frac{1}{\hbar^2} \frac{\partial^2 E}{\partial^2 \vec{k}}
\]

The electrons effective mass or holes effective mass can be defined as the partial differential at the upper edge of the valence band or at the lower edge of the conduction band. Based on the detailed description of effective mass, we have computed it about Pnnm-SiC, Pm-SiC, and \( \beta \)-SiC as follows. The lattice directions and magnitude of effective mass of SiC in different phases are abstracted and enumerated in table 4. By analyzing the results of table 4, the electronic effective mass and the hole effective mass of \( \beta \)-SiC are in excellent agreement with previous calculation results [60–62] because of the minute difference 0.01 between this calculation work and previous calculation work. In addition, we find that a high electron effective mass is 5.638 \( m_0 \) and hole effective mass is 0.1872 \( m_0 \) in the Pnnm-SiC. Moreover, the electronic effective mass and the hole effective mass of Pm-SiC are all larger than Pnnm-SiC, respectively. The electronic effective mass of Pm-SiC and Pnnm-SiC shows different calculation results in different directions, so both of SiC in different phases have effective mass anisotropy.

### Table 3. The values of maximum and minimum of Young’s modulus, shear modulus MAX and MIN, Poisson’s ratio MAX and MIN of SiC in different phases.

| Materials   | Method   | Young’s modulus Max | Young’s modulus Min | Shear modulus MAX Max | Shear modulus MAX Min | Shear modulus MIN Max | Shear modulus MIN Min | Poisson’s ratio MAX Max | Poisson’s ratio MAX Min | Poisson’s ratio MIN Max | Poisson’s ratio MIN Min |
|-------------|----------|---------------------|---------------------|-----------------------|-----------------------|-----------------------|-----------------------|------------------------|------------------------|------------------------|------------------------|
| Pnnm-SiC    | PBE-D3   | 479.34              | 364.08              | 217.64                | 152.20                | 185.35                | 144.93                | 0.25                   | 0.07                   | 0.16                   | 0.06                   |
| Pm-SiC      | PBE-D3   | 443.18              | 318.03              | 212.21                | 143.77                | 183.76                | 124.72                | 0.29                   | 0.08                   | 0.16                   | 0.02                   |

Figure 5. The band structure of Pnnm-SiC (a) and Pm-SiC (b), respectively, and the size of the blue, purple, green and yellow represents the projected weight of C\( s \), C\( p \), Si\( s \), Si\( p \) orbitals, respectively.
Table 4. Direction vector is along the three principal lattice \((a, b, c)\) and magnitude (in \(m_a, m_b, \) and \(m_c\)) of the effective mass of \(\beta\)-SiC, \(Pnnm\)-SiC and \(Pm\)-SiC, respectively.

| Carrier type | Materials | \(m_a\) | \(m_b\) | \(m_c\) |
|-------------|-----------|---------|---------|---------|
| electrons   | \(Pnnm\)-SiC | 0.4007  | 0.2991  | 0.2975  |
|             | \(Pm\)-SiC  | 3.2573  | 0.5291  | 0.4045  |
|             | \(\beta\)-SiC| 0.65    | 0.22    | 0.22    |
|             | Cal.\(^a\) | 0.68    | 0.23    | 0.23    |
| holes       | \(Pnnm\)-SiC | 1.8509  | 0.7891  | 1.5295  |
|             | \(Pm\)-SiC  | 4.1004  | 0.1872  | 5.6380  |
|             | \(\beta\)-SiC| 0.590   | 0.390   | 0.390   |
|             | Cal.\(^c\) | 0.593   | 0.393   | 0.393   |

\(^a\) Reference [60].
\(^b\) Reference [61].
\(^c\) Reference [62].

Table 5. Effective constant of elastic (in GPa), the constant of deformation potential (in eV) and carrier mobility (in \(10^3\) cm\(^2\) V\(^{-1}\)s\(^{-1}\)) of \(\beta\)-SiC, \(Pnnm\)-SiC, and \(Pm\)-SiC.

| Carrier type | Materials | \(C_{\text{eff},1}\) | \(C_{\text{eff},2}\) | \(E_i\) | \(E_{i1}\) | \(E_{i2}\) | \(\rho_i\) | \(\mu_{i1}\) | \(\mu_{i2}\) |
|-------------|-----------|-----------------|-----------------|-------|---------|---------|-------|---------|---------|
| electrons   | \(Pnnm\)-SiC | 469             | 455             | 494   | 15.21   | 24.25   | 8.64  | 1.64    | 0.84    | 7.20    |
|             | \(Pm\)-SiC  | 441             | 449             | 438   | 21.70   | 24.88   | 17.09 | 0.02    | 0.13    | 0.27    |
|             | \(\beta\)-SiC| 390             | 390             | 390   | 15.02   | 15.02   | 15.02 | 0.71    | 0.71    | 0.71    |
|             | Cal.\(^b\) | 0.75             | 0.75             |       |         |         |       | 0.75    | 0.75    |         |
| holes       | \(Pnnm\)-SiC | 469             | 455             | 494   | 19.81   | 23.12   | 8.72  | 0.03    | 0.04    | 0.17    |
|             | \(Pm\)-SiC  | 441             | 449             | 438   | 18.31   | 20.41   | 13.92 | 0.01    | 0.06    | 0.01    |
|             | \(\beta\)-SiC| 390             | 390             | 390   | 28.51   | 28.51   | 28.51 | 0.11    | 0.11    | 0.11    |
|             | Cal.\(^c\) | 0.12             | 0.12             |       |         |         |       | 0.12    | 0.12    | 0.12    |

\(^a\) Reference [64].
\(^b\) Reference [65].
\(^c\) Reference [66].

3.4. Carrier mobility

As for carrier mobility, a phonon-limited scatter model is adopted, in which we ignore ionized impurity scattering and the optical branch scattering, and the reason is that the main mechanism limiting carrier mobility is acoustic phonon scattering in intrinsic semiconductor. A three-dimensional carrier mobility of a solid can be computed as [63]:

\[
\mu_{3D} = \frac{2\sqrt{2\pi}}{3} \frac{\rho \mu_i^2 h^4 e}{E_i^2 m_i^6 (m_i^3 + \lambda_i^3 (k_b T)^{3/2})}
\]  

(8)

Where \(h\) is the reduced Plank constant; the value of \(k_b T\) is about 0.026 eV (\(T = 300\) K); the term \(E_i = \frac{1}{2}(|\Delta W_{i+}^+| + |\Delta W_{i-}^-|) / (\Delta I / \Delta I_0)\) shows the deformation potential constant of the valence band maximum about holes, or the minimum of conduction band about electrons. What is more, the energy change value in the \(i\) band under appropriate strain are \(\Delta W_{i+}^+\) and \(\Delta W_{i-}^-\), and 1% compression and dilatation have been applied in this calculation work. \(\lambda_i\) is the lattice constant of the transport orientation and \(\Delta I\) is the deformation relative to \(\lambda_i\); \(\rho\) and \(\nu\) mean the density of crystal and the velocity of acoustic. As for the relationship between \(\rho\) and \(\nu\), which can be defined as \(C_{\text{eff}} = \rho \nu^2\), and \(C_{\text{eff}}\) is the effective constant of elasticity.

The deformation potential constant (in eV), effective elastic constant (in GPa), and carrier mobility (in \(10^3\) cm\(^2\) V\(^{-1}\)s\(^{-1}\)) are displayed in table 5. The carrier mobilities \(\mu_{i1}, \mu_{i2}\), and \(\mu_{i3}\) are computed by utilizing the above equation (8), and the temperature (\(T\)) is set to 300 K. The carrier mobility of \(\beta\)-SiC is computed to prove the precision of the results of SiC in different phases. According to table 5, the calculated carrier mobilities (\(\mu_{e} = 710\) cm\(^2\) V\(^{-1}\)s\(^{-1}\), \(\mu_{b} = 110\) cm\(^2\) V\(^{-1}\)s\(^{-1}\)) of \(\beta\)-SiC are in fabulous accordance with the experimental results (\(\mu_{e} = 750\) cm\(^2\) V\(^{-1}\)s\(^{-1}\), \(\mu_{b} = 120\) cm\(^2\) V\(^{-1}\)s\(^{-1}\)) [64–66]. A high electron mobility (270 cm\(^2\) V\(^{-1}\)s\(^{-1}\)) and hole mobility (60 cm\(^2\) V\(^{-1}\)s\(^{-1}\)) is found in the \(Pm\)-SiC, but for the \(Pnnm\)-SiC has higher electron mobility (7200 cm\(^2\) V\(^{-1}\)s\(^{-1}\)) and hole mobility (170 cm\(^2\) V\(^{-1}\)s\(^{-1}\)) than the \(Pm\)-SiC, which indicates the \(Pnnm\)-SiC has good transport properties and more potential applications. However, both of SiC in different phases shows different calculation results in different directions, which indicates \(Pnnm\)-SiC and \(Pm\)-SiC all have carrier mobility anisotropy. In addition, we find that even if the effective mass of \(\beta\)-SiC is smaller than the \(Pnnm\)-SiC, the electron mobility of \(Pnnm\)-SiC is larger than \(\beta\)-SiC. There are two reasons for the result: on the one hand the
Phm-SiC (494 GPa) has larger effective elastic constant than β-SiC (390 GPa), and the other hand the deformation potential constant of β-SiC (15.02 eV) is larger than Phm-SiC (8.64 eV). so the Phm-SiC has larger electron mobility with a value of 7200 cm² V⁻¹ s⁻¹. Due to its high carrier mobility, the Phm-SiC has good transport properties and that is promising materials in the microelectronics area.

4. Conclusions

The structural, mechanical, and electronic properties, as well as anisotropy, and carrier mobility of SiC in different phases have been investigated using first principle calculations in view of DFT. The phonon spectra and elastic constants calculations illustrate that Phm-SiC and Phm-SiC are dynamically and mechanically stable under ambient pressure. What is more, through an analysis of elastic modulus, both of SiC in different phases are mechanically anisotropic, and Phm-SiC and Phm-SiC are naturally brittle materials because they have small values of Poisson’s ratio v (< 0.26). The calculations of band structure predict that Phm-SiC is an indirect semiconductor with a value of 3.12 eV, while Phm-SiC is a quasi-direct semiconductor with a value of 2.64 eV, which demonstrates the Phm-SiC has large potential applications in the optoelectronic devices area. The effective mass calculations show that effective mass of Phm-SiC is smaller than Phm-SiC, and both of SiC in different phases all have effective mass anisotropy. Finally, carrier mobilities of all different phases of SiC are calculated using a phonon-limited scatter model, and the result shows that a high electronic mobility (7200 cm² V⁻¹ s⁻¹) and hole mobility (170 cm² V⁻¹ s⁻¹) in the Phm-SiC, and both of SiC in different phases all have carrier mobility anisotropy.

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ORCID iDs

Yanxing Song https://orcid.org/0000-0002-5026-1431
Wei Zhang https://orcid.org/0000-0001-5802-9488

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