Corrigendum: Effects of boron doping on the fabrication of dense 6H-SiC ceramics by high-temperature physical vapor transport (2021 J. Phys.: Conf. Ser. 2045 012001)

B B Liu¹, J Huang² and J F Yang¹
¹ State Key Laboratory for Mechanical Behavior of Materials, Xi'an Jiaotong University, Xi'an 710049, PR China.
² College of Chemistry and Chemical Engineering, Xi'an Shiyou University, Xi'an 710065, PR China.

Page 4

Figure 2 in this paper was based upon a figure first published in reference [14] in the paper. The authors apologise for failing to include this citation in their figure caption.

[14] Dai P Y, Wang Y Z 2011 Fabrication of highly dense pure SiC ceramics via the HTPVT method Acta Mater. 59 6257-6263

Page 5, 6

Since publishing this article, it has come to the author’s attention that equations 6 and 7 in the article contain some inaccuracies. The correct equations are:

\[ \Delta H = E_{\text{total}} - \left( N_{\text{Si}} E_{\text{Si(atom)}} + N_{\text{C}} E_{\text{C(atom)}} + N_X E_{\text{X(atom)}} \right) \] (6)

\[ \Delta_{\text{defect}}(X) = E_{\text{total}}(Doped,cell) - E_{\text{total}}(Pure,cell) - \sum \eta_i \mu_i + \Delta V \] (7)
Effects of boron doping on the fabrication of dense 6H-SiC ceramics by high-temperature physical vapor transport

B B Liu¹, *, J Huang², *, J F Yang¹

¹ State Key Laboratory for Mechanical Behavior of Materials, Xi’an Jiaotong University, Xi’an 710049, PR China.
² College of Chemistry and Chemical Engineering, Xi’an Shiyou University, Xi’an 710065, PR China.

*Corresponding emails: yupiner2003@163.com (B B Liu); huangjian1290@163.com (J Huang)

Abstract. In this paper, boron-doped dense 6H-SiC ceramics was fabricated by the high-temperature physical vapor transport (HTPVT) method. The effect of B doping on the crystal structure stability of 6H-SiC was investigated based on density functional theory (DFT). The results show that B doping can be realized even under thermodynamical equilibrium conditions. Nevertheless, it is found that the B doping effects on the (0001) of Si-plane and (000-1) of C-plane are significantly different. The doping experiments demonstrated that B can observably change the crystal growth morphology, leading to the formation of elongated 6H-SiC crystals.

1. Introduction
Dense SiC ceramics can be applied as high-performance structural components by virtue of their attractive high-temperature properties, such as high temperature strength, corrosion resistance, good thermal conductivity, oxidation resistance, and a relatively low thermal expansion coefficient [1, 2]. Much attention has been paid to doping technology for the improvement of SiC density by controlling the crystal growth processes [3-6]. An important way is gas phase doping which allows the vapor containing target elements (such as N, Al, B, etc.) to be doped in the ceramics or crystals at high temperature during the crystal growth process. It is found that the doped element concentration in SiC crystals is not proportional to its calculated value in the growing environment, but tends to remain at a certain level [7-9]. This characteristic is the result of the competition between the doping elements and Si or C in the crystal growth process. However, the underlying reasons for the competition mechanism are still unclear [10-12]. Density functional theory (DFT), which has become one of the key approaches in the field of material design, makes it possible to understand the structure of doped materials and their properties after doping from a fundamental point of view [13]. Furthermore, the doping effect on crystal growth is systematically discussed. Therefore, it is of great theoretical value and practical significance to explore the deep-seated causes of the doping effect on the fabrication of dense SiC ceramics or single crystals [14-16].
2. Experimental procedure

2.1. Raw materials
Commercial SiC powders with the average size of 120 µm (purity 99.9%; specific surface area 0.018 m²·g⁻¹; Zaozhuang Li-yuan SiC Co., Ltd., Zao-zhuang, China) were used as the main raw materials. B₄C powder with the mean size of 5 µm (purity 99.99%) purchased from Alfa Aesar Company was used as the additive. Mixtures of SiC powder and B₄C powder with different weight percentage of B₄C (0, 0.2, 0.4, 1, 2, 4, and 7 wt%) were used as the raw materials.

2.2. Fabrication process
The SiC ceramic samples were prepared by the high-temperature physical vapor transport (HTPVT) method using a medium frequency vacuum induction furnace (3.5 kHz, Model ZGRS-160/2.55 Jinzhou Electric Furnace Co., Ltd., Jinzhou, China). The fabrication process consisted of the following steps. Firstly, a graphite crucible packed with the raw materials was loaded into the induction furnace, and then the vacuum pump was turned on to evacuate the furnace chamber to 0.01 Pa. Subsequently, the crucible was heated to 1000°C to burn out the adsorbed contaminants. Thirdly, the vacuum pump was turned off and the crucible was gradually heated up to 2350°C under an argon pressure of 50 kPa. Then the ambient pressure in the furnace chamber was evacuated down to 10 kPa to trigger the deposition of SiC ceramics. During the deposition period, the heating power was maintained constant to keep the temperature of the bottom of the crucible at 2350°C (the temperature measured at the top of the crucible was about 2200°C, which implies a mean temperature gradient of about 30°C/cm). After firing for 1 h, the heating was stopped (by switching off the heating power) and an argon pressure of approximately 1 atm was introduced to the furnace to prevent the SiC ceramics from further decomposition. In this manner a polycrystalline SiC specimen with 10 mm in diameter and 8 mm in thickness could be obtained.

2.3. Characterization and calculation
The phase composition of SiC samples was characterized by X-Ray diffraction (XRD, Bruker D8 Advance, Germany) using Cu Ka radiation, the microstructures were observed by scanning electronic microscopy (SEM, Hitachi S4800, Japan), and the bulk densities of specimens were measured by the Archimedes method. The electrical resistance of the specimens was measured by a digital four-probe tester (DFPT, JG ST2253, China). The total energy and electronic structure calculations were carried out with the Cambridge Serial Total Energy Package (CASTEP)5 (DFT)6 code based on density function theory with the plane-wave ultrasoft pseudopotential method. [15]

3. Results and discussion

3.1. Effects of B₄C doping contents on the microstructure of SiC ceramics
Figure 1 shows the XRD patterns of SiC ceramics fabricated by HTPVT for 60 min with different contents of B₄C (0 wt%, 0.4 wt%, 1 wt% and 2 wt%) in the raw materials. It could be seen that when the B₄C content was 0.4 wt% or below, only two diffraction peaks were observed, located at 35.6° and 75.4°, corresponding to the (0006) and (00012) crystal faces of 6H-SiC, respectively, demonstrating that the crystal grains of 6H-SiC maintained the preferential growth characteristic and preferred to grow along the [0001] direction. When increasing the B₄C content to 1 wt%, the peak intensity corresponding to the (0006) plane of the SiC ceramic sample was significantly weakened, and the peak of the (00012) plane even disappeared completely, but peaks of (1 0 1 0), (1 0 1 3), (1 0 1 8), and (1 1 2 6) planes appeared and gradually increased, indicating that the preferred orientation along the [0001] was obviously weakened. As B₄C content was increased to 2 wt% in the raw materials, it was found that the relative intensities of the diffraction peaks corresponding to the (0006) and (00012) crystal faces is further weakened, indicating further weakening of the preferred orientation. Therefore,
it is observed that introducing B$_4$C in the raw materials can change the preferred grain (crystallite) orientation in SiC ceramics, which has a significant influence on the properties of SiC ceramics.

Figure 1. XRD patterns of SiC ceramics fabricated with different contents of B$_4$C in the raw materials: (a) 0 wt%, (b) 0.4 wt%, (c) 1 wt% and (d) 2 wt%.

3.2. Effects of the contents of B$_4$C on the growth morphology of SiC ceramics

Figure 2 shows the low-magnification SEM micrographs of SiC ceramics fabricated from raw materials with different boron carbide contents. It can be seen that when the content of B$_4$C content is 0 wt% and 0.2 wt%, as shown in Figure 2a and Figure 2b, the angle between the two adjacent sides of the grain sections of the original silicon carbide ceramic surface is relatively close to 120°, and the corresponding grain morphology is hexagonal, distributed parallel to the surface of SiC ceramics. Notably, the text that the SEM micrographs were taken from the (untreated) specimen surface, not from a fracture surface and not from a thermally etched section. These growth morphology characteristics demonstrated that the grains of SiC ceramics have a preferred orientation of [0001], which is in accord with the result measured by XRD.

When the B$_4$C content was increased to 0.4 wt%, as shown in Figure 2c, the grains on the surface of silicon carbide ceramics are not single flakes, but flakes and strips interpenetrate and are randomly distributed, which means that the preferred orientation in the direction of [0001] is disturbed. However, there is still a large number of thick plates like grains on the ceramic surface, showing a certain preferred orientation. According to the XRD results, the exposed crystal surface should be (1 1 2 6) crystal surface.
Figure 2. Low-magnification SEM micrographs of SiC ceramics fabricated from raw materials with different B$_4$C contents. (a) 0 wt%; (b) 0.2 wt%; (c) 0.4 wt%.

It can also be observed that the silicon carbide ceramics prepared by HTPVT doped with B$_4$C have many “pores” on the boundary of the silicon carbide grains, as shown in Figure 2 (b, c). Based on the shapes and sizes, the holes can be called “pore channels defects”. These pore channels would inevitably decrease the densities of SiC ceramics doped with B. Since micropipe defects usually exist only along the direction of [0 0 0 1], when the contents of B$_4$C in the raw materials is lower than 0.2 wt%, the grain orientation in the corresponding silicon carbide ceramic along the (0 0 0 1) crystal plane is obvious [17]. With increasing B$_4$C content in the raw materials the orientation of the preferred orientation of the corresponding silicon carbide ceramic along the (0 0 0 1) crystal plane is gradually reduced. As a result, the proportion of the (0 0 0 1) crystal plane gradually decreases and the number of micropipes gradually decreases as well. However, the grain size becomes larger, resulting in a gradual increase in the density of the silicon carbide ceramic, as shown in Table 1. Moreover, as shown in Table 1, it is found that B doping in SiC ceramics also has a great influence on the bending strength and the resistance of SiC ceramics, which also correlates with the change of growth morphology of SiC ceramics. So, it is necessary to investigate the effect of B doping on the growth of the grains in SiC ceramics during the HTPVT process. The electrical resistance was estimated using the following formula: [12]

$$m = \frac{Cs \times w \times A}{K \times \gamma \times G}$$

where m is the doping amount (wt %), w is silicon carbide density (g/cm$^3$), atomic weight of boron (NA), G is target resistivity (Ω·cm), Cs is doping concentration (at %), A is atomic weight (NA), K is equilibrium constant (NA), γ is segregation coefficient (NA) and the calculated values of G are listed in Table 1 [10].
and thermal energies of the bulk.

In the eutectic product, carbide grains, and finally leading to the increase of the rate area under the act temperature gradient and concentrationorque.

If the temperature gradient and concentration of the temperature was substituted by an X atom, the ion of the temperature gradient and concentration.

−

The ceramic has a complex composition, including eutectic compounds Si

the number of atoms, respectively.

= 23

Si

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atom

atomic Density, bending strength and resistance of SiC ceramics.

Table 1. Density, bending strength and resistance of SiC ceramics.

| Sample | 0% B4C | 0.4% B4C | 1% B4C | 2% B4C | Standard Deviation |
|--------|--------|----------|--------|--------|--------------------|
| Theoretical Density (g/cm³) | 3.07 | 2.95 | 3.02 | 2.99 | ± 0.02 |
| Strength (MPa) | 335.00 | 311.00 | 285.00 | 271.00 | ± 17.00 |
| Resistance (Ω·cm) | 14.70 × 10⁹ | 9.30 × 10³ | 6.90 × 10³ | 3.25 × 10³ | ± 0.20 × 10³ |

3.3. Effect mechanism of doping B in SiC ceramics

Above 2100°C, B4C decomposes into C, B, BC2 and B2C, and the gas phase is mainly B and BC2, the quantity of B and BC2 being much higher than that of B2C. This gas mixture diffuses to the low temperature substrate area under the action of the temperature gradient and concentration gradient together with the decomposed gas phase of silicon carbide. The introduction of boron can effectively increase the diffusion coefficient of silicon and carbon [18, 19], accelerating the condensation process of gas molecules on the surface of silicon carbide grains, and finally leading to the increase of the grain growth rate in the silicon carbide ceramics. The eutectic transformation of the B-Si-C liquid phase system was studied by Chen et al. [20] At 2250°C the main products of the eutectic transformation of the B-Si-C liquid phase system are silicon carbide and boron carbide. The temperature is continuously decreasing, and the main reactions of eutectic transformation are [21]:

\[
\text{Liquid} + (\text{C}) \rightarrow \text{SiC} + \text{B}_4\text{C} \quad (1)
\]

\[
\text{Liquid} + (\text{B}) \rightarrow \text{B}_4\text{C} + \text{SiB}_6 \quad (2)
\]

\[
\text{Liquid} + \text{SiB}_6 \rightarrow \text{B}_4\text{C} + \text{SiB}_6 \quad (3)
\]

\[
\text{Liquid} + \text{B}_4\text{C} \rightarrow \text{SiB}_6 + \text{SiC} \quad (4)
\]

\[
\text{Liquid} \rightarrow \text{SiC} + \text{SiB}_6 + (\text{Si}) \quad (5)
\]

According to the literature [22], when the cooling rate is slow, the SiC in the eutectic product is mainly α-SiC, which increases the cooling rate of the liquid phase. In addition, the SiC in the eutectic product also have some extra β phase. Therefore, in addition to α-SiC and β-SiC, the boron-rich region of the original surface of the silicon carbide ceramic has a complex composition, including eutectic reaction products such as B4C and SiB6.

The theoretical formation enthalpy (ΔH) was calculated to validate the thermodynamic stability of the 6H-SiC-X structure, the formula for which is expressed as follows [23, 24]:

\[
\Delta H = \frac{1}{N_{\text{Si}} + N_{\text{C}} + N_{\text{X}}} [E_{\text{total}} - (N_{\text{Si}}E_{\text{Si(atom)}} + N_{\text{C}}E_{\text{C(atom)}} + N_{\text{X}}E_{\text{X(atom)}})],
\]

where \( E_{\text{total}} \) is the total energy of the bulk compound, and \( E_{\text{Si(atomic)}} \), \( E_{\text{C(atomic)}} \) and \( E_{\text{X(atomic)}} \) represent the energy of pure Si, C, and X atoms with equilibrium lattice parameters, and \( N_{\text{Si}} \), \( N_{\text{C}} \) and \( N_{\text{X}} \) are the number of atoms, respectively. \( E_{\text{SiC24X}} \) and \( E_{\text{Si24C23X}} \) represent the total energies of the bulk compounds \( \text{Si}_{24}\text{C}_{23}\text{X} \) and \( \text{Si}_{24}\text{C}_{23}\text{X} \), in which the Si atom or the C atom was substituted by an X atom, respectively. These are the two most typical SiC compounds, one carbon atom or one silicon atom is easily replaced. \( E_{\text{Si}} \) and \( E_{\text{C}} \) are the calculated results for \( \text{Si}_{24}\text{C}_{23}\text{X} \) and \( \text{Si}_{24}\text{C}_{23}\text{X} \), respectively, by formula (6). \( E_{\text{sub}} \) is defined as the substitution formation enthalpy, which is calculated by formula (7).
\[ E_{\text{site}} = E_C - E_{\text{Si}} \]  

(7)

If the value of \( E_{\text{site}} \) is positive, the X atom will replace the Al atom preferentially, or the X atom will replace the Fe atom. These elements (Al or Fe) could be originated from the interfacial Al or Fe atoms. When the temperature is raised to 700°C, the molten aluminum is hydraulically poured into the SiC prefabricated part in the graphite mold, and the pressure is maintained for 10 min for impregnation. Finally, when the infiltration temperature was reduced to 300°C, the sample will be cooled down to room temperature and the Al/SiC composite can be obtained by demoulding.

| Table 2. Calculated values of \( E_{\text{total}}, \Delta H \) and \( E_{\text{site}} \) in 6H-Si-X (X=Fe, C or B). |
|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| Phase | \( E_{\text{total}}(C)(\text{eV}) \) | \( E_{\text{total}}(\text{Si})(\text{eV}) \) | \( \Delta H_C(\text{eV}) \) | \( \Delta H_{\text{Si}}(\text{eV}) \) | \( E_{\text{site}}(\text{eV}) \) |
| C | — | -6353.61 | — | -7.59 | — |
| B | -6229.44 | -6276.84 | -7.48 | -7.56 | 0.07 |

Usually, the equilibrium lattice parameters were evaluated by measuring by analyzing X-ray diffraction patterns using Rietveld’s method. Here, the equilibrium lattice parameters have been calculated via the CASTEP software of the National Supercomputing Center in Shenzhen, China. All calculated results are listed in Table 2 and Table 3. It is found that all \( E_{\text{site}} \) exhibit positive values, suggesting that these (Al/Fe/B) ternary additions have stronger preference for the Si sites than for the C sites.

It can be seen from the calculation results in the table that the cohesive energy and the generated enthalpy of all doping models are less than zero, which indicates that 6H-SiC polycrystals can exist stably within a certain doping concentration range (as shown in practice). However, the inclusion of these doping elements is generally difficult to perform under thermodynamic equilibrium conditions, the defect formation energy of other doping defects is significantly greater than zero except for the substitution of N-substituted C and B for Si.

| Table 3. Calculated lattice constants, cohesive energies, formation enthalpy and defect formation of 6H-SiC with different doping types (formula unit is abbreviated to f.u.) [25, 26]. |
|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| Doped crystal | Lattice constant /Å | Total energy /eV (cell) | Cohesive energy /eV (f.u.) | Formation enthalpy /eV (f.u.) | Defect energy /eV (cell) |
| 6H-SiC | 3.088 | 15.147 | -1577.354 | -15.175 | -0.774 | — |
| Si6C5B | 3.099 | 15.565 | -1497.112 | -14.338 | -0.392 | 2.297 |
| Si5C6B | 3.040 | 14.822 | -1552.999 | -15.228 | -1.759 | -5.906 |

Boron B is known to be able to substitute for carbon atoms in all families of carbon materials, i.e. diamond, fullerenes and also graphite. N-substitution involved the intramolecular or intermolecular nitrogen atoms electrophilic or nucleophilic substitution reaction, in which one atom or functional group is replaced by other atoms or specific functional groups owing to the electron absorption effect of nitrogen. [22] The calculation results show that in the growth process of SiC polycrystal, B in the atmosphere can spontaneously enter the crystal lattice, and thus B can be blended faster with SiC under thermodynamic equilibrium conditions, which is consistent with the experimental observations.

Figure 3 shows SEM micrographs of SiC crystals obtained at 2300°C after different sintering times (1 h and 2 h, respectively) with 7 wt% B₄C content in the raw materials. It can be seen that there are obvious voids in the crystal grown for 1 h, the crystal orientation is weak, and the voids at the interface exhibit triangular cross sections.
As the sintering time increases, the voids at the crystal interfaces disappear and there is obviously further grain growth; boron doping increases the grain growth rate in silicon carbide ceramics and changes the texture characteristics of the preferred orientation of the grains. Because the doping defect formation energy of B on the (000-1) C plane is (2.297 eV/cell) much larger than the doping defect formation energy (-5.906 eV/cell) on the (0001) Si plane, doping produces large fluctuations with the crystal plane arrangement of SiC along the c-axis [27, 28].

When the B content in the gas phase is high, the difference in doping characteristics on different crystal faces leads to the enrichment of B on the (0001) Si planes to form second phase B inclusion particles, and then through the growth step of the bypass model in the crystal a large number of defects is introduced, which seriously damages the quality of the crystal. [25] The expansion rate of this crystal plane direction is then higher than that of other crystal planes, which ultimately leads to the texture characteristics of the silicon carbide crystal grains which are preferentially oriented along the (0 0 0 1) crystal plane.

After boron nitride is added to the raw material powder, a gas phase such as B and BC₂ is introduced into the gas phase of the growth system, and these boron-containing gas phases are attached to the surface of the silicon carbide crystal grains, and the specific surface free energy of the crystal grain surface is reduced. It had been found that the first-order Raman spectra of B-doped 6H-SiC were shifted to higher frequency when comparing with undoped samples, revealing that there existed low free carrier concentration, possibly induced by the deep energy level effect of B impurity [29, 24].

It is worth noting that the presence of boron not only reduces the specific surface free energy of the (0 0 0 1) crystal plane, but also reduces the specific surface free energy of other crystal faces, that is, the introduction of boron causes silicon carbide crystals. The free energy of each surface of the particles is reduced, so that the difference between the growth rates of the grains in all directions becomes smaller, and the growth rate of the crystal grains along the (0 0 0 1) crystal plane is reduced. The doping experiments demonstrated that B can observably change the crystal growth morphology, which led to the preferred orientation of SiC ceramic grains decreases, and tends to be isotropic random orientation with the increase of boron nitride content in the raw material powder.

4. Conclusions
The effects of doping B on the chemical stability and crystal structure and the microstructure of SiC ceramics are studied by experiments and calculations based on DFT theory. It is found that the cohesive energy and the formation enthalpy of the doping B is less than zero, but the doping defect formation energy is obviously greater than zero. The doping characteristics of B on (0001) Si surface and (000-1) C surface of 6H-SiC crystal are different, which may lead to the enrichment of B in (0001) Si and the formation of B-rich inclusion particles, leading to a large number of micropipe defects formed in the grains of SiC ceramics. As a result, the density, bending strength and electrical
resistance of SiC ceramics were reduced. 6H-SiC polycrystals could exist stably in a certain doping concentration range, and the introduction of doping elements is generally difficult under thermodynamic equilibrium conditions, because the defect formation energy of doping defects is significantly greater than zero.

Acknowledgments
This work was supported by the National Natural Science Foundation of China (No. 51072157, 50821140308), Natural Science Basic Research Plan in Shaanxi Province of China (No. 2019JQ-490), and Doctoral Fund of Ministry of Education of China (No. 20100201110036). We also acknowledge the support of the CASTEP software of National Supercomputing Center in Shenzhen and the Modern Analysis and Testing Center of Xi’an Shiyou University.

References
[1] Lee S K, Kim Y C, Kim C H 1994 Microstructural development and mechanical properties of pressureless-sintered SiC with plate-like grains using Al$_2$O$_3$-Y$_2$O$_3$ additives J. Mater. Sci. 29 5321-5329
[2] Ravi B G, Omotoye O A, Srivatsan T S 2000 The microstructure and hardness of silicon carbide synthesized by plasma pressure compaction J. Alloy Compd. 299 292-296
[3] Nawaz A, Mao W G, Lu C, Shen Y G 2017 Mechanical properties, stress distributions and nanoscale deformation mechanisms in single crystal 6H-SiC by nanoindentation J. Alloy Compd. 708 1046-1053
[4] Lilov S K 1993 Study of the equilibrium processes in the gas phase during silicon carbide sublimation Mater. Sci. Eng. B 21 65-69
[5] Yoshida K, Mukai H, Imai M 2007 Reaction sintering of two-dimensional silicon carbide fiber-reinforced silicon carbide composite by sheet stacking method J. Nucl. Mater. 367 769-773
[6] Jun H W, Lee H W, Song H, Kim B H 2004 Reaction-bonded silicon carbide tube fabricated by continuous sintering of double-walled preform Ceram. Int. 30 533-537
[7] Zhang X F, Yang Q, Jonghe L C 2003 Microstructure development in hot-pressed silicon carbide: effects of aluminum, boron, and carbon additives Acta Mater. 51 3849-3860
[8] Yuan R, Kruzie J J, Zhang X F 2003 Ambient to high-temperature fracture toughness and cyclic fatigue behavior in Al-containing silicon carbide ceramics Acta Mater. 51 6477-6491
[9] Gallardo-Lopez A, Munoz A, Marti nez-Fernandez 1999 High-temperature compressive creep of liquid phase sintered silicon carbide Acta Mater. 47 2185-2195
[10] Guo X Z, Yang H, Zhang L J 2010 Sintering behavior, microstructure and mechanical properties of silicon carbide ceramics containing different nano-TiN additive Ceram. Int. 36 161-165
[11] Cupid D M, Fabrichnaya O, Seifert H J 2007 Thermodynamic aspects of liquid phase sintering of SiC using Al$_2$O$_3$ and Y$_2$O$_3$ Int. J. Mater. Res. 98 976-986
[12] Kim Y W, Lee S H, Nishimura T, Mitomo M 2005 Heat-resistant silicon carbide with aluminum nitride and scandium oxide Acta Mater. 53 4701-4708
[13] Wu Q J, Xie J P, Wang A Q, Wang C Q 2019 Effects of vacancies at Al(111)/6H-SiC(0001) interfaces on deformation behavior: A first-principle study Comput. Mater. Sci. 158 110-116
[14] Dai P Y, Wang Y Z 2011 Fabrication of highly dense pure SiC ceramics via the HTPVT method Acta Mater. 59 6257-6263
[15] Van Rijswijk W, Shanafiel D J 1990 Effects of carbon as a sintering aid in silicon carbide J. Am. Ceram. Soc. 73 148-149
[16] Shi Y G, Yang J F, Dai P Y 2012 Fabrication and mechanism of 6H-type silicon carbide whiskers by physical vapor transport technique J. Cryst. Growth 349 68-74
[17] Tajima Y, Kingery W D 1982 Solid solubility of aluminum and boron in silicon carbide J. Am. Ceram. Soc. 65(2) C27-C29
[18] Hildenbrand D L, Hall W F 1964 The decomposition pressure of boron carbide and the heat of sublimation of boron J. Chem. Phys 68(5) 989-993
[19] Friederich K M, Coble K L 2010 Influence of boron on chemical interdiffusion in SiC during conversion of silicon fibers to SiC J. AM. Ceram. Soc. 66(8) 141-142
[20] Bracht H, Stolwijk N A, Laube M, et al. 2000 Diffusion of boron in silicon carbide: Evidence for the kick-out mechanism Appl. Phys. Lett. 77(20) 3188-3190
[21] Chen H M, Qi H Y, Zheng F, et al. 2009 Thermodynamic assessment of the B-C-Si system J. Alloy Compd. 481(1-2) 182-189
[22] Shaffer P T B 1969 The SiC phase in the system SiC-B$_4$C-C Mater. Res. Bull. 4(3) 213-219
[23] Liu B B, Yang J F 2019 Mg on adhesion of Al(111)/3C-SiC(111) interfaces from first principles study J. Alloy Compd. 791 530-539
[24] Liu B B, Yang J F, Shi Y G, Dai P Y 2020 Fabrication of Highly Dense Pure 6H-SiC Ceramics via the PVT Method Using sub-micron SiC powders Ceram-Silikáty 64 (2) 135-144.
[25] Sudarshan T S, Maximenko S I 2006 Bulk growth of single crystal silicon carbide Microelectron. Eng. 83(1) 155-159
[26] Hurle D I J 1994 Handbook of Crystal Growth Amsterdam: Elsevier Science 2 615
[27] Geiger G H, Poirier D R 1973 Transport phenomena in metallurgy New Jersey: Addison-Westley Publising Company press 204
[28] Kitanin E L, Ramm M S, Ris V V, et al. 1998 Heat transfer through source powder in sublimation growth of SiC crystal Mater. Sci. Eng. B 55(3):174-183
[29] Li X B, Chen Z Z, Shi E W 2012 Effect of impurities on the Raman scattering of 6H-SiC crystals Physica B Condensed Matter 405(10) 2423-6