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The 6*H*-SiC structure model: Further refinement from SCXRD data from a terrestrial moissanite

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ABSTRACT

The crystal structure of a terrestrial 6*H*-SiC moissanite has been refined in the $P6_3mc$ *S.G.* from area detector single crystal X-ray data, down to an *R*-index on the observed reflections of 0.0205. The cell parameters refined over all the collected reflections are $a = 3.0810(2)$ and $c = 15.1248(10)$ Å. The average Si-C bond lengths are 1.8898 Å, with average bonds along the stacking direction (1.8993 Å) slightly longer than those along the bilayer (1.8862 Å). The interlayer distances, defined as the distances along [0001] between Si-Si layers, which may occur either in cubic (*c*) or hexagonal (*h*) configurations, are maximal at the *c*-*h* interface (2.5270 Å) and minimal at the *h*-*c* interface (2.5165 Å), entailing that the *h*-bilayer is not equidistant from either *c*-bilayers. All the tetrahedral angles are identical within the experimental error and close to the ideal value of 109.47°, but those at the *c*-*h* interface, where a significant distortion of 0.15° is recorded. Finally, the anisotropic displacement factors are utterly very small, identical among different atoms within the experimental error, and significantly spherical. It thus appears that the 6*H*-SiC structure is affected by a slight relaxation along the [0001] stacking direction with respect to the ideal cubic structure, and that the relaxation is mainly accomplished at the *c*-*h* interface, i.e., at the twin-like boundary, where a bilayer in cubic configuration links a bilayer in antiparallel, hexagonal configuration. As far as we know this is the first crystal structure refinement of a natural 6*H*-SiC moissanite. Possible implications on the polytype stability in the light of these results are briefly discussed.

Keywords: 6*H*-SiC, moissanite, structure, SCXRD

INTRODUCTION

Silicon carbide was first found in terrestrial rocks by Bobrievich et al. (1957) in the diamond pipes of Yakutia, Russia, and was identified as the hexagonal α-SiC polymorph (moissanite *s.s.*). Since then, several works reported the terrestrial occurrence of SiC in a variety of rocks and petrogenetic environments (for a list of occurrences see Filippidis 1993). However, their significance has been extensively debated since the matter of laboratory contamination from cutting and grinding tools was often not rigorously addressed (Milton and Vitaliano 1984, 1985).

Recent studies, however, have confirmed the natural occurrence of SiC at least in kimberlites rocks, either as inclusions in diamond (Jaques et al. 1989; Moore and Gurney 1989; Otter and Gurney 1989; Leung 1990) or as mineral concentrates (Leung et al. 1990; Mathez et al. 1995) and, in one case, SiC has been reported as rock-forming mineral (Di Pierro et al. 2003). The reason for such enthusiasm surrounding natural SiC is that, like diamond and graphite, SiC may be an important C-bearing phase in the Earth's mantle. It may provide information about carbon cycling (Leung 1990; Leung et al. 1990) and redox condition, which in turn affects the volatiles composition in deep Earth, the occurrence of partial melting, and the geochemistry of chalcophile and siderophile elements (Mathez et al. 1995 and references therein).

In applied fields, SiC is largely exploited for its high hardness (the ceramic form of SiC—carborundum, H ~ 9¼—is one of the most employed abrasives), redox properties, thermal, and chemical resistance. However, the most attractive application of SiC relates to the fabrication of semiconductors. Actually, SiC has been proven capable of outperforming silicon in high-power, high-temperature, and high-frequency applications, though the difficulties in growing crystals with sufficiently low density of defects have represented an obstacle for the employment of SiC in electronic devices. Recently, a new seeded sublimation growth technique, named the repeated *a*-face (Nakamura et al. 2004), has been shown to produce "virtually dislocation-free" wafers, thus renewing the interest in SiC microchips.

The basic SiC structure can be described as a closed packed framework of Si atoms with C atoms occupying half of the tetrahedral sites. Of course, reciprocity exists between Si and C atoms. Alternatively, the structure may be seen as a covalent diamond derivative, formed by alternating Si and C atoms, linked through a sp^3 bond network. Because of the different ways of stacking SiC bilayers (a bilayer being defined by Si and C atoms overlapping along the direction of stack, see Fig. 1), silicon carbide exhibits an extensive range of defined structures, referred

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as polytypes after Baumhauer (1912). The most common phases are the hexagonal 2*H*, 4*H*, 6*H*, and 15*R* (referred also as α-SiC) and the cubic 3*C* (or β-SiC). In these symbols, numbers refer to the number of layers in a repeat unit along the stacking direction, and letters to the symmetry of the cell (Ramsdell 1947). Most of the long-period polytypes may be described through these basic structures. Because of the peculiarity of its structure, i.e., the occurrence of polytypism and frequent stacking disorder, SiC was used as an example by Dornberger-Schiff (1956) to set the basis of the OD (Order-Disorder) theory (see also Ďurovič 1997, and references therein).

This report is on the crystal structure refinement of a 6*H*-SiC moissanite, which represents the high-temperature polymorph of SiC (stable above ~2400 K; see review article of Pandey and Krishna 1983 and Cheng et al. 1990a) and the most abundant polytype occurring in terrestrial rocks. As far as we know, this is the first crystal structure refinement of a terrestrial 6*H*-SiC and the second refinement of a natural SiC after the recent report of Lee et al. (2006), who refined the structure of a 33*R*-SiC from Luobusa harzburgite in Tibet. A detailed analysis of the geometrical features of the 6*H*-SiC structure and a comparison with literature data is presented in this paper. Relative stability of SiC polytypes in the light of the present results is briefly discussed.

THE 6*H*-SIC STRUCTURE

The 6*H*-SiC structure can be described by the sequence *A*α*B*β*C*γ*A*α*C*γ*B*β, where the Roman letters denote positions of the Si atoms and the Greek letters those of C atoms. Since the positions of C atoms are fixed with respect to the position of Si atoms, it is customary to omit the Greek letters and write the structure as *ABCACB*. This notation tells us that for a given layer with atoms in 000 position, say the *A*-layer, there is one layer above with atoms at 1/3 2/3 1/6 (*B*-layer), another layer with atoms at 2/3 1/3 2/6 (*C*-layer), and so on. While the sequences $A \rightarrow B \rightarrow C \rightarrow A$ involve a vector translation 1/3 2/3 1/6, the sequences $A \rightarrow C \rightarrow B \rightarrow A$ involve a vector translation 2/3 1/3 1/6. If one denotes the former by a plus (+) sign and the latter by a minus (–) sign, the *ABCACB* sequence can thus be described as (+ + + – – –). It turns out that when a (+) sequence switchs to a (–) sequence, a kink along the stacking direction occurs and, if the change is periodic, a zigzag pattern is formed. In the case of the 6*H*-SiC, kinks occur every three layers. Since layers on the opposite side of each kink are in antiparallel configuration, i.e., they are not just translated but also rotated by π, a twin-like boundary separates a (+) layer from a (–) layer. It follows that the 6*H* structure can also be described in terms of a cubic *ABC* sequence in which periodic twins occur with π-rotation around [111] as twin operator (Jepps and Page 1983). Finally, a layer is said to be in hexagonal (*h*) configuration if it is surrounded on either side by layers of the same type. Conversely, it is said to be in cubic (*c*) configuration if it is surrounded on either side by layers of different type. The 6*H*-SiC structure can thus be described also as *hcchcc*.

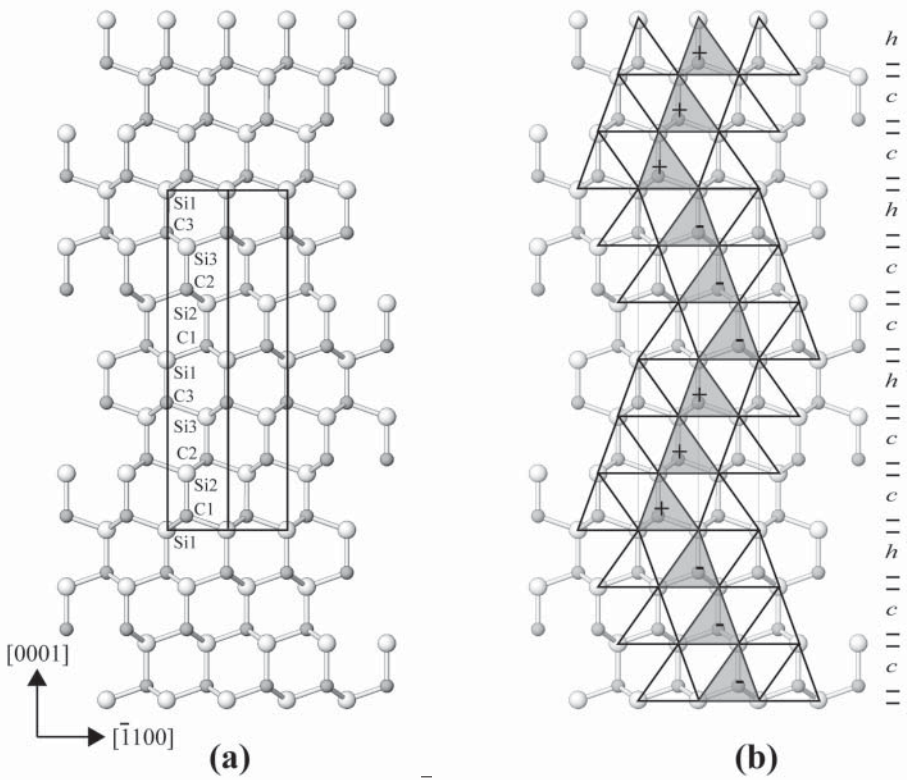

FIGURE 1. (**a**) The refined 6*H*-SiC structure as projected on the (11$\bar{2}$0) plane. (**b**) Same as before, but with superposition of the stacking scheme. For description see text.

SAMPLE AND METHODS

The moissanite crystal studied here was selected from a batch of crystals discovered in a volcanic rock pebble collected along the Turkish cost, around 150 km NW from Izmir. As pointed out by Di Pierro et al. (2003), the sample is practically free of impurities (e.g., Al), at least within the electron microprobe detection limit. Furthermore, the nature of the inclusions, the mineral assemblage, and the isotope signature, all point to the natural, terrestrial origin of the sample.

Single crystals were mounted on glass fibers and X-ray diffraction data collected at the Dipartimento Geomineralogico of Bari with a Bruker AXS X8APEX system equipped with a four-circle Kappa goniometer and a 4K CCD detector. All data were collected with a combination of φ–ω scans. A crystal-to-detector distance of 40 cm was employed to collect up to 1195 frames, with a scan width of 1° and a counting time 10 to 15 s per frame. Cell refinement and data reduction were performed with the SAINT+ v. 6.02 software (Bruker AXS-9/19/01). Raw intensity data were corrected for absorption using the SADABS v. 2.03 program (Sheldrick 1996). Relevant crystal data and experimental parameters for the studied sample are summarized in Table 1.

The crystal structure of the 6*H*-SiC was refined in the $P6_3mc$ space group with SHELXL-97 (Sheldrick 1997). Starting atomic coordinates were from Wyckoff (1963). All carbon and silicon atoms occur in special positions, with x and y coordinates constrained by the hexagonal axes, and z free to move. Anisotropic displacement parameters, a weighting scheme $w \approx 1/\sigma^2(\mathrm{I})$, and a secondary extinction parameter were employed during the refinement.

RESULTS

A preliminary survey of as-received, sub-millimeter sized moissanite crystals with the area detector diffractometer showed matrix indexing problems due to polytypic disorder. By contrast, electron diffraction and high-resolution imaging of the same crystals showed no stacking faults at the TEM scale and unambiguous 6*H* structure. These observations made us aware that the disorder was discrete and on a sub-millimeter scale, and that the faulted regions were possibly removed after the size-reduction occurred for preparation of the TEM sample. We were thus induced to attempt a single-crystal X-ray data collection on one of the crystals used for TEM observations.

The crystal was indexed as hexagonal and the matrix refinement over all the recorded reflections gives the following cell constants $a = 3.0810(2)$ and $c = 15.1248(10)$ Å, which upgrade $a = 3.080(1)$ and $c = 15.12(1)$ Å of Di Pierro et al. (2003). The average interlayer distance is 2.5208 Å with c/na ratio 0.8182 ($n = 6$ for a 6*H*-SiC). The ideal value for a close packed structure should be 0.8165 (diamond or β-SiC).

The refined atomic coordinates are reported in Table 2 and the Si-C bond lengths in Table 3. Si-C distances are all very similar (average value 1.8898 Å) but with the "in-plane" bonds (i.e., Si1-C1, Si2-C2, and Si3-C3, Fig. 1a) slightly shorter (average value 1.8862 Å) than the "off-plane" bonds (i.e., Si1-C3, Si2-C1, and Si3-C2; average value 1.8933 Å). The above experimental observations indicate a slight relaxation of the 6*H* structure along the stacking direction, i.e., an evidence of a hexagonal deviation from the cubic symmetry.

All the tetrahedral angles are identical within the experimental error and close to the ideal value of 109.47°, with the exception of those involving the central Si1. In fact, the Si1 tetrahedron shows a minor distortion, with the "in-plane" angle C1-Si1-C1 slightly higher (109.62°) than the ideal value, and the "off-plane" angle C1-Si1-C3 slightly smaller (109.32°), as if the central atoms (Si1) were dislocated toward the basal plane defined by the C1 atoms (or the C1 atom toward the Si1 plane).

With respect to the interlayer distances, defined as the distance between Si-Si layers along [0001], the Si1-Si3 distance (2.5270 Å) is significantly larger than the Si1-Si2 and the Si2-Si3 distances (2.5165 and 2.5189 Å, respectively). In other words, the *h*-bilayer is not equidistant from the adjacent *c*-bilayers (Fig. 1b).

Finally, the anisotropic displacement factors (Table 4) are utterly very small and identical among different atoms within the experimental error and significantly spherical. This is not surprising since the Debye temperature of SiC is high (1400–1800 K, Gomes de Mesquita 1967) and in agreement with the substantial degree of order observed at the TEM and the lack of impurities in the bulk composition.

DISCUSSION

A previous report of a 6*H*-SiC moissanite from northwest Bohemian volcanic breccias (Bauer et al. 1963) shows in comparison a shorter a parameter (3.06 Å) and an exceedingly long c parameter

TABLE 1. Crystal data and experimental parameters for 6*H*-SiC moissanite

Empirical formula/Z	SiC/6
Formula weight	40.10
Temperature	293(2) K
Wavelength	0.71073 Å
Space group	$P6_3mc$
Unit-cell dimensions	$a = 3.0810(2)$ Å; $c = 15.1248(10)$ Å
Volume	124.338(14) Å^3
Density (calculated)	3.213 Mg/m^3
Absorption coefficient	1.551 mm^{-1}
F(000)	120
Crystal size	0.60 × 0.20 × 0.05 mm^3
Theta range for data collection	2.69 to 36.32°
Index ranges	$-5 \le h \le 4$, $-3 \le k \le 5$, $-25 \le l \le 24$
Reflections collected	3257
Independent reflections	295 [R(int) = 0.0512]
Completeness to theta = 36.32°	94.1%
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	295/0/19
Goodness-of-fit on F^2	1.157
Final R indices [I>2σ(I)]	$R1 = 0.0205$, w$R2 = 0.0400$
R indices (all data)	$R1 = 0.0250$, w$R2 = 0.0431$
Absolute structure parameter	–0.2(2)
Extinction coefficient	2.53(11)
Largest diff. peak and hole	0.465 and –0.831 e·Å^{-3}

TABLE 2. Atomic coordinates (×10^4) and equivalent isotropic displacement parameters (Å^2× 10^3) for 6*H*-SiC moissanite

	x	*y*	*z*	*U*(eq)
Si1	0	0	0	5(1)
Si2	3333	6667	1664(1)	5(1)
Si3	6667	3333	3329(1)	5(1)
C1	3333	6667	412(2)	5(1)
C2	6667	3333	2080(2)	5(1)
C3	0	0	3746(2)	5(1)

Note: U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

TABLE 3. Bond lengths (Å), angles (°), thickness of the interlayer (Å), relative changes (%) of the bond lengths, and of the interlayer thickness for 6*H*-SiC moissanite

Si1-C1	1.8850(8)	C1-Si1-C1	109.62(6)	<Si-C>	1.8898	$\Delta L_1/L_0$	0.381
Si1-C3	1.897(3)	C1-Si1-C3	109.32(7)	<$\mathrm{Si_n}$-$\mathrm{C_n}$>	1.8862	$\Delta L_2/L_0$	0.169
Si2-C2	1.8867(9)	C2-Si2-C2	109.47(7)	<$\mathrm{Si_n}$-$\mathrm{C_m}$>	1.8933	$\Delta L_3/L_0$	0.010
Si2-C1	1.893(2)	C2-Si2-C1	109.47(7)	Si1-Si2	2.5165 (8)	$\Delta d_1/d_0$	–0.171
Si3-C3	1.8869(9)	C3-Si3-C3	109.45(8)	Si2-Si3	2.5189 (7)	$\Delta d_2/d_0$	–0.075
Si3-C2	1.890(2)	C3-Si3-C2	109.49(8)	Si3-Si1	2.5270 (8)	$\Delta d_3/d_0$	0.246

Note: Si1-Si2, etc. = distances between planes defined by the named atoms; $\Delta L_1/L_0$ = [(Si1-C1) – (<Si-C>)]/(<Si-C>) and so on; $\Delta d_1/d_0$ = [(Si1-Si2) – (<Si-Si>)]/(<Si-Si>) and so on.

TABLE 4. Anisotropic displacement parameters ($Å^2 \times 10^3$) for 6*H*-SiC moissanite

	U_{11}	U_{22}	U_{33}	U_{12}
Si1	5(1)	5(1)	5(1)	2(1)
Si2	5(1)	5(1)	5(1)	2(1)
Si3	5(1)	5(1)	6(1)	2(1)
C1	6(1)	6(1)	4(1)	3(1)
C2	5(1)	5(1)	5(1)	2(1)
C3	5(1)	5(1)	5(1)	3(1)

Note: The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2\,h\,k\,a^*\,b^*\,U_{12}]$.

(15.88 Å), which leads to an unrealistic *c*/*na* distortion of 0.8649. Our results match better with the report of Leung (1990) for two crystals of moissanite included in diamond from Fuxian (China) kimberlites: (1) $a = 3.077(3)$, $c = 15.09(1)$; and (2) $a = 3.082(3)$, $c = 15.12(1)$ Å, which also gives reasonable *c*/*na* distortions (0.8174 and 0.8177, respectively).

High-precision cell constants determined for synthetic Lely grown 6*H*-SiC single crystals, which could deviate from natural crystals since the growth conditions are different, gives indeed similar results: $a = 3.0806(5)$, $c = 15.1173(8)$ Å, $c/na = 0.8179$ (Taylor and Jones 1959, as quoted in Gomes de Mesquita 1967); $a = 3.08129(4)$, $c = 15.11976(6)$ Å, $c/na = 0.8178$ (Bauer et al. 1998).

From the Results section, it appears that the 6*H*-SiC structure is affected by a slight relaxation along the [0001] stacking direction with respect to the ideal cubic structure and that the relaxation is mainly accomplished at the *c*-*h* interface, indicating that the *h*-bilayer is not equidistant from either *c*-bilayers. In other words, most of the distortion features of the 6*H* structure occur at a twin-like boundary (*TLB*), where a bilayer in cubic configuration links a bilayer in antiparallel, hexagonal configuration (Fig. 1b).

This relaxation was first envisaged by Taylor and Laidler (1950) after high-resolution Debye-Scherrer studies of synthetic silicon carbide powders. However, those authors did not realize that relaxation occurs at different degrees in different interlayers along the stacking direction.

Gomes de Mesquita (1967) refined a synthetic 6*H*-SiC and correctly found that relaxation along the *c*-axis is mostly accomplished by the *h*-*c* interface. However, faced with the difficulties to precisely locate the *h*-bilayer, the author arbitrarily assumed equidistance between the *h* and *c* bilayers.

More recently, Bauer et al. (1998, 1999) determined the atomic coordinates in synthetic 6*H*-SiC by a combination of precise single-crystal X-ray diffraction and first principles calculations. They found relative changes of the interlayer thickness as high as 0.102% and fluctuations of the Si-C bond lengths along [0001] as high as 0.32%. Our results show changes in the interlayer thickness more than twice as much, and slightly higher Si-C bond fluctuations (Table 3). However, because of the ambiguity of the method used, those authors could not define the sign of the relaxation parameters, i.e., which specific bilayer, hexagonal or cubic, contracts or expands in the stacking sequence. Moreover, the bond lengths in both cubic layers were assumed identical.

The ambiguity was solved by Bauer et al. (2001) through two independent methods: (1) by gathering additional phase information of the measured "quasiforbidden" reflections by collecting Renninger-scans (ψ-scans) profiles and comparing them with theoretically calculated profiles for each possible relaxation model; (2) by comparing bond lengths between atoms which have equivalent vicinities in the polytypes 6*H* and *4H* (i.e., their respective *hc* parts were assumed similar). In both methods Si-C bond lengths in the hexagonal bilayer were longer than in the cubic bilayer. Also in this case, however, the cubic bilayers were assumed equivalent.

In conclusion, the most relevant result of this study is that in the *hcc* sequence of 6*H*-SiC moissanite, the two cubic bilayers are noticeably different, since one of them is in parallel configuration with respect the adjacent *h*-bilayer, while the other is in antiparallel configuration, i.e., the latter forms a *TLB* with the *h*-bilayer, which accomplishes most of the relaxation. Since longer interatomic distances are present at the *TLBs*, we may tentatively infer that substitutional impurities with larger atomic radius than silicon, such as aluminum for instance, may stabilize polytypes with higher percentage of *h*-layers in the structure, i.e., with higher frequency of *TLBs*: 2*H* (2/2) > 4*H* (2/4) >15*R* (2/5)> 6*H* (2/6). Indeed, as reviewed by Pandey and Krishna (1983), Al as an impurity has been shown to stabilize the 4*H*-SiC structure at higher temperatures with respect the 6*H* structure. To confirm this issue, further studies coupling structure refinements and ion microprobe analyses of additional SiC polytypes are needed.

One of the main concerns about SiC polytypism relates to whether polytypes are genuine equilibrium phases or phases controlled by growth factors. At least for polytypes with short repeat distances along the *c*-axis, ab initio total-energy calculations indicate that stability might correspond to free-energy minima under certain conditions of growth (e.g., Cheng et al. 1988, 1990a; Park et al. 1994). In contrast, there are plausible growth mechanisms for the origin of higher-order polytypes (Pandey and Krishna 1983), although the energetic effects of long-range interactions cannot be excluded (Cheng et al. 1990a). In this respect, the relaxation energy associated with the distortion at *TLBs* may have some consequences on polytype stability (Cheng et al. 1990b; Käckell et al. 1994). It has been shown by experiment that with increasing growth temperature, the percentage of *h*-layers in the SiC structure decreases (Knippenberg 1963; Inomata et al. 1968). Since the frequency of twin faults in the structure is directly related to the percentage of *h*-layers, it is very probable that the relaxation energy at *TLBs* might influence the polytype stability. We believe that our results may represent an experimental reference, hopefully along with similar results on other polytypes, for further refinement of energy calculation schemes, eventually aiming to solve the issue of polytypism in SiC.

Finally, as pointed out by Käckell et al. (1994), atomic relaxations play an important role in finding the correct structural properties of SiC polytypes. Since the physical properties of materials depend on the structural properties, we believe that our results may be of some help in the future design of electronic devices riding the wave of the renewed interest in SiC semiconductors. For instance, the conduction band structures of the 6*H*-SiC would be more precisely assessed if theoretical calculations could be fine-tuned on the base of this improved structural model.

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