

08.3-15 THE NEW TERNARY INTERMETALLIDE WITH GIGANT UNIT CELL $Tb_{117}Fe_{52}Ge_{112}$. By O.I.Rodak, E.I.Gladyshevsky, V.K.Pecharsky and P.K.Starodob, Faculty of Chemistry, Lvov State University, Lvov, USSR.

Crystal structure of the new ternary compound $Tb_{117}Fe_{52}Ge_{112}$ solved by combined direct and Patterson methodes (SHELX-76, XTLSM). All calculations were performed on SM-4 mini-computer. Adaptation of programs was done by V.K.Pecharsky, P.Yu.Zavaliy, L.G.Akselrud, Yu.N.Gryn' and E.I.Gladyshevsky.

Unit cell is cubic: sp.gr. $Fm\bar{3}m$, $a=28.580(6)\text{\AA}$. Intensities (475 non-equivalent, observed reflections) were measured on P3 NICOLET diffractometer. Final R-factors are 0.054 (isotropic) and 0.047 (anisotropic approximation). List of atomic parameters is given below.

Atom	Position	x	y	z
Tb1	96k	0.1793	0.1793	0.4084
Tb2	96k	0.1995	0.1995	0.0663
Tb3	96k	0.0681	0.0681	0.1557
Tb4	96j	0.2550	0.1036	0
Tb5	48i	0.1158	0.1158	0.5
Tb6	24e	0.3384	0	0
Tb7	8c	0.25	0.25	0.25
Tb8	4a	0	0	0
Fe1	96k	0.1676	0.1676	0.2302
Fe2	32f	0.3983	0.3983	0.3983
Fe3	48h	0.0723	0.0723	0
Fe4	32f	0.4503	0.4503	0.4503
Ge1	48h	0.1447	0.1447	0
Ge2	48i	0.2906	0.2906	0.5
Ge3	24e	0.2150	0	0
Ge4	32f	0.1464	0.1464	0.1464
Ge5	32f	0.3088	0.3088	0.3088
Ge6	96k	0.1071	0.1071	0.2423
Ge7	24e	0.1152	0	0
Ge8	48g	0.25	0.25	0.1395
Ge9	96k	0.0738	0.0738	0.3228

Co-ordination polyhedra of small atoms (Fe and Ge) are distorted trigonal prisms, tetragonal antyprisms, cubooctahedra and icosahedra. The structure one can build from the polyhedra, mentioned above.

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08.3-16 THE CRYSTAL STRUCTURES OF THE RARE EARTH BINARY GALLIDES. By E.I.Hladyshevsky, Ya.P.Yarmolyuk, Yu.N.Hryn', Chair of Inorganic Chemistry, Lvov State University, Lvov, USSR.

During the investigation of the phase equilibria in the ternary systems RE - Ga - 3d-transition metal we found 21 new binary gallides of rare earths. Their crystal structures have been studied by X-ray single crystal and powder methods. They belong to 5 structure types:

Compound	Structure type	Space group	a, Å	b, Å	c, Å
Tm_3Ga_5	Tm_3Ga_5	$Fm\bar{3}m$	6.001	9.651	11.293
Sm_9Ga_4	Sm_9Ga_4	$I4/m$	11.940		5.081
Gd_3Ga_2	Gd_3Ga_2	$I4/mcm$	11.666		15.061
Ho_5Ga_3	Cr_5B_3	$I4/mcm$	7.590		14.001
YGa_6	$PuGa_6$	$P4/nbm$	5.947		7.549

The isotypic to Tm_3Ga_5 compounds were obtained in the systems with Y, Tb, Dy, Ho, Er, Lu. The Tm_3Ga_5 structure is closely related to Bi_3Y_5 , $\beta-Sb_3Yb_5$, UPb_2Se_5 (these four structures relate to one another due to small deformation) and together with Pu_3Pd_5 forms the new series of homogeneous linear structures. The structures of this series have the symmetry of 6 orthorhombic and monoclinic space groups: $Cmcm$, $Fm\bar{3}m$, $Pma2$, $Pmn2_1$, $P2_1/m$, Fm . The Sm_9Ga_4 structure is the substructure to $Nb_5Cu_4Si_4$. The unit cell of Sm_9Ga_4 contains the big details of closest packed structure of $AuCu_3$ type. The isotypic phases occur with Pr and Nd. The full structure determination of Gd_3Ga_2 establishes that its real unit cell has four times greater cell volume, as has been reported in former publications. The Gd_3Ga_2 structure is built from some fragments as $Pu_{31}Sn_{20}$, Y_3Rh_2 , W_5Si_3 , $Sm_{26}(Ga,Co)_{17}$. The isotypic phases have been found in the systems with Nd, Sm, Tb, Dy, Ho, Er, Tm, Y. The formerly unknown phases with Cr_5B_3 structure type are the high-temperature modifications of Ho_5Ga_3 and Er_5Ga_3 compounds existing at $600^\circ C$. The YGa_6 compound finishes the series of rare earth hexagallides with $PuGa_6$ structure type. The $PuGa_6$ structure is related to a well known structure AlB_2 by means of double substitution of the part of R atoms by the pairs of X atoms (R and X are atoms with different radii: $r_R > r_X$). The rare earth atoms in the described structures have in most cases big coordination numbers (13 - 20), The gallium atoms have 9 - 12 nearest neighbours, its coordination polyhedrons are icosahedron, cubooctahedron and their related variants.