STRUCTURE AND PROPERTIES OF RCr_6Ge_6 GERMANIDES

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A series of RCr_6Ge_6 compounds (R = Y, Gd, Tb, Dy, Ho, Er, Tm, Yb, and Lu) was synthesized by arc-melting, annealed at 1070 K and characterized by XRPD and EDX analyses. Several new representatives of this series: $TmCr_6Ge_6$, $YbCr_6Ge_6$, and $LuCr_6Ge_6$ were found and appeared to be isotype to the previously studied RCr_6Ge_6 germanides with Y, Gd-Er, which crystallize in the $MgFe_6Ge_6$ structure type (space group *P*6/*mmm*). In addition, for $ErCr_6Ge_6$ and YCr_6Ge_6 compounds, a differential thermal analysis (synchronous LINSEIS STA PT 1600 thermoanalyzer) was performed and showed that they exist up 1126 K and 1120 K, respectively.

Performed phase analysis of the compounds with Y, Gd, Tb, Dy, Ho, Er confirmed that they belong to the $MgFe_6Ge_6$-type according to the literature data [1]. Because at the time of our study there are no data in the

literature about the isotypic compounds with R=Tm, Yb, Lu, we decided to synthesize them. Analysis of the X-ray powder pattern reflections of the corresponding samples clearly showed the formation of the $TmCr_6Ge_6$, $YbCr_6Ge_6$ and $LuCr_6Ge_6$ compounds which are isostructural to the previously studied RCr_6Ge_6 (R=Y, Gd-Er). Calculated lattice parameters and EPMA data of the RCr_6Ge_6 germanides are given in Table 1.

Table 1

Crystallographic parameters of the RCr_6Ge_6 compounds

Compound	EPMA data, at. %	Lattice parameters, nm		*V*, nm^3
		a	*c*	
YCr_6Ge_6	$Y_{8.01}Cr_{45.88}Ge_{46.11}$	0.5169(2)	0.8264(9)	0.1912
$GdCr_6Ge_6$	$Gd_{7.89}Cr_{46.34}Ge_{45.77}$	0.5177(7)	0.8283(2)	0.1925
$TbCr_6Ge_6$	$Tb_{7.65}Cr_{45.78}Ge_{46.57}$	0.5166(1)	0.8278(3)	0.1913
$DyCr_6Ge_6$	$Dy_{7.44}Cr_{46.05}Ge_{46.51}$	0.5163(1)	0.8272(3)	0.1910
$HoCr_6Ge_6$	$Ho_{7.58}Cr_{45.75}Ge_{46.67}$	0.51617(1)	0.82745(8)	0.1909
$ErCr_6Ge_6$	$Er_{7.61}Cr_{46.94}Ge_{45.45}$	0.5153(3)	0.8265(6)	0.1901
$TmCr_6Ge_6$	$Tm_{6.85}Cr_{44.50}Ge_{48.65}$	0.51506(6)	0.82648(8)	0.1898
$YbCr_6Ge_6$	$Yb_{7.46}Cr_{45.57}Ge_{46.97}$	0.51452(3)	0.82570(5)	0.1893
$LuCr_6Ge_6$	$Lu_{6.68}Cr_{45.04}Ge_{48.28}$	0.5143(1)	0.8256(3)	0.1891

The crystal structure of the $TmCr_6Ge_6$, $YbCr_6Ge_6$ and $LuCr_6Ge_6$ compounds was determined using X-ray powder diffraction method (Fullprof suite program package). The powder patterns of the samples were indexed on the basis of the hexagonal lattice with cell parameters *a* = 0.51506(6), *c* = 0.82649(8) nm (Tm), *a*=0.51452(3), *c*=82570(5) nm (Yb), *a*=0.5143(1), *c*=0.8256(3) nm (Lu) and indicated that these compounds belongs to the $MgFe_6Ge_6$ type structure (space group *P*6/*mmm*). Refined atomic coordinates and displacement parameters of the $TmCr_6Ge_6$

compound are listed in Table 2. The observed, calculated and difference in X-ray patterns of the $Tm_8Cr_{46}Ge_{46}$ sample are shown in Fig. 1.

Table 2

Atomic coordinates and isotropic displacement parameters for $TmCr_6Ge_6$ compound (R_p = 0.0847, R_{wp} = 0.0565, R_{Bragg} = 0.0566)

Atom	Wyckoff Position	*x*	*y*	*z*	occupancy	B_{iso}, Å^2
Lu	1*a*	0	0	0	1	1.8(3)
(Cr,Ge)	6*i*	1/2	0	0.2510(3)	5.44/0.56	0.6(0)
Ge1	2*d*	1/3	2/3	1/2	1	0.7(5)
Ge2	2*c*	1/3	2/3	0	1	0.6(1)
Ge3	2*e*	0	0	0.3482(4)	1	1.6(2)

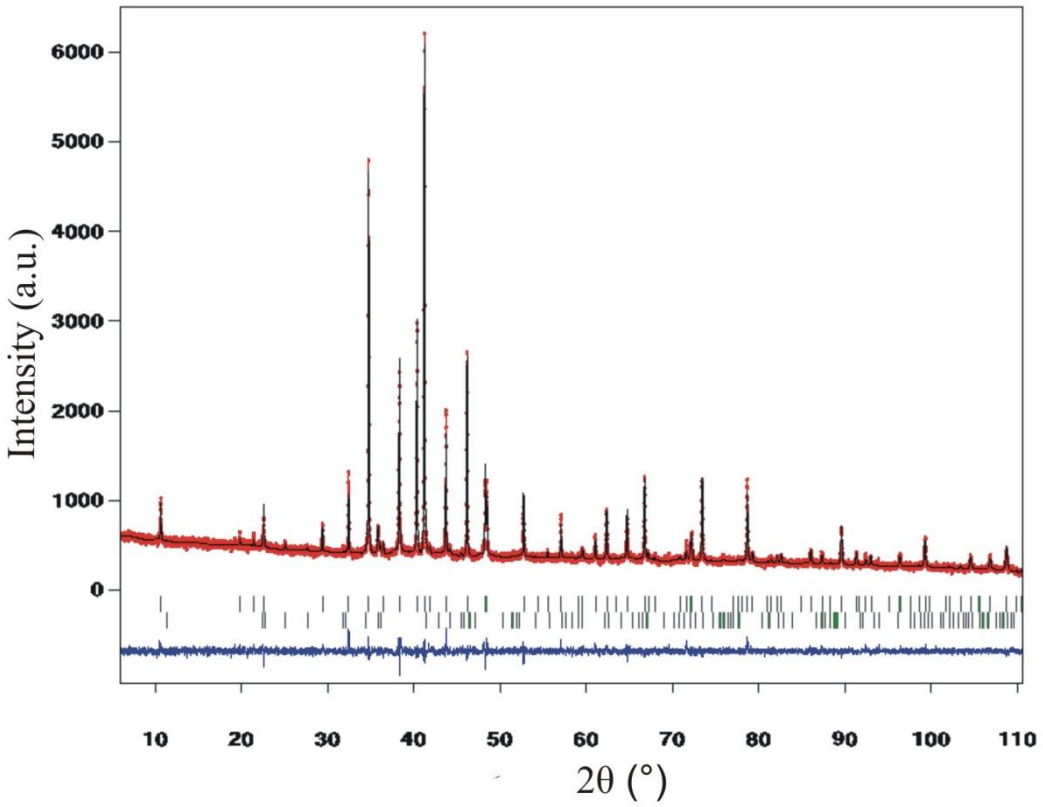

Fig. 1. The observed, calculated and difference in X-ray patterns of the $TmCr_6Ge_6$ compound (second phase is $TmCr_{1-x}Ge_2$)

The temperature dependencies of the electrical resistivity were measured in the temperature range 11-300 K using the helium cryostat with a closed cycle (Advanced Research Systems, USA). A character of the electrical resistivity indicates a metallic type of conductivity for all studied compounds in the whole temperature region. For $GdCr_6Ge_6$ and $TbCr_6Ge_6$ the anomalies on the resistivity curves are observed (Fig. 2) at temperatures that correspond to their magnetic ordering [1,2].

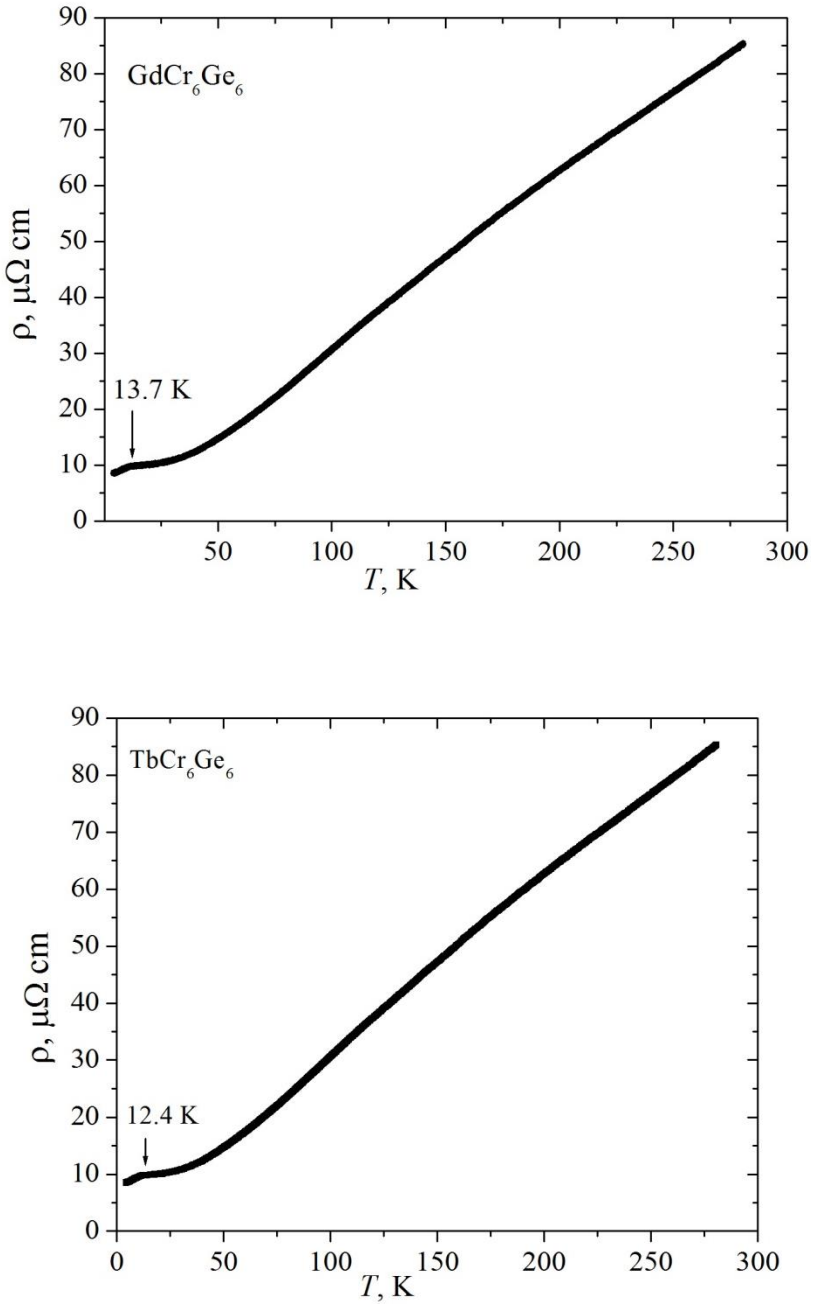

Fig. 2. Temperature dependences of the electric resistivity of the $GdCr_6Ge_6$ and $TbCr_6Ge_6$ compounds

In the paramagnetic region, the resistivity data of the RCr_6Ge_6 germanides can be approximated by the Bloch–Gruneissen–Mott (BGM). For YCr_6Ge_6 and $LuCr_6Ge_6$ the DFT modeling was performed and is in agreement with transport data.

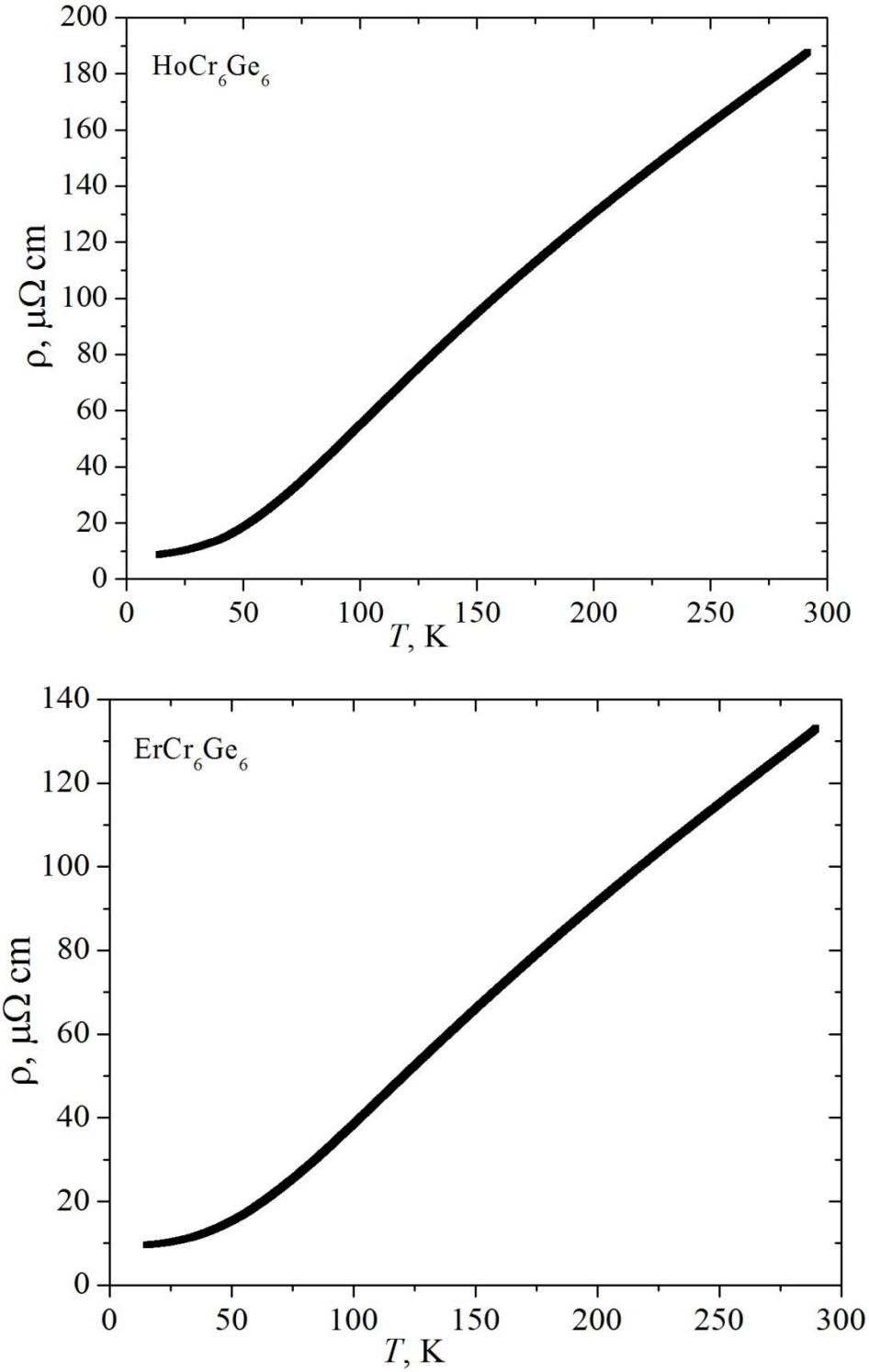

Fig. 3. Temperature dependences of the electric resistivity of the $HoCr_6Ge_6$ and $ErCr_6Ge_6$ compounds

Table 2

Parameters of the temperature dependencies of electrical resistivity of the RCr_6Ge_6 germanides

Compound	$\rho_{290\ K}$, μΩ·cm	$\rho_{11\ K}$, μΩ·cm	$T_{order.}$, K	
			R*	M**
YCr_6Ge_6	86.7	3.5		–
$GdCr_6Ge_6$	87.5	9.8	13.7	15
$TbCr_6Ge_6$	84.4	7.0	12.4	11
$DyCr_6Ge_6$	11.,5	5.8		3.0
$HoCr_6Ge_6$	124.6	8.9		
$ErCr_6Ge_6$	133.2	9.5		2.5
TmCr6Ge6	131.6	9.2		
$LuCr_6Ge_6$	89.3	2.5		–

R* Data of the electric property measurements
M** Data of the magnetic property measurements

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