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High-resolution X-ray Diffraction to elucidate Homogeneity Ranges in Intermetallics

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In course of a detailed analysis of various intermetallic compounds derived from the AlB_2 type structure, high-resolution X-ray diffraction on single crystals proved very powerful in deriving precise composition of individual phases. E.g., the homogeneity ranges of $EuGa_2$ and $SrGa_2$ were determined and associated structure distortions induced by changes in composition were analyzed. The structural models derived are also discussed on the basis of solid state NMR data and in comparison to quantum chemical calculations.

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Refinement of the crystal structure of a terrestrial 6H-SiC

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This contribution is part of a more comprehensive research project that includes the characterization of structural defects in SiC polytypes and their relations with the growth conditions [1],[2]. The structure of a 6H-SiC moissanite, previously described by ref. [3], has been refined anisotropically in the $P6_3mc$ S.G. from area detector single crystal X-ray data, down to an R index over the observed reflections of 0.0205 (see Figure). The cell parameters, refined over all the collected reflections, are $a = 3.0810(2)$, $c = 15.1248(10)$ Å, giving an average SiC-bilayer thickness of 2.5208 Å and a c/na ratio of 0.8182. The average Si-C bond lengths are 1.8898 Å, but with bonds along the stacking direction slightly longer (1.8993 Å) than bonds along the bilayer (1.8862 Å). The bilayer thickness, defined as the distance along [0001] between Si-Si layers, is maximum at the $c-h$ interface (2.5270 Å) and thinner at the $h-c$ and $c-c$ interfaces (2.5165 and 2.5189 Å, respectively). All the tetrahedral angles are identical within the experimental error and close to the ideal value of 109.47°, but those involved with Si1 central, that is to say at the $c-h$ interface, where a significant distortion is recorded. Finally, the anisotropic displacement factors are utterly very small, identical among different atoms within the experimental error, and significantly spherical. From the present study thus appears that the 6H-SiC structure is affected by a slight relaxation along the [0001] stacking direction with respect to the ideal cubic analogue, and that the relaxation is mainly accomplished at the $c-h$ interface, entailing that the h -bilayer is not equidistant from the c -bilayers on the opposite sides. In other words, most of the distortion features of the 6H structure occur at the antiphase boundary where a bilayer in ccp configuration links a bilayer in antiparallel, hcp configuration. As far as we know this is the first crystal structure refinement of a terrestrial SiC.



- [1] Agrosi G., Fregola R.A., Monno A., Scandale E., Tempesta G., Materials Science Forum, 2005, 483-485, 311.
[2] Tempesta G., Agrosi G., Capitani G.C., Fregola R.A., Scandale E., 2006, This congress.
[3] Di Pierro, S., Gnos, E., Grobèty, B. H., Armbruster, T., Bernasconi, S. M., Ulmer, P., Am. Mineral., 2003, 88, 1817.