

CRYSTAL STRUCTURE OF THE NEW TERNARY COMPOUND  $\text{Gd}_2\text{Ge}_{2.88}\text{Sb}_{0.65}$ 

Dankevych R. V., Tokaychuk Ya. O., Gladyshevskii R. E.

Department of Inorganic Chemistry, Ivan Franko National University of Lviv,

Kyryla i Mefodiya St., 6, 79005 Lviv, Ukraine

roman.dankevych@lnu.edu.ua

A systematic investigation of the Gd–Ge–Sb ternary system indicated the formation of a new ternary compound with high germanium content. Its crystal structure was refined by the Rietveld method using X-ray powder diffraction pattern of an alloy of nominal composition  $\text{Gd}_{37.5}\text{Ge}_{52.5}\text{Sb}_{10}$  collected at room temperature on a powder diffractometer STOE Stadi P (Cu  $K\alpha_1$ -radiation, angular range  $6^\circ \leq 2\theta \leq 110^\circ$ , step  $0.015^\circ$ ). The sample was synthesized from pure elements ( $\geq 99.8$  mass%) by arc melting under argon atmosphere and annealed under vacuum at  $600^\circ\text{C}$  for 720 h. Phase analysis of the sample revealed the presence of three phases: a new ternary compound (82.3(8) mass%),  $\text{Gd}_3\text{Ge}_5$  (structure type  $\text{Y}_3\text{Ge}_5$ , Pearson symbol  $oF64$ , space group  $Fdd2$ , 15.7(3) mass%), and  $\text{GdSb}$  (NaCl,  $cF8$ ,  $Fm-3m$ , 2.0(1) mass%). Refinement of the profile and structure parameters was performed using the FullProf Suite software package [1]. The composition of the new ternary compound was confirmed by energy-dispersive X-ray spectroscopy performed on a Tescan Vega3 LMU scanning electron microscope:  $\text{Gd}_{2.1(3)}\text{Ge}_{2.9(5)}\text{Sb}_{0.7(2)}$ .

The crystal structure of the ternary compound  $\text{Gd}_2\text{Ge}_{2.88(5)}\text{Sb}_{0.65(2)}$  belongs to the orthorhombic structure type  $\text{Gd}_2\text{Ge}_{2.94}\text{Sn}_{0.82}$ , Pearson symbol  $oS32$ , space group  $Cmcm$ ,  $a = 4.0198(2)$ ,  $b = 30.3729(18)$   $c = 4.1340(2)$  Å,  $R_B = 0.0580$ ,  $R_F = 0.0559$ . It is characterized by two sites for Gd atoms, four sites for Ge atoms, and one site for a statistical mixture of Ge and Sb atoms (Table). A particular feature of the structure is local positional disorder of part of the Ge atoms, which was modeled by split positions  $8f$  and  $4c$ , occupied to 27 and 39 % respectively, instead of one 4-fold site. The refined distances of the split sites are: 1.26(5) Å for Ge3–Ge3 and 0.65(6) Å for Ge3–Ge4.

Table. Atomic coordinates and isotropic displacement parameters  
in the structure of  $\text{Gd}_2\text{Ge}_{2.88(5)}\text{Sb}_{0.65(2)}$

Site	Wyckoff position	$x$	$y$	$z$	$B_{\text{iso}}, \text{\AA}^2$
Gd1	4c	0	0.44138(19)	1/4	0.52(4)
Gd2	4c	0	0.83411(17)	1/4	0.45(4)
0.35(2)Ge + 0.65(2)Sb	4c	0	0.2497(2)	1/4	0.81(6)
Ge1	4c	0	0.0907(17)	1/4	1.21(15)
Ge2	4c	0	0.6460(3)	1/4	1.17(14)
Ge3 (Occ. = 0.27(3))	8f	0	0.0085(9)	0.088(5)	1.2(-)
Ge4 (Occ. = 0.39(4))	4c	0	0.014(4)	1/4	1.2(-)

The structure type  $\text{Gd}_2\text{Ge}_{2.94}\text{Sn}_{0.82}$  belongs to the homologous series of structures containing triple layers of trigonal prisms and square nets, representing linear intergrowth of  $\text{AlB}_2$ - and  $\text{CaF}_2$ -type slabs.

[1] J. Rodríguez-Carvajal, *Commission on Powder Diffraction (IUCr), Newsletter* 26 (2001) 12-19.