

CRYSTAL STRUCTURE OF THE TERNARY COMPOUND GdAg₂Ge₂Parashchuk A., *Klymentiy N.*, Semuso N., Pukas S., Gladyshevskii R.

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

Kyryla i Mefodiya St. 6, 79005 Lviv, Ukraine

nastasia.klymentiy@lnu.edu.ua

Four ternary compounds, GdAg₂Ge₂, ~GdAgGe₃, Gd₃Ag₄Ge₄, and GdAgGe, were observed in the Gd–Ag–Ge system at 500 °C [1]. Later [2] the existence of two more compounds: Gd₂AgGe₆ and GdAg_{0.6}Ge_{1.4}, was reported at 600 °C in the same system. For the compound GdAgGe a complete structure determination was performed [3], whereas for the compounds Gd₃Ag₄Ge₄, Gd₂AgGe₆, and GdAg_{0.6}Ge_{1.4} cell parameters were determined and structure types were assigned [1,4]. For the compound ~GdAgGe₃ orthorhombic cell parameters were reported [1], whereas for the compound GdAg₂Ge₂ the structure type CeAl₂Ga₂ was assigned [1]. The aim of the present work was to confirm the existence of the ternary compounds GdAg₂Ge₂ and ~GdAgGe₃ at 600 °C and refine their crystal structures.

Alloys of nominal compositions Gd₂₀Ag₄₀Ge₄₀ and Gd₂₀Ag₂₀Ge₆₀ were synthesized from high-purity metals (Gd ≥ 99.86 mass%, Ag ≥ 99.999 mass%, Ge ≥ 99.999 mass%) by arc melting and annealed at 600°C for 720 h. The overall compositions of the samples and of the individual phases were investigated by means of energy-dispersive X-ray spectroscopy (scanning electron microscope TESCAN Vega 3 LMU) and the crystal structures of the phases present in the alloys were established by X-ray powder diffraction (diffractometer STOE Stadi P, Cu Kα₁ radiation).

According to the analysis by energy-dispersive X-ray spectroscopy, it was found that the alloy Gd₂₀Ag₄₀Ge₄₀ was single-phase and contained the ternary compound GdAg₂Ge₂ (Gd_{19.1(2)}Ag_{39.7(5)}Ge_{41.2(7)}), whereas the alloy Gd₂₀Ag₂₀Ge₆₀ contained three phases: two ternary compounds, Gd₂AgGe₆ (Gd_{22.1(3)}Ag_{12.7(6)}Ge_{65.2(6)}) and GdAg₂Ge₂ (Gd_{20.5(3)}Ag_{40.9(5)}Ge_{38.6(7)}), and elementary Ge. The experimentally determined overall composition, Gd_{20.9(3)}Ag_{19.3(5)}Ge_{59.8(6)}, is in good agreement with the nominal value Gd₂₀Ag₂₀Ge₆₀.

The phase content of the alloys was confirmed by X-ray powder diffraction. The compound GdAg₂Ge₂ in the Gd₂₀Ag₄₀Ge₄₀ alloy crystallizes with a CeAl₂Ga₂-type structure (Pearson symbol *tI10*, space group *I4/mmm*, cell parameters *a* = 4.19856(4), *c* = 11.0886(1) Å). In the sample Gd₂₀Ag₂₀Ge₆₀ the main phase (55(1) mass%) is Gd₂AgGe₆ and its crystal structure belongs to the Ce₂CuGe₆-type (*oS18*, *Amm2*, *a* = 4.19572(4), *b* = 4.06743(4), *c* = 21.1765(9) Å); the second phase (31(1) mass%) is GdAg₂Ge₂ (CeAl₂Ga₂, *tI10*, *I4/mmm*, *a* = 4.19938(6), *c* = 11.0898(9) Å) and the third phase (14(2) mass%) is elementary Ge.

A complete determination of the crystal structure of the compound GdAg₂Ge₂ was carried out (*R*_B = 0.0435, *R*_P = 0.0410, *R*_{wp} = 0.0538). Each kind of atom occupies a distinct Wyckoff position of the space group *I4/mmm*: Gd in *2a* (atomic coordinates 0 0 0, displacement parameter *B*_{iso} = 1.41(3) Å²), Ag in *4d* (0 ½ ¼, *B*_{iso} = 1.79(3) Å²), Ge in *4e* (0 0 0.3922(2), *B*_{iso} = 1.83(4) Å²). The ternary compound ~GdAgGe₃ was not observed under the experimental conditions applied here.

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