Crystal structures of the compounds R_3CuSe_6 (R = Gd, Tb and Dy) and $TbCu_{0.34}Te_2$

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Abstract

The crystal structures of the compounds R_3CuSe_6 (R = Gd, Tb and Dy) (Sm_3CuSe_6 structure type, space group *Pbcm*, Pearson symbol *oP40*) and $TbCu_{0.34}Te_2$ ($LaCu_{0.28}Te_2$ structure type, space group *Pbcm*, Pearson symbol *oP13.36*) were determined by means of X-ray powder diffraction: $a = 0.70902(3)$ nm, $b = 0.77850(3)$ nm, $c = 1.68576(7)$ nm, $R_I = 0.0882$ (Gd_3CuSe_6); $a = 0.70630(3)$ nm, $b = 0.77396(3)$ nm, $c = 1.67913(8)$ nm, $R_I = 0.0806$ (Tb_3CuSe_6); $a = 0.70463(4)$ nm, $b = 0.76962(4)$ nm, $c = 1.6680(1)$ nm, $R_I = 0.0928$ (Dy_3CuSe_6); $a = 0.75580(3)$ nm, $b = 0.81753(3)$ nm, $c = 0.60828(2)$ nm, $R_I = 0.0864$ ($TbCu_{0.34}Te_2$).
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1. Introduction

The existence of the Sm_3CuSe_6 and $Y_3Cu_{0.685}Se_6$ compounds (Sm_3CuSe_6 structure type, space group *Pbcm*) have been reported in Refs. [1,2], respectively. The crystal structure of the $LaCu_{0.28}Te_2$ compound ($LaCu_{0.28}Te_2$ structure type, space group *Pbcm*) has been determined in Ref. [3]. The formation of the compounds RCu_xTe_2 (R = Ce, Pr, Nd, Sm, Gd and Dy) isostructural to $LaCu_{0.28}Te_2$ have been established in Refs. [4–6].

This paper presents part of a systematic investigation of ternary rare earth chalcogenides with transition metals. The crystal structures of the new ternary compounds R_3CuSe_6 (R = Gd, Tb and Dy) and $TbCu_{0.34}Te_2$ are given.

2. Experimental details

The alloys were prepared by fusion of the high purity elements (the purity of the ingredients was better than 99.9 wt.%) in evacuated quartz ampoules. The synthesis was realized in a shaft furnace. The ampoules with the components were heated with a rate of 30 K/h to the maximal temperature of the synthesis, i.e. to 1420 K. The samples were kept at the maximal temperature during 4 h. After that they were cooled slowly to 870 K with a rate of 10 K/h and annealed at this temperature during 240 h. After annealing the ampoules with the samples were quenched in cold water.

X-ray powder diffraction pattern of the samples were recorded using a DRON-4-13 powder diffractometer (Cu Kα radiation, $10° \leq 2\Theta \leq 80°$, step scan mode with a step size of 0.05° and counting time of 1 s per data point). Phase analysis was carried out. X-ray powder diffraction patterns of the samples for the crystal structure determination were recorded using a DRON-4-13 powder diffractometer (Cu Kα radiation, $10° \leq 2\Theta \leq 100°$, step scan mode with a step size of 0.05° and counting time of 20 s per data point).

The crystal structure determination was performed using the CSD [7].

3. Results

3.1. Crystal structures of the R_3CuSe_6 (R=Gd, Tb and Dy) compounds

The existence of the R_3CuSe_6 (R = Gd, Tb and Dy) compounds was established during the investigation of the phase relations in the R−Cu−Se (R = Gd, Tb and Dy) systems.

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Table 1
Results of the crystal structure determination of the R_3CuSe_6 (R = Gd, Tb and Dy) compounds

Compound	Gd_3CuSe_6	Tb_3CuSe_6	Dy_3CuSe_6
Structure type	Sm_3CuSe_6	Sm_3CuSe_6	Sm_3CuSe_6
Number of formula units per unit cell	4	4	4
Space group	*Pbcm*	*Pbcm*	*Pbcm*
a (nm)	0.70902(3)	0.70630(3)	0.70463(4)
b (nm)	0.77850(3)	0.77396(3)	0.76962(4)
c (nm)	1.68576(7)	1.67913(8)	1.6680(1)
Cell volume (nm^3)	0.9305(1)	0.9179(1)	0.9045(2)
Number of atoms in cell	40	40	40
Calculated density (g/cm^3)	7.2023	7.3374	7.525
Absorption coefficient (cm^{-1})	1669.85	1386.34	1466.57
Radiation and wavelength (nm)	Cu 0.154178	Cu 0.154178	Cu 0.154178
Diffractometer	Powder DRON-4-13	Powder DRON-4-13	Powder DRON-4-13
Mode of refinement	Full profile	Full profile	Full profile
Number of atom sites	7	7	7
Number of free parameters	27	27	27
2Θ and $\sin\Theta/\lambda$ (max)	99.71 0.496	99.77 0.496	99.65 0.496
R_I, R_P	0.0882 0.1545	0.0806 0.1582	0.0928 0.1739
Scale factor	1.057(6)	1.114(8)	0.978(5)
Texture axis and parameter	[1 0 0] 1.00(2)	[1 0 0] 0.96(2)	[1 0 0] 1.04(3)

The similarity of the X-ray powder diffraction patterns of the compounds R_3CuSe_6 (R = Gd, Tb and Dy) and the recently reported compound $Y_3Cu_{0.685}Se_6$ (Sm_3CuSe_6 structure type) [2] allows it us to assume that these compounds are isostructural to Sm_3CuSe_6. The peaks of the X-ray powder diffraction patterns of these samples were indexed in an orthorhombic unit cell with the lattice parameters (Table 1) close to those reported for Sm_3CuSe_6. No extra peaks were present in the X-ray powder diffraction patterns of the R_3CuSe_6 (R = Gd, Tb and Dy) samples. The results of the crystal structure determination of the R_3CuSe_6 (R = Gd, Tb and Dy) compounds are given in Table 1. The atomic coordinates and isotropic
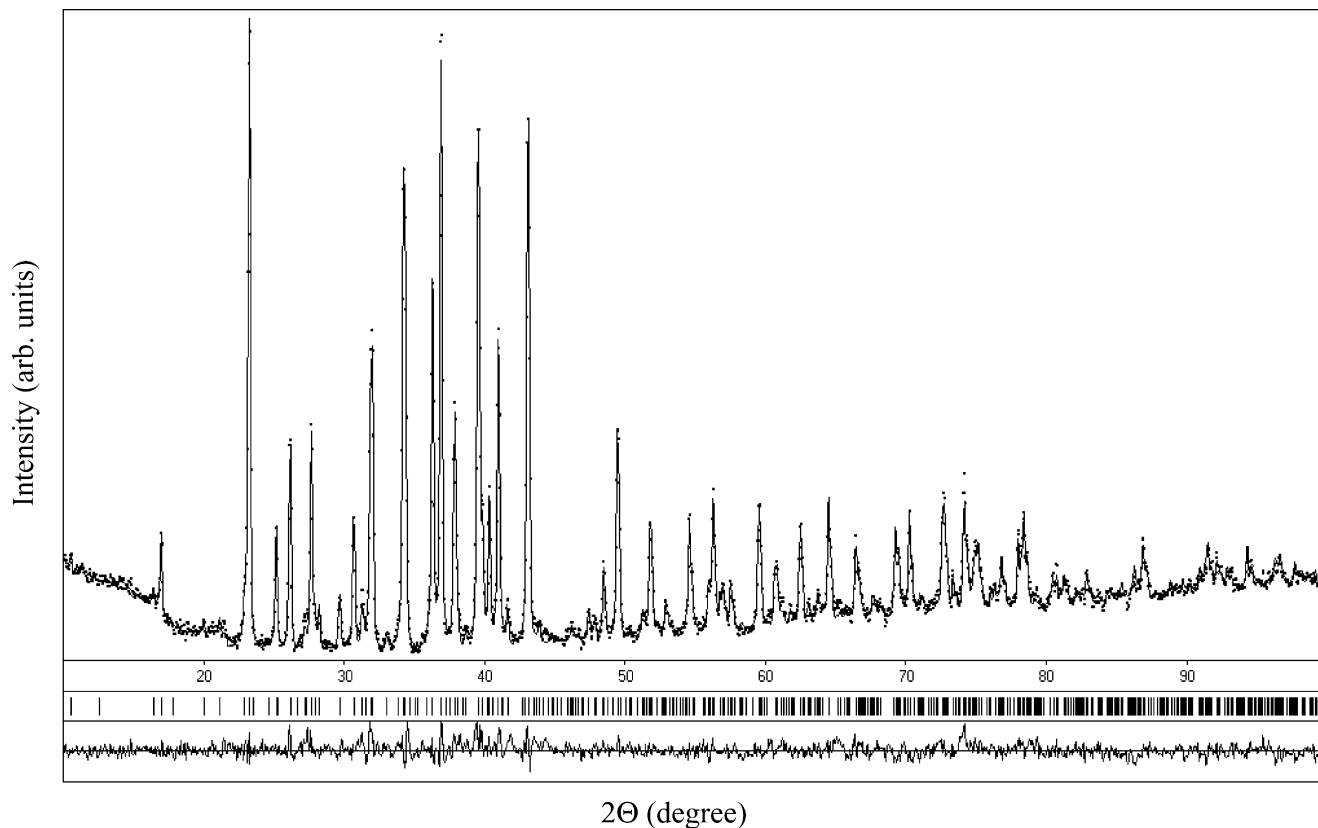

Fig. 1. The experimental and calculated diffractograms and the corresponding difference diagram for Gd_3CuSe_6.