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Phase Equilibria in The Gd–Cr–Ge System at 1070 K

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The isothermal section of the phase diagram of the Gd–Cr–Ge ternary system was constructed at 1070 K over the whole concentration range using X-ray diffractometry, metallography and electron microprobe (EPM) analysis. Three ternary compounds are realized in the Gd–Cr–Ge system at the temperature of annealing: $Gd_{117}Cr_{52}Ge_{112}$ ($Tb_{117}Fe_{52}Ge_{112}$ structure type, space group *Fm*-3*m*, Pearson symbol *cF*1124, *a* = 2.8971(6) nm), $GdCr_6Ge_6$ ($SmMn_6Sn_6$ structure type, space group *P*6/*mmm*, Pearson symbol *hP*16, *a* = 0.51797(2), *c* = 0.82901(4) nm) and $GdCr_{1-x}Ge_2$ ($CeNiSi_2$ structure type, space group *Cmcm*, Pearson symbol *oS*16, *a* = 0.41569(1)-0.41593(8), *b* = 1.60895(6)-1.60738(3), *c* = 0.40318(1)-0.40305(8) nm). For the $GdCr_{1-x}Ge_2$ compound the homogeneity range was determined (*x* = 0.73 - 0.69).

Keywords: intermetallics; ternary system; phase equilibria; crystal structure.

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Introduction

Experimental data of the study of the components interaction in the metallic systems provide important information on the formation, temperature and concentration stability and crystal structure of intermediate phases to search for new materials with valuable properties.

Among the ternary systems R-M-Ge (R - rare earth metal, M - *d*-element) phase equilibrium diagrams of the systems involving rare earth metals, chromium and germanium are constructed for R = Nd, Y and Er [1-3], for other elements the structural and physical characteristics of individual ternary compounds were investigated. According to the literature data for rare earth metals of the yttrium subgroup, the existence of the ternary compounds RCr_6Ge_6 (R = Y, Tb − Er) [4, 5] has been established, which belong to the $HfFe_6Ge_6$ (or $MgFe_6Ge_6$) structure type. Information cornerning the $GdCr_6Ge_6$ compound is reported in Ref. [6], the authors of which studied the $GdMn_{6-x}Cr_xGe_6$ solid solution with $HfFe_6Ge_6$ structure type. Neutronographic studies of the $TbCr_6Ge_6$ compound showed that the structure of the germanide is a partially disordered derivative of the $HfFe_6Ge_6$ structure type [7]. Analysis of the literature data shows that RCr_xGe_2 germanides with a structure of the $CeNiSi_2$ type are formed with rare-earth metals as Sm, Y, Gd – Er [8, 9] and are characterized by defects in the crystallographic position of the transition metal. Samples of the corresponding compositions for both series of the compounds (RCr_6Ge_6, RCr_xGe_2) were obtained at an annealing temperature of 1070 K. No ternary compounds were observed during the study of the Y–Cr–Ge system at 870 K [10], and the results of further studies of the system at 1070 K established the existence of two ternary compounds YCr_6Ge_6 ($HfFe_6Ge_6$ structure type) and $YCr_{0.23}Ge_2$ ($CeNiSi_2$ structure type) [1]. According to the results of differential thermal analysis, the YCr_6Ge_6 and $ErCr_6Ge_6$ germanides exist in a sufficiently wide temperature range up to ~1120 K [1, 3]. For rare earth metals, where R = La, Ce, Pr, Nd, Sm, compounds of stoichiometric composition $RCrGe_3$ with the structure of perovskite $BaNiO_3$ are realized [11], the existence of the compounds $Nd_{117}Cr_{52}Ge_{112}$ and $Sm_{117}Cr_{52}Ge_{112}$ with a cubic structure of the $Tb_{117}Cr_{52}Ge_{112}$ type is reported in Refs. [2, 12].

In this paper, we present the experimental results of the study of the components interaction in the Gd–Cr–Ge system at a temperature of 1070 K and the structural characteristics of the ternary compounds.

I. Methods and materials

To construct a phase equilibrium diagram of the Gd–Cr–Ge system, the samples were synthesized by the arc-melting method of the initial components (the content of the main component is not less than 99.9 wt.%). The losses of the charge during melting were controlled by re-weighing and, if the mass of the sample did not deviate from the mass of the charge by more than 1 - 2 %, the composition of the alloy was considered to be the same for the charge. To bring the alloys to equilibrium state, homogenizing annealing was performed at 1070 K for 700 h, followed by quenching in cold water without first breaking the ampoules. X-ray phase analysis was performed on the diffraction patterns of the samples obtained on the diffractometer DRON-4.0 (FeK_α-radiation). The elemental composition of the synthesized samples was controlled by X-ray fluorescence spectroscopy (analyzer ElvaX Pro). The microstructure of individual alloys was examined using an electron microscope TESKAN VEGA 3 LMU, equipped by an X-ray analyzer with energy dispersive spectroscopy (EDS). Calculations and indexing of powder diffraction patterns were performed using the WinCSD software package [13] (determination of the lattice parameters). The diffraction data for the crystal structure refinements were collected at room temperature using STOE STADI P diffractometer (graphite monochromator, Cu $K\alpha_1$ radiation). The coordinates of atoms, occupancy of the crystallographic sites, and isotropic displacement parameters were refined and theoretical intensities were calculated with the FullProf Suite software package [14], using the Rietveld calculation algorithm [15].

II. Results and discussion

To construct a phase equilibrium diagram of the Gd–Cr–Ge ternary system, 33 ternary and 12 binary alloys were synthesized and homogenized at 1070 K for 700 hours. Annealed samples were examined by X-ray phase, X-ray spectral (EDXS) and X-ray fluorescence (XRFA) analyzes. As example, in Table 1 the results of the elemental composition for individual samples according to EDXS and XRFA data are given which agree satisfactorily with the initial compositions of alloys.

Phase equilibrium diagram of the Gd−Cr−Ge system was constructed at 1070 K based on the results of X-ray phase and electron probe microanalyses (Fig. 1). The

Table1

EDXS and XRFA data for individual alloys of the Gd−Cr−Ge system

Nominal composition, at. %	Experimantal composition, at. %	
	EDXS	XRFA
$Gd_9Cr_{43.5}Ge_{47.5}$	$Gd_{10.26}Cr_{43.15}Ge_{46.59}$	$Gd_{10.7}Cr_{42.9}Ge_{46.4}$
$Gd_{33}Cr_7Ge_{60}$	$Gd_{34.87}Cr_{8.58}Ge_{56.55}$	$Gd_{32.6}Cr_{7.4}Ge_{60}$
$Gd_{62.5}Cr_{10}Ge_{27.5}$	$Gd_{63.58}Cr_{9.3}Ge_{27.12}$	$Gd_{60.5}Cr_{11.8}Ge_{27.7}$
$Gd_{25}Cr_{32}Ge_{43}$	$Gd_{25.21}Cr_{33.47}Ge_{41.32}$	$Gd_{26.3}Cr_{32.0}Ge_{41.7}$
$Gd_{45}Cr_{10}Ge_{45}$	$Gd_{43.89}Cr_{11.23}Ge_{44.88}$	$Gd_{44.6}Cr_{10.3}Ge_{45.1}$
$Gd_{45}Cr_{20}Ge_{35}$	$Gd_{43.98}Cr_{21.05}Ge_{34.97}$	$Gd_{44.4}Cr_{20.7}Ge_{34.9}$

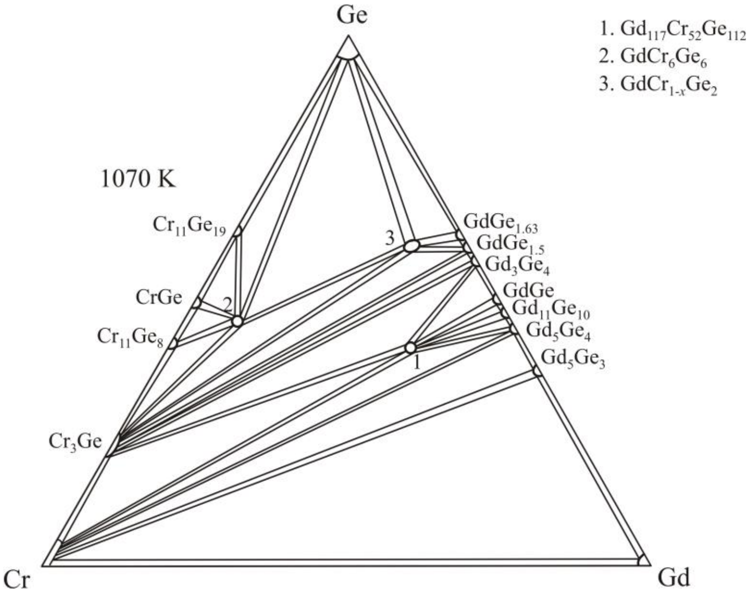

Fig. 1. Isothermal section of the Gd−Cr−Ge system at 1070 K.

Table 2

EPMA data and crystallographic characteristics of the selected alloys of the Gd-Cr-Ge system annealed at 1070 K

Nominal composition, at. %	Phase	Structure type	Lattice parameters, nm			EPMA data, at. %		
			a	*b*	*c*	Gd	Cr	Ge
$Gd_{20}Cr_{60}Ge_{20}$	Cr	Cr	0.4581(3)					
	$Gd_{117}Cr_{52}Ge_{112}$	$Tb_{117}Cr_{52}Ge_{112}$	2.8980(5)					
$Gd_{63}Cr_{10}Ge_{27}$	Gd_5Ge_3	Mn_5Si_3	0.8594(3)		0.6428(5)	66.73		33.27
	Cr	Cr	0.4580(4)				100.0	
	Gd	Mg	0.3678(4)		0.5858(5)	100.0		
$Gd_{25}Cr_{32}Ge_{43}$	Cr_3Ge	Cr_3Si	0.4626(3)				74.18	25.82
	Gd_3Ge_4	Er_3Ge_4	0.4100(3)	1.0751(5)	1.4310(6)	56.64		43.36
$Gd_{30}Cr_{35}Ge_{35}$	Cr_3Ge	Cr_3Si	0.4628(3)					
	$Gd_{117}Cr_{52}Ge_{112}$	$Tb_{117}Cr_{52}Ge_{112}$	2.898(5)					
$Gd_{50}Cr_{15}Ge_{35}$	Gd_5Ge_3	Mn_5Si_3	0.8594(3)		0.6429(4)	65.18	0.95	33.87
	Gd_5Ge_4	Sm_5Ge_4	0.7696(3)	1.4830(6)	0.7785(5)	55.32		44.68
	Cr	Cr	0.4581(4)				100.0	
$Gd_{40}Cr_{25}Ge_{35}$	$Gd_{117}Cr_{52}Ge_{112}$	$Tb_{117}Cr_{52}Ge_{112}$	2.899(4)			43.47	17.33	39.20
	Gd_5Ge_4	Sm_5Ge_4	0.7695(5)	1.4828(6)	0.7784(5)	54.49		45.51
	Cr	Cr	0.4582(5)				100.0	
$Gd_{20}Cr_{40}Ge_{40}$	Cr_3Ge	Cr_3Si	0.4629(5)					
	$GdGe_{1.5}$	AlB_2	0.3976(3)		0.4202(5)			
$Gd_{10}Cr_{45}Ge_{45}$	$GdCr_6Ge_6$	$SmMn_6Sn_6$	0.5177(3)		0.8288(5)	8.07	47.21	44.72
	Cr_3Ge	Cr_3Si	0.4631(4)				74.92	25.08
	$GdCr_{1-x}Ge_2$	$CeNiSi_2$	0.4157(4)	1.6088(6)	0.4030(5)	30.75	10.34	58.91
$Gd_{45}Cr_{10}Ge_{45}$	GdGe	TlI	0.4320(3)	1.080(5)	0.3974(5)	49.78		50.22
	$Gd_{117}Cr_{52}Ge_{112}$	$Tb_{117}Cr_{52}Ge_{112}$	2.8991(5)			41.62	17.44	40.94
	Gd_3Ge_4	Er_3Ge_4	0.4101(4)	1.0749(6)	1.4311(6)	41.96		58.04
$Gd_5Cr_{50}Ge_{45}$	CrGe	FeSi	0.4780(3)					
	$GdCr_6Ge_6$	$SmMn_6Sn_6$	0.5176(3)		0.8289(6)			
	$Gd_{11}Ge_8$	$Gd_{11}Ge_8$	(traces)					
$Gd_{25}Cr_{25}Ge_{50}$	$GdCr_{1-x}Ge_2$	$CeNiSi_2$	0.4156(3)	1.6089(6)	0.4028(4)			
	Cr_3Ge	Cr_3Si	0.4630(5)					
	$GdGe_{1,5}$	AlB_2	0.3976(3)		0.4202(5)			
$Gd_{20}Cr_{25}Ge_{55}$	$GdCr_6Ge_6$	$SmMn_6Sn_6$	0.5177(4)		0.8290(6)	8.20	46.25	45.55
	$GdCr_{1-x}Ge_2$	$CeNiSi_2$	0.4160(4)	1.6088(6)	0.4031(4)	30.86	9.51	59.63
	Ge	C	0.5650(3)					100.0
$Gd_5Cr_{35}Ge_{60}$	$GdCr_6Ge_6$	$SmMn_6Sn_6$	0.5178(4)		0.8290(5)			
	Ge	C	0.5649(4)					
	$Cr_{11}Ge_{19}$	$Mn_{11}Si_{19}$	(traces)					
$Gd_{33}Cr_7Ge_{60}$	$GdCr_{1-x}Ge_2$	$CeNiSi_2$	0.4159(3)	1.6073(6)	0.4029(4)	30.65	8.07	61.28
	$GdGe_{1,5}$	AlB_2	0.3977(3)		0.4200(5)	40.26		59.74
$Gd_{30}Cr_5Ge_{65}$	$GdCr_{1-x}Ge_2$	$CeNiSi_2$	0.4159(3)	1.6074(5)	0.4030(4)			
	Ge	C	0.5650(3)					
	$GdGe_{1.63}$	$ThSi_2$	(traces)					

phase composition and EPMA data for selected alloys are summarized in Table 2, microphotographs of some alloys are shown in Fig. 2.

In our study of the Gd−Cr−Ge system, information on the phase diagrams of the Gd−Ge, Gd−Cr, and Cr−Ge binary systems, which limit the studied ternary system, and the structural data of the corresponding binary compounds were used from handbooks [16, 17]. According to the literature [17], intermediate binary phases were not detected in the Gd–Cr system, which was confirmed during the study of the Gd–Cr–Ge system. According to the results of X-ray phase and electron microprobe analyzes, the samples in the ternary region Gd_5Ge_3–Gd–Cr of the Gd−Cr−Ge system contain three phases in equilibrium - the binary compound Gd_5Ge_3, Gd and Cr (Fig. 2, b). At the used annealing temperature in the Cr–Ge binary system the existence of the binary compounds Cr_3Ge (Cr_3Si-type), $Cr_{11}Ge_8$ ($Cr_{11}Ge_8$-type), CrGe (FeSi-type) and $Cr_{11}Ge_{19}$ ($Mn_{11}Si_{19}$-type) was confirmed. The Cr_5Ge_3compound with the W_5Si_3 structure type at the temperature of the study was not identified. According to X-ray phase analysis, the sample of the corresponding composition contained in equilibrium two binary compounds: Cr_3Ge and $Cr_{11}Ge_8$. The obtained result is consistent with the literature data [18], according to which the Cr_5Ge_3 compound exists in the high temperatures range 1269 - 1535 K.

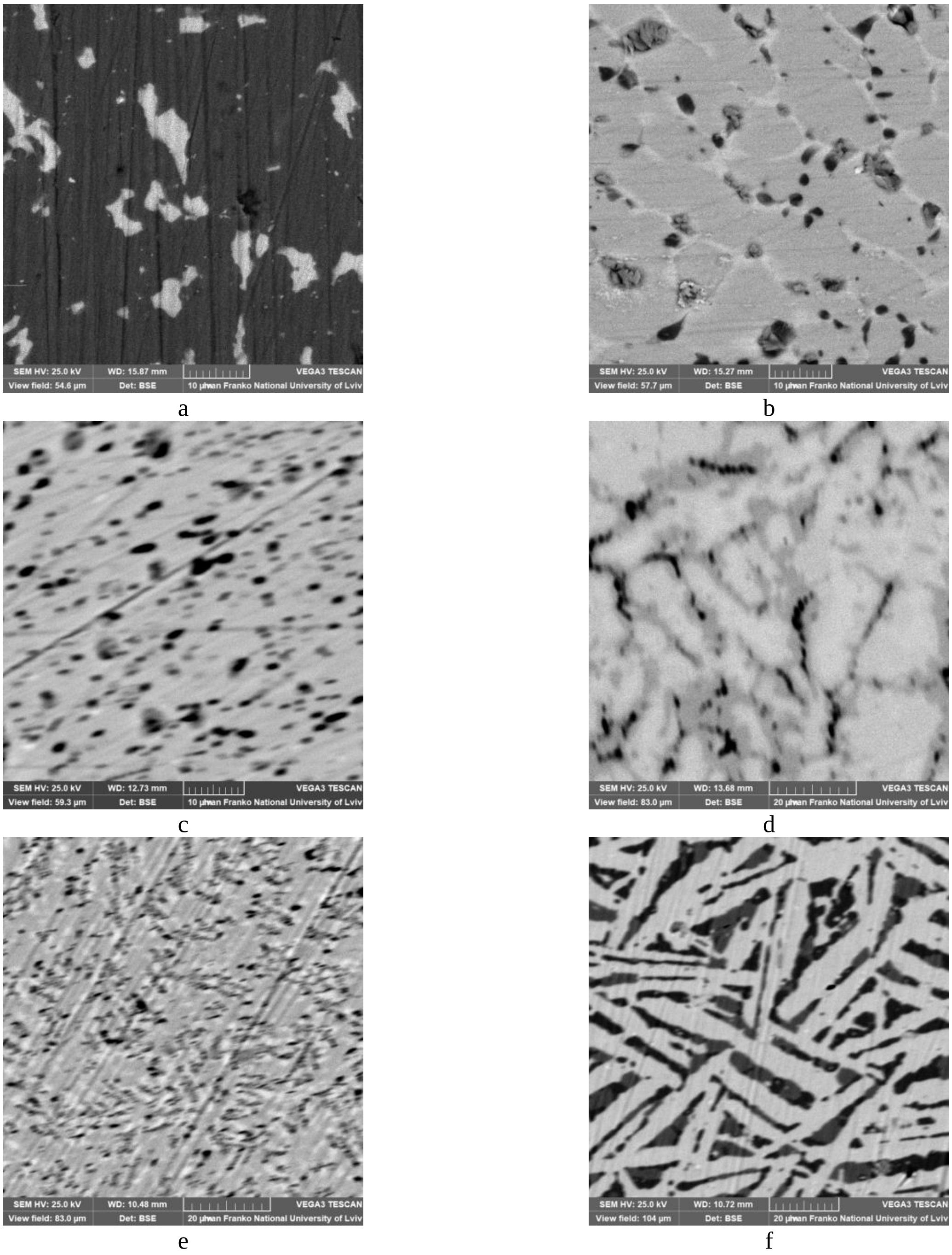

Fig. 2. Electron microphotographs of the Gd−Cr−Ge alloys: a) $Gd_{10}Cr_{45}Ge_{45}$ – $GdCr_6Ge_6$ (dark phase); $GdCr_{1-x}Ge_2$ (light phase); Cr_3Ge (black phase); b) $Gd_{63}Cr_{10}Ge_{27}$ – Gd_5Ge_3 (grey phase); Cr (black phase); Gd (light phase); c) $Gd_{50}Cr_{15}Ge_{35}$ – Gd_5Ge_3 (grey phase); Gd_5Ge_4 (dark grey phase); Cr (black phase); d) $Gd_{45}Cr_{10}Ge_{45}$ – GdGe (light phase); $Gd_{117}Cr_{52}Ge_{112}$ (dark grey phase); Gd_3Ge_4 (dark phase); e) $Gd_{40}Cr_{25}Ge_{35}$ − Gd_5Ge_4 (light phase); $Gd_{117}Cr_{52}Ge_{112}$ (dark grey phase); Cr_3Ge (dark phase); f) $Gd_{20}Cr_{25}Ge_{55}$− $GdCr_{1-x}Ge_2$ (light phase); $GdCr_6Ge_6$ (dark grey phase); Cr_3Ge (dark phase).

In the Gd–Ge binary system according to the reported state diagram [16] the existence of binary compounds at the used annealing temperature was confirmed: Gd_5Ge_3 (Mn_5Si_3-type), Gd_5Ge_4 (Sm_5Ge_4-type), GdGe (TlI-type), $GdGe_{1.5}$ (AlB_2-type), $GdGe_{1.63}$ ($ThSi_2$-type) (Fig. 1). Since the information of the Gd_3Ge_4 and $Gd_{11}Ge_{10}$ compounds which are absent in the phase diagram of the Gd–Ge system are reported in the literature [19, 20], we additionally synthesized the samples of the corresponding stoichiometric compositions. X-ray phase analysis of the prepared and annealed at 1070 K alloys showed the formation of the Gd_3Ge_4 (Er_3Ge_4-type) and $Gd_{11}Ge_{10}$ ($Ho_{11}Ge_{10}$-type) compounds at the studied annealing temperature.

According to EPMA data the solubility of the third component in the binary compounds of the Cr–Ge and Gd–Ge systems does not exceed 1 - 2 at. % under the conditions of our study.

According to the performed analysis of experimental data three ternary compounds are formed in the Gd–Cr–Ge system at 1070 K, the crystallographic characteristics of which are given in Table 3. During the study the existence of the $GdCr_6Ge_6$ and $GdCr_{1-x}Ge_2$ compounds was confirmed at 1070 K, and the formation of a new compound in the $Gd_{40}Cr_{20}Ge_{40}$ sample was established. Analysis of the X-ray diffraction pattern of the $Gd_{40}Cr_{20}Ge_{40}$ sample and the calculated lattice parameter indicated that the new compound belongs to the $Tb_{117}Fe_{52}Ge_{112}$ structure type. The formation and composition of the $Gd_{117}Cr_{52}Ge_{112}$ compound was confirmed by EDXS analysis (Fig. 2 d, e, Table 2). According to the performed structural studies, the $GdCr_6Ge_6$ compound belongs to the $SmMn_6Sn_6$ structure type, which is a partially disordered variant of the $HfFe_6Ge_6$ structure type. As reported in the literature [7] similar results based on neutronographic studies were obtained for the isostructural $TbCr_6Ge_6$ compound which belongs to the $SmMn_6Sn_6$ structure type with a partial distribution of Tb and Ge1 atoms in two crystallographic positions.

The crystal structure refinements was performed for the $GdCr_{1-x}Ge_2$ compound, using the powder diffraction data of the $Gd_{30}Cr_{10}Ge_{60}$ sample (Fig. 3). Experimental details of the structure refinements, atomic coordinates, isotropic displacement parameters are gathered in Tables 4, 5.

According to the results of X-ray phase and EPM analyses the existence of a small homogeneity range within the content of Cr 0.27-0.31 was established for the $GdCr_{1-x}Ge_2$ germanide. The values of the lattice parameters are given in Table. 3.

A comparison of the investigated Gd–Cr–Ge system with the previously studied {Nd, Y, Er}−Cr−Ge shows that the Gd–Cr–Ge system concerning the character of the phase equilibria and crystal structure of the ternary compounds is similar to the Y−Cr−Ge (1070 K) and Er–Cr–Ge (1070 K) systems [1, 3]. These systems are characterized by the formation of the RCr_6Ge_6 compounds ($HfFe_6Ge_6$ and $SmMn_6Ge_6$ structure types) and $RCr_{1-x}Ge_2$ with structure of $CeNiSi_2$ type, for which, as well as for isostructural compounds $RM_{1-x}Ge_2$ with other *d*-elements (M = Mn, Fe, Co, Ni, Cu), the defect in crystallographic position of the transition metal was observed [21]. In contrast to RCr_6Ge_6 germanides, which are formed with rare-earth elements of the yttrium subgroup, $R_{117}Cr_{52}Ge_{112}$ compounds with a cubic structure of the $Tb_{117}Fe_{52}Ge_{112}$ type are realized for the elements of cerium subgroup such as Nd and Sm [2, 12]. According to performed in our work studies, a similar compound is formed in the Gd–Cr–Ge system. Taking into account the small number of the ternary compounds formed in the studied systems {Y, Gd, Er}−Cr−Ge, it is

Table 3

Crystallographic characteristics of the compounds in the Gd−Cr−Ge system

Compound	Space group	Structure type	Lattice parameters, nm		
			a	*b*	*c*
$GdCr_6Ge_6$	*P*6/*mmm*	$SmMn_6Sn_6$	0.51797(2)	–	0.82901(4)
$GdCr_{1-x}Ge_2$	*Cmcm*	$CeNiSi_2$	0.41569(1)- 0.41593(8)	1.60895(6)- 1.60738(3)	0.40318(1)- 0.40305(8)
$Gd_{117}Cr_{52}Ge_{112}$	*Fm*-3*m*	$Tb_{117}Fe_{52}Ge_{112}$	2.8971(6)	–	–

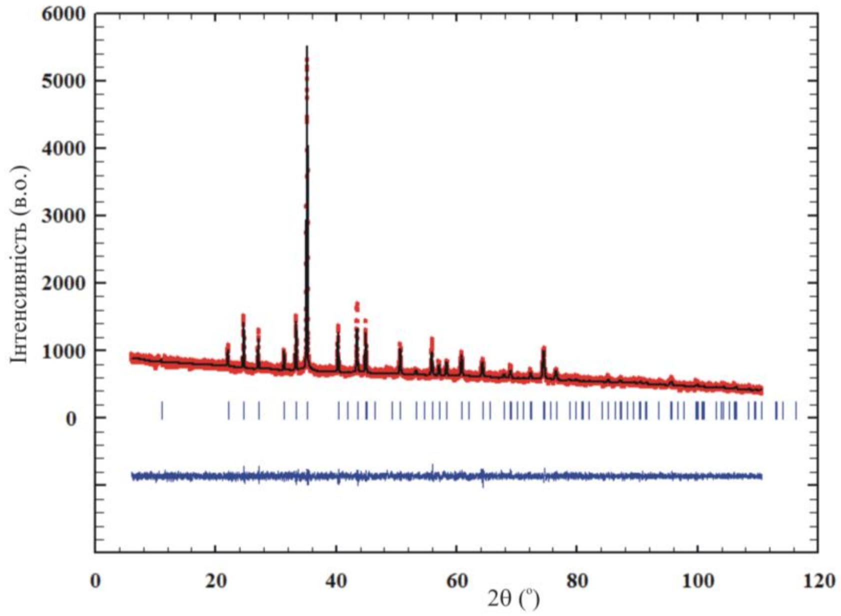

Fig. 3. The experimental (circles), calculated (line) and difference (bottom) X-ray diffraction patterns for $Gd_{30}Cr_{10}Ge_{60}$ sample.

possible to predict the interaction of the components in the related systems with other rare earth metals, particularly, Tb, Dy, and Ho, for which the RCr_6Ge_6 and $RCr_{1-x}Ge_2$ compounds were studied. It is possible to predict the formation of isostructural RCr_6Ge_6 and $RCr_{1-x}Ge_2$ compounds also with R = Tm, Yb and Lu, for which currently information on ternary compounds in the literature is absent or limited.

Table 4

Experimental details and crystallographic data for $GdCr_{0.31}Ge_2$ compound
($CeNiSi_2$-type; space group *Cmcm*; Z = 4)

Alloy composition		$Gd_{30}Cr_{10}Ge_{60}$
Refined composition		$GdCr_{0.31(5)}Ge_2$
Pearson symbol		*oS*16
Lattice parameters:	*a*, nm	0.415699(1)
	b, nm	1.60895(6)
	c, nm	0.40318(1)
Volume cell	*V*, nm^3	0.2696(6)
Number of atoms		12.92
Calculated density D_x, g/см^3		7.847
Diffractometer		STOE STADI P
Radiation, wavelength λ,		Cu K_α, 1.54056
Scanning method		$\theta/2\theta$
Interval 2θ,°		6–120
Scanning step, °scan time at the point, s		0.015/220
Refinement mode		Fullprof
Mixing parameter η		0.349(9)
Half width parameters :	*U*	0.142(4)
	V	0.006(20)
	W	0.015(4)
Asymmetry parameter:	A_1	0.081(7)
	A_2	0.038(2)
Reliability factors:	R_{Bragg}	0.0413
	R_f	0.0510
	χ^2	1.16

Table 5

Fractional atomic coordinates, site occupations (G) and isotropic displacement parameters B_{iso}
for $GdCr_{0.31}Ge_2$ compound

Atom	Wyckoff position	*x*	*y*	*z*	G	B_{iso}, Å^2
Gd	4*c*	0	0.3969(4)	1/4	1	0.29(1)
Cr	4*c*	0	0.1984(9)	1/4	0.31(5)	1.52(1)
Ge1	4*c*	0	0.0506(7)	1/4	1	1.19(3)
Ge2	4*c*	0	0.7514(6)	1/4	1	1.79(3)

Conclusions

According to the results of an experimental study of the components interaction in the ternary Gd–Cr–Ge system over the whole concentration range at 1070 K, the formation of the ternary germanides $GdCr_6Ge_6$ and $GdCr_{1-x}Ge_2$ was confirmed and the formation of a new ternary compound $Gd_{117}Cr_{52}Ge_{112}$ with cubic structure of $Tb_{117}Fe_{52}Ge_{112}$-type was determined. Structural studies of the $GdCr_6Ge_6$ compound have shown that it belongs to the $SmMn_6Sn_6$ structure type, which is a partially disordered variant of the $HfFe_6Ge_6$ structure type. It was found that the $GdCr_6Ge_6$ compound is characterized by a point composition, and for the $GdCr_{1-x}Ge_2$ compound with a structure of the $CeNiSi_2$ type a small homogeneity range was established, which is limited by the $GdCr_{0.27}Ge_2$ and $GdCr_{0.31}Ge_2$ compositions.

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Фазові рівноваги в системі Gd–Cr–Ge при 1070 K

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Методами рентгенофазового, рентгеноструктурного і рентгеноспектрального аналізів досліджено взаємодію компонентів та побудовано ізотермічний переріз діаграми стану потрійної системи Gd–Cr–Ge при 1070 K у повному концентраційному інтервалі. У системі Gd–Cr–Ge за температури відпалювання утворюються три тернарні сполуки: $Gd_{117}Cr_{52}Ge_{112}$ (структурний тип $Tb_{117}Fe_{52}Ge_{112}$, просторова група *Fm*-3*m*, символ Пірсона *cF*1124, *a* = 2,8971(6) нм), $GdCr_6Ge_6$ (структурний тип $SmMn_6Sn_6$, просторова група *P*6/*mmm*, символ Пірсона *hP*16, *a* = 0,51797(2), *c* = 0,82901(4) нм) та $GdCr_{1-x}Ge_2$, для якої рентгенівським дифракційним методом порошку проведено уточнення кристалічної структури (структурний тип $CeNiSi_2$, просторова група *Cmcm*, символ Пірсона *oS*16, *a* = 0,41569(1), *b* = 1,60895(6), *c* = 0,40318(1) нм, R_{Bragg} = 0,0413, R_p = 0,0510). Для сполуки $GdCr_{1-x}Ge_2$ визначено область гомогенності (*x* = 0.73 – 0,69).

Ключові слова: інтерметаліди, потрійна система, фазові рівноваги, кристалічна структура.