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

GIAN CARLO CAPITANI,1,* SIMONPIETRO DI PIERRO,2,† AND GIOACCHINO TEMPESTA

1Dipartimento Geomineralogico—Università degli Studi di Bari, Via Orabona 4, I-70125 Bari, Italy
2Ecole Normale Supérieure de Lyon—U.M.R. 5570—Laboratoire “Sciences de la Terre” 46, Allée d’Italie, 69364 Lyon Cedex 07, France

ABSTRACT

The crystal structure of a terrestrial 6H-SiC moissanite has been refined in the P63mc 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 6H-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 6H-SiC moissanite. Possible implications on the polytype stability in the light of these results are briefly discussed.

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

INTRODUCTION

Silicon carbide was first found in terrestrial rocks by Bobrie
dich et al. (1957) in the diamond pipes of Yakutia, Russia, and was identified as the hexagonal \(\alpha\)-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, \(H \approx 9\frac{3}{4}\)—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 to as polytypes.