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

Gian Carlo Capitani,[1,*] Simonpietro Di Pierro,[2,†] and Gioacchino Tempesta[1]

[1]Dipartimento Geomineralogico—Università degli Studi di Bari, Via Orabona 4, I-70125 Bari, Italy
[2]Ecole 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 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