CRYSTAL STRUCTURE OF NEW PHASES IN THE Zr−Ru−Ga SYSTEM IN THE REGION OF HIGH Ga CONTENT

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The Zr−Ru−Ga system has been partially studied in the region of 0−50 at. % Ga in [1−3], which revealed the existence of two ternary compounds with the $MgZn_2$-type structure (space group (SG) *P*6$_3$*/mmc*): $ZrRu_xGa_{2-x}$ ($0.60 < x < 0.96$), a = 5.2475(5) − 5.2557(1), c = 8.3923(7) − 8.2854(1) Å [1] and $Zr_{1-x}Ga_xRu_2$ (x = 0.18), a = 5.1399(1), c = 8, 4888(2) Å [2], and solid solutions based on binary RuGa and ZrRu compounds with the CsCl-type structure (SG *Pm*-3*m*) [3]. In this work the Zr−Ru−Ga system was investigated in the region of high Ga content (>50 at. %) at 870 K.

The samples for the study were prepared by melting a charge of compact high-purity metals in an electric arc furnace under a purified argon atmosphere. The heat treatment of the alloys consisted of homogenizing annealing at 870 K for 720 hours. Phase analysis of the alloys was performed using an array of powder X-ray diffraction data (XRD) obtained using DRON-2.0M (FeK_α radiation) and STOE STADI P (Cu$K_{\alpha1}$ radiation) powder diffractometers. The energy dispersive X-ray spectroscopy (EDX) was used to confirm the atomic ratio of elements in each phase. Single crystal data for $Zr_7Ru_6Ga_{17}$ were collected at room temperature on a Bruker D8 Venture diffractometer with monochromatized Mo$K\alpha$ radiation.

In the studied concentration range, the existence of the ternary compound $Zr_7Ru_{6+x}Ga_{17-x}$ ($0 \le x \le 2.0$) and solid solutions of substitution based on binary compounds $RuZr_xGa_{2-x}$ ($0<x<0$, 32, ST $TiSi_2$, SG *Fddd*, a = 4.749 − 4.7501(7), b = 8.184 − 8.195(1), c = 8.696 − 8.708(2) Å), $ZrRu_xGa_{3-x}$ ($0< x <0.33$, ST $ZrAl_3$, SG *I*4*/mmm*, a = 3.960−3.9640(4), c = 8.72 − 8.741(3) Å) was established. The limiting solubility of the third component in binary intermetallics was confirmed by EDX and XRD analyses.

The crystal structure of the galide $Zr_7Ru_6Ga_{17}$ was investigated by the single-crystal method. The compound $Zr_7Ru_6Ga_{17}$ crystallizes in a new structure type (Pearson's symbol *cF*120, space group *Fm*-3*m*, a = 12.409(1) Å, Z = 4, R_1 = 0.037, wR_2 = 0.091 for 172 independent reflexes with $I_o > 2\sigma(I_o)$ and 19 refined parameters). An decrease of the unit cell parameters indicates homogeneity range of $Zr_7Ru_{6+x}Ga_{17-x}$ ($0 \le x \le 2.0$) for the compound at 870 K along the isoconcentrate of 23.3 at. % Zr. It is a solid solution of substitution of Ru for Ga with the limits from 50.0 to 56.7 at. % Ga.

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