NEW $R_3T_{1-x}Zn_x$ COMPOUNDS WITH $AuCu_3$ STRUCTURE TYPE

O. Zelinska, P. Solokha, V. Pavlyuk, A. Zelinskiy

Inorganic Chemistry Department, Ivan Franko National University of Lviv, Kyryla and Mefodiya Str., 6, 79005 Lviv, Ukraine

INTRODUCTION

For the first time ternary compounds with the $AuCu_3$ type of structure in the systems R–T–Zn (where R - rare earth and T - transition metals) were reported by authors [1, 2]. Among them $CeFe_{1.2}Zn_{1.8}$ (a = 0.5415 (1) nm) and $CeNi_{1.2}Zn_{1.8}$ (a = 0.5415 (1) nm).
This paper is devoted to investigation of the new representatives of the $AuCu_3$ structure type in the systems La–{Co, Cu}–Zn and Ce–Co–Zn with something another redistribution of the atoms in the Wyckoff positions.

EXPERIMENTAL

The samples were synthesized by arc melting of pure metals (lanthanum and cerium with a purity of 99,87 wt. %, cobalt and copper – 99,99 wt. %, zinc – 99,9 wt. %) in argon atmosphere at a pressure of 100 kPa. The alloys were annealed in evacuated quartz ampoules at 470 K for 2000 h and quenched in cold water. Powder patterns of the alloys were obtained by powder diffractometer HZG-4a (FeKα-radiation, $20° \leq 2\theta \geq 125°$, 0.02° step of scanning, 8 sec./one point speed of scanning). Determination and refinement of the crystal structure were performed by DBW-3.2S program [3].

RESULTS AND DISCUSSION

During systematic investigation of the phase equilibria in the La–Co–Zn, Ce–Co–Zn and La–Cu–Zn systems new ternary compounds in the rare earth-rich range were observed. X-ray powder patterns of the compounds were indexed in a cubic unit cell. Lattice parameters, intensities of the reflections and composition of the samples proved that these compounds are isostructural with the $AuCu_3$ structure type (space group $Pm\bar{3}m$, Pearson code cP4). Two of them have a homogeneity range of 3 at. % and their lattice parameters are a = 0,5332(2)÷0,5305(3) nm for $La_3Co_{0,40\text{-}0,52}Zn_{0,60\text{-}0,48}$ and a = 0,5307(4)÷0,5281(5) nm for $Ce_3Co_{0,40\text{-}0,52}Zn_{0,60\text{-}0,48}$. The refined lattice parameter for $La_3Cu_{0.48}Zn_{0.52}$ is equal a = 0.53108(2) nm.
Further refinement of the crystal structure of the $La_3Cu_{0.48}Zn_{0.52}$ ternary compound was performed by Rietveld method. It reveals that in the structure of this compound La are in the position of Cu (3c) and statistical mixture (Co+Zn) in the positions of Au (1a). The refined atomic and isotropic thermal

displacement parameters for $La_3Cu_{0.48}Zn_{0.52}$ are listed in Table 1. The values of the agreement factors R_p and R_{wp} are equal to 0.0276 and 0.0357 respectively. The interatomic distances have acceptable values for intermetallic compounds and are listed in Table 2.
Experimental X-ray powder pattern, calculated and difference diffraction profiles for the $La_3Cu_{0.48}Zn_{0.52}$ ternary compound are present in Fig. 1.

Table 1. Atomic and isotropic thermal displacement parameters of the $La_3Cu_{0.48}Zn_{0.52}$

Atoms	Site	x/a	y/b	z/c	$B_{iso}\cdot10^2$, nm^2
T (48 % Cu + 52 % Zn)	1a	0	0	0	1.19(2)
La	3c	0	1/2	1/2	0.65(1)

Table 2. Interatomic distances δ and coordination numbers (C.N.) in the $La_3Cu_{0.48}Zn_{0.52}$

Atoms		δ, nm	C.N.	Atoms		δ, nm	C.N.
La –	8La	0.37548(1)	12	T –	12La	0.37548(1)	12
	4T	0.37548(1)					

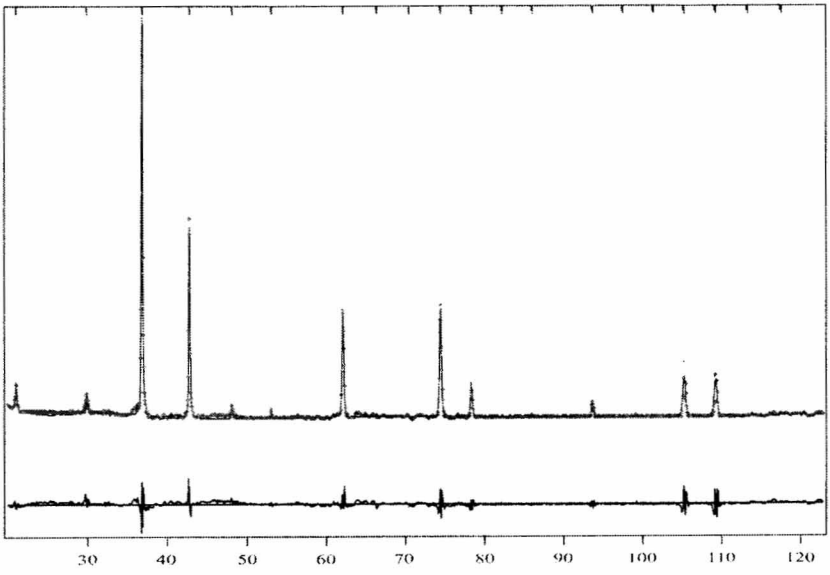

Figure 1. Experimental X-ray diffraction pattern, calculated and difference diffraction profiles for $La_3Cu_{0.48}Zn_{0.52}$

The projection of the $La_3Cu_{0.48}Zn_{0.52}$ unit cell on the xy plane is present in Fig. II. In the structure of $La_3Cu_{0.48}Zn_{0.52}$ compound the coordination polyhedra for all atoms are cuboctahedrons (C.N. = 12).

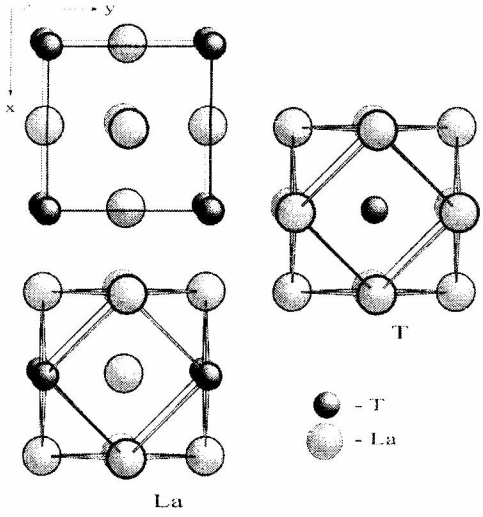

Figure 2. Projection of the $La_3Cu_{0.48}Zn_{0.52}$ unit cell on the xy plane and coordination polyhedra of the atoms.

Experimental investigation of the R–T–Zn systems shows that ternary compounds with the $AuCu_3$ structure are formed only in the systems where R = La or Ce. Moreover in the structure of the compounds rare earth metal can occupy the positions either of Au atoms 1a (in the compounds where T = Fe, Ni) or Cu atoms 3c (in the compounds where T = Co, Cu). Resembling redistribution of the atoms in the Wyckoff positions is typical for the binary compounds R_3X and RX_3 (where X = Al, In) and confirms the similarity of Zn to the elements of IIIa-group.

REFERENCES

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