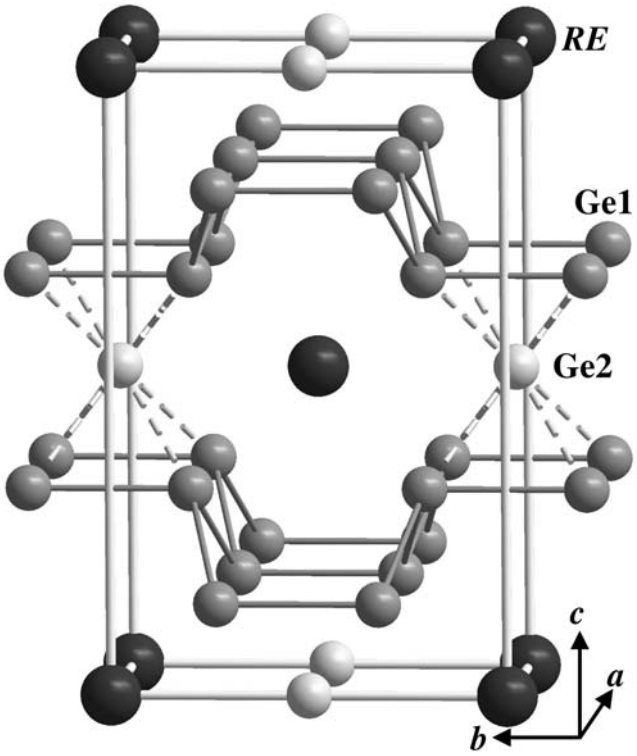
© by Oldenbourg Wissenschaftsverlag, München

Crystal structure of samarium pentagermanide, $SmGe_5$

Katrin Meier[I], Cevriye Koz[II], Alexander Kerkau[I] and Ulrich Schwarz[*,I]

[I] Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden, Germany
[II] Koç University, Rumelifeneri Yolu, 34450 Sariyer Istanbul, Turkey

Received May 28, 2009, accepted and available on-line June 24, 2009; CSD no. 710015



Abstract

Ge_5Sm, orthorhombic, *Immm* (no. 71), a = 3.9805(7) Å, b = 6.1522(9) Å, c = 9.839(2) Å, V = 240.9 Å^3, Z = 2, $R_{gt}(F)$ = 0.093, $wR_{ref}(I)$ = 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; H_2O, O_2 < 0.1 ppm). An X-ray powder diffraction pattern of the prereacted mixture evidenced the presence of $SmGe_2$ (*tI*12) [2] and unreacted Ge (*cF*8) [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 $SmGe_{4.84(4)}$ for the main phase according to EDXS measurements.

Experimental details

Lattice parameters were obtained by a least-squares refinement of 18 reflections with LaB_6 as internal standard (a = 4.15692 Å, Huber Image Plate Guinier camera G670, $CuK_{\alpha 1}$ radiation, λ = 1.54056 Å, $3° \le 2\theta \le 100°$). 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 $SmGe_5$ crystallizes isostructurally to $LaGe_5$ [7].

Discussion

The structure of $LaGe_5$ [7] and the isotypic germanides $GdGe_5$ and $NdGe_5$ [8] can be described as consisting of condensed corrugated Ge layers (Ge1 in 8*l*). These segments are linked by germanium (Ge2 in 2*d*) and samarium atoms (Sm1 in 2*a*) 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 *Imm*2, *I*222, and *I*12/*m*1. The results show no significant improvement in comparison to a disordered model in space group *Immm*. After introducing the split position 8*m* for Ge2, the U_{iso} 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 1. Data collection and handling.

Powder:	black, particle size < 63 μm
Wavelength:	0.4 Å
μ:	107.7 cm^{-1}
Diffractometer:	Beamline ID31 at ESRF
$2\theta_{max}$, stepwidth:	33.4°, 0.002°
$N(hkl)_{measured}$:	255
$N(param)_{refined}$:	16
Programs:	WinCSD [5], DIAMOND [9]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site		x	y	z	U_{iso}
Sm(1)	2*a*		0	0	0	0.0055(1)
Ge(1)	8*l*		½	0.29399(8)	0.83068(5)	0.0069(2)
Ge(2)	8*m*	0.25	0.016(1)	½	0.0078(4)	0.0070(3)

* Correspondence author (e-mail: schwarz@cpfs.mpg.de)

Acknowledgments. We like to thank S. Leipe for supporting high-pressure syntheses and Dr. H. Borrmann, Dr. R. Cardoso-Gil, S. Hückmann, Dr. Yu. Prots for X-ray experiments. Dr. S. Hoffmann and S. Müller are gratefully acknowledged for measuring thermal properties. We thank Dr. U. Burkhardt, T. Vogel and P. Scheppan for EDXS analysis and Prof. Yu. Grin for valuable discussions.

References

1. Meier, K; Schnelle, W.; Schwarz, U.: Homonuclear 8-fold coordinated Ge in rare-earth metal pentagermanides. Z. Kristallogr., Supplement **29** (2009) 81.
2. Iandelli, A.: Intermetallic compounds of the rare earth metals. National physical laboratory, U.K., symposium **1** (1959) 3F-2-3F-11.
3. Swanson, H. E.; Tatge, E.: Standard X-ray diffraction powder patterns I. Nat. Bureau of Standards **539** (1953) 1-95.
4. Walker, D.; Carpenter, M. A.; Hitch, C. M.: Some simplifications to multianvil devices for high pressure experiments. Am. Mineral. **75** (1990) 1020-1028.
5. Akselrud, L. G.; Zavalii, P. Y.; Grin, Yu.; Pecharsky, V. K.; Baumgartner, B.; Wölfel, E.: Use of the CSD program package for structure determination from powder data. Mater. Sci. Forum **133-136** (1993) 335-340.
6. Fitch, A.: The High Resolution Powder Diffraction Beam Line at ESRF. J. Res. Nat. Inst. Stand. Technol. **109** (2004) 133-142.
7. Fukuoka, H.; Yamanaka, S.: High-pressure synthesis and superconductivity of $LaGe_5$ containing a tunnel germanium network. Phys. Rev. **B67** (2003) 094501.
8. Meier, K.; Kerkau, A; Schwarz, U.: Crystal structure of gadolinium pentagermanideand, $GdGe_5$ and neodymium pentagermanide, $NdGe_5$. Z. Kristallogr. NCS **224** (2009) 373-374.
9. Brandenburg, K.: DIAMOND. Visual Crystal Structure Information System. Version 2.0f. Crystal Impact, Bonn, Germany 1998.