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Interaction of Components in the Zr–Zn–Si System at 600°C

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The development of new materials requires systematic investigations of the interactions between the components in ternary and multicomponent systems, their phase diagrams, the composition and crystal structures of the compounds obtained. In this respect it is interesting to study the variation of the interactions of the components in Zr–Zn–X systems (where: X = an element of the 4 group).

The interaction of zirconium with zinc and silicon over the whole range of concentrations has not yet been studied. Phase equilibria in the side systems bounding the Zr–Zn–Si ternary system are complicated [1]. Crystallographic characteristics for the binary compounds of the Zn–Zr and Si–Zr according to [2] are listed in Table 1.

Table 1. Crystallographic parameters of the binary compounds of the Zn–Zr and Si–Zr systems [2].

Compound	Type	Space group	a, nm	b, nm	c, nm
SiZr	BFe	Pnma	0.6995(3)	0.3786(2)	0.5296(3)
	BCr	Cmcm	0.3757	0.9915	0.374
$SiZr_2$	Al_2Cu	I4/mcm	0.6609(3)		0.5298(3)
Si_2Zr	Si_2Zr	Cmcm	0.3721	1.468	0.3683
Si_2Zr_3	Si_2U_3	P4/mbm	0.7082		0.3714
Si_3Zr_5	Mn_5Si_3	P4			
Si_4Zr_5	Si_4Zr_5	$P4_12_12$	0.7123(1)		1.3002(1)
ZnZr	ClCs	$Pm\bar{3}m$	0.3336		
$ZnZr_2$	$MoSi_2$	I4/mmm	0.3303		1.126
Zn_2Zr	Cu_2Mg	$Fd\bar{3}m$	0.73950		
Zn_3Zr	--------	--------	0.816		1.623

In this communication we present our results of the isothermal section of the Zr–Zn–Si system at 600°C and data of new ternary compounds.

Isothermal section of the phase diagram of Zr–Zn–Si system has been constructed by X-ray phase analysis of 49 alloys. The alloys were prepared by sintering in quartz ampoules under vacuum at 600°C for 240 h with the following arc melting in argon.

Then they were annealed in quartz ampoules under vacuum at 600°C for 240 h. The purity of the starting metals was better than 99.9%. The powder diffraction patterns were obtained by using the diffractometers DRON-2 (FeK_α-radiation) SIEMENS (CoK_α-radiation). The lattice parameters and crystal structure refinement were calculated by means of LATCON and RIETVELD ANALYSES programs [3].

The phase diagram of the Zr–Zn–Si ternary system at 600°C is shown in Fig. 1. Five ternary compounds $Zr_5Zn_4Si_4$, $ZrZnSi_2$, $Zr_3Zn_5Si_2$, $Zr_6Zn_{23}Si$, and Zr_6ZnSi_3 were found. Lattice parameters for three of these compounds are presented in Table 2. Our investigation has shown, that the $Zr_5Zn_4Si_4$ compound crystallizes in the $Nb_5Cu_4Si_4$ structure type. The atoms of zirconium occupy positions 8(h): x y 0 (x = 0.3714, y = 0.3042) and 2(a): 0 0 0, like niobium atoms in the $Nb_5Cu_4Si_4$ structure. The atoms of zinc occupy positions 8(h): x y 0 (x = 0.1031, y = 0.4184), as atoms of copper. The atoms of silicon occupy positions 8(h): x y 0 (x = 0.2519, y = 0.0596) (R = 0.0542). Compound $ZrZnSi_2$ crystallizes in FeB structure type. The atoms of silicon occupy positions 4(c): x y z (x = 0.0396, y = 0.2500, z = 0.6300), like boron atoms in the FeB structure. The atoms of zirconium and zinc are statistically arranged in the position 4(c): x y z (x = 0.1777, y = 0.2500, z = 0.1244) (50% Zr + 50% Zn), as atoms of iron (R = 0.0462).

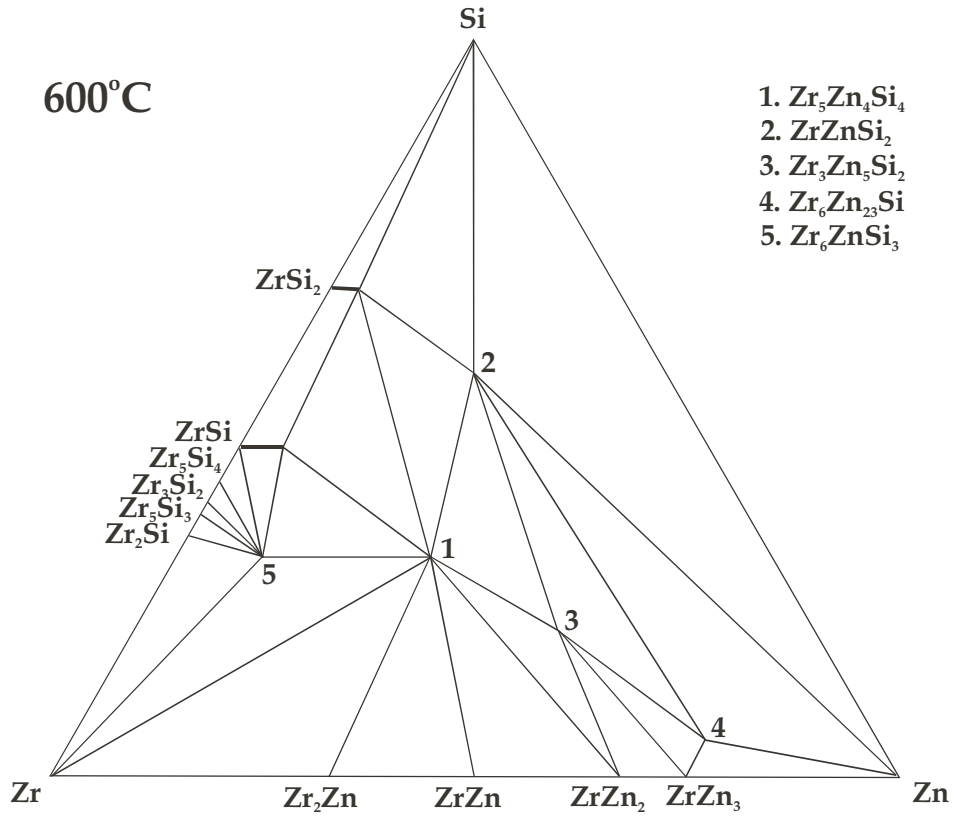

Figure 1. Isothermal section of the Zr–Zn–Si system at 600°C.

Table 2. Crystallographic characteristics of the ternary compounds of the Zr–Zn–Si system.

Compound	Structure type	Space group	a, nm	b, nm	c, nm
$Zr_5Zn_4Si_4$	$Nb_5Cu_4Si_4$	I4/m	1.0340(5)		0.3587(3)
$ZrZnSi_2$	FeB	Pnma	0.7034(4)	0.3773(2)	0.5328(3)
$Zr_3Zn_5Si_2$					
$Zr_6Zn_{23}Si$	$Zr_6Zn_{23}Si$	$Fm\bar{3}m$	1.2556(5)		
Zr_6ZnSi_3					

Our investigation confirms the existence of the compound $Zr_6Zn_{23}Si$, which is presented in [4]. The $Zr_6Zn_{23}Si$ compound is a superstructure to $Sc_{11}Ir_4$ or "filled" variant of the Th_6Mn_{23} structure type. Interrelation of the structure types, which can be obtained from an initial type structure Th_6Mn_{23} by the ordered substitution, insertion and redistribution of atoms are presented in Table 3. The crystal structures of the $Zr_3Zn_5Si_2$ and Zr_6ZnSi_3 ternary compounds are not known.

Table 3. Distribution of atoms on Wyckoff sites for Th_6Mn_{23}, $Mg_6Cu_{16}Si_7$, $Sc_{11}Ir_4$ and $Zr_6Zn_{23}Si$ structure types.

Wyckoff sites	Th_6Mn_{23}	$Mg_6Cu_{16}Si_7$	$Sc_{11}Ir_4$	$Zr_6Zn_{23}Si$
32f	Mn1	Cu1	Sc1	Zn1
32f	Mn2	Cu2	Sc2	Zn2
24e	Th	Mg	Sc3	Zr
24d	Mn3	Si1	Ir1	Zn3
4b	----	----	Ir2	Zn4
4a	Mn4	Si2	Ir3	Si

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