Crystal structure of samarium pentagermanide, SmGe₅

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Abstract
GesSm, orthorhombic, Immm (no. 71), \(a = 3.9805(7) \) Å, \(b = 6.1522(9) \) Å, \(c = 9.839(2) \) Å, \(V=240.9 \) Å³, \(Z = 2\), \(R_g(\hat{F})=0.093, \) \(wR_{int}(\hat{F})=0.110, \) \(T = 295 \) K.

Source of material
Samarium pentagermanide was synthesized by a high-pressure high-temperature reaction as earlier reported in [1]. The precursor mixture was prepared by arc melting of samarium (Techn. Büro Dr. G. Lamprecht, 99.9 %, sublimed) and germanium (Chempur, 99.9999+ %) in a mass ratio 1:5. Precursor synthesis, sample loading and product recovery was performed in an argon atmosphere of a glove box (MBraun; H₂O, O₂ < 0.1 ppm). An X-ray powder diffraction pattern of the prereacted mixture evidenced the presence of SmGe₂ (JCPDS) [2] and unreacted Ge (cF8) [3]. High-pressure and high-temperature treatment at 10(1) GPa and 1123(100) K was realized in a multi-anvil press equipped with a Walker-type module [4]. The sample obtained by the high-pressure experiment exhibits a composition of SmGe₄.84(4) for the main phase according to EDXS measurements.

Experimental details
Lattice parameters were obtained by a least-squares refinement of 18 reflections with LaB₆ as internal standard (\(a = 4.15692 \) Å, Huber Image Plate Guinier camera G670, CuKα₁ radiation, \(\lambda = 1.54056 \) Å, \(3° < 2\theta < 100°\)). For the crystal structure refinement an X-ray powder diffraction measurement with synchrotron radiation at beamline ID31 of the European Synchrotron Radiation Facility [6] was performed. The results show that the intermetallic compound SmGe₅ crystallizes isostructurally to LaGe₅ [7].

Discussion
The structure of LaGe₅ [7] and the isotypic germanides GdGe₅ and NdGe₅ [8] can be described as consisting of condensed corrugated Ge layers (Gel in 2d). These segments are linked by germanium (Ge2 in 2d) and samarium atoms (Sm1 in 2a) which are located in channels oriented parallel to [100] [8]. The large displacement parameter of Ge2 motivated refinements of the crystal structure in the subgroups Imml, 1222, and /12/ml. The results show no significant improvement in comparison to a disordered model in space group Immm. After introducing the split position 8m for Ge2, the Uiso parameters of the germanium atoms are the same within experimental error.

The phase stability of the new samarium germanide at ambient pressure was investigated by DTA measurements between 300 K and 1473 K with a heating and cooling rate of 10 K/min. An irreversible exothermic multistage decomposition is observed in the temperature range from 545 K to 645 K evidencing the metastable character of the compound.

<table>
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<th>(y)</th>
<th>(z)</th>
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References