CRYSTAL STRUCTURE OF THE NEW TERNARY COMPOUND $Zr_5Al_{0.41}Sn_{2.59}$

Maryskevych D. T., Tokaychuk Ya. O., Gladyshevskii R. E.
Department of Inorganic Chemistry, Ivan Franko National University of Lviv,
Kyryla i Mefodiya St. 6, 79005 Lviv, Ukraine
danylo.maryskevych@lnu.edu.ua

A new ternary compound was found at 62.5 at.% Zr during the investigation of the phase equilibria in the system Zr–Al–Sn at 600 °C. Its crystal structure was refined by the Rietveld method using X-ray powder diffraction pattern of a single-phase alloy of nominal composition $Zr_{62.5}Al_5Sn_{32.5}$ collected at room temperature on a powder diffractometer STOE Stadi P (Cu $K\alpha_1$-radiation, angular range $6^\circ \le 2\theta \le 110^\circ$, step 0.015º). The sample was synthesized from pure metals (≥ 99.9 mass%) by arc melting under argon atmosphere and annealed under vacuum at 600 °C for 720 h. Refinement of the profile and structure parameters was performed using the FullProf Suite software package [1].

The new compound, with refined composition $Zr_5Al_{0.412(11)}Sn_{2.588(11)}$, crystallizes with a ternary derivative of the W_5Si_3 type, the structure type Nb_5SiSn_2 (Pearson symbol *tI*32, space group *I*4/*mcm*, a = 11.1852(13), c = 5.5557(7) Å, R_B = 0.0688, R_F = 0.0646) and is characterized by statistical distribution of Al and Sn atoms in Wyckoff position 4*a*. Sn atoms alone occupy the second *p*-element site (8*h*). The composition of the compound as determined by energy-dispersive X-ray spectroscopy carried out on a Tescan Vega3 LMU scanning electron microscope ($Zr_{4.97(8)}Al_{0.43(7)}Sn_{2.60(9)}$), is fully consistent with the results of the Rietveld refinement.

The structure of the title compound is built from two types of column along the 4-fold axes (Fig.). On the one hand there are tetragonal antiprisms composed of Zr atoms from the Wyckoff position 16*k* site, centered by atoms of the statistical mixture Al/Sn ($d_{(Al/Sn)-Zr1}$ = 2.9464(19) Å), which share square faces, and on the other hand tetrahedra composed of Sn atoms centered by Zr atoms from the Wyckoff position 4*b* (d_{Zr2-Sn} = 2.9532(16) Å), connected via common edges. The shortest interatomic distance in the structure (2.7729(4) Å) is observed between atoms of the statistical mixture Al/Sn, indicating strong interaction.

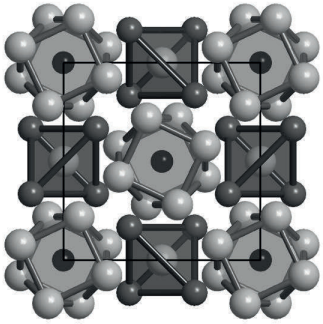

Fig. Projection of the structure of $Zr_5Al_{0.41}Sn_{2.59}$ onto the *xy* plane, emphasizing columns of tetragonal antiprisms $(Al/Sn)Zr_8$ and tetrahedra $ZrSn_4$ running along the crystallographic direction [001]

Table. Atomic coordinates and isotropic displacement parameters in the structure of $Zr_5Al_{0.412(11)}Sn_{2.588(11)}$

Site	Wyckoff position	x	y	z	B_{iso}, Å^2
Zr1	16*k*	0.0780(2)	0.21896(19)	0	0.58(5)
Zr2	4*b*	0	1/2	1/4	1.04(10)
Sn	8*h*	0.16485(15)	0.66485(15)	1/4	1.27(6)
0.588(11)Al + 0.412(11)Sn	4*a*	0	0	1/4	1.1(2)

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