

08.3-17 THE STRUCTURES OF $Y_{2m+2n}Ga_{2n}Co_{2m+2n}$ SERIES. By Yu.N.Hryn', Ya.P.Yarmolyuk and R.E.Hladyshevsky, Chair of Inorganic Chemistry, Lvov State University, Lvov, USSR.

There exist five compounds in the ternary Y - Ga - Co system at 600°C on the YCo - YGaCo section, including new binary YCo phase. Crystal structure of the compounds has been investigated by means of single crystal and powder techniques.

Compound	Structure type	Space group	a, Å	b, Å	c, Å
YCo	α -JT1	Cmcm	4,106	10,358	3,906
Y_5GaCo_5	Y_5GaCo_5	Cmcm	4,123	10,289	20,539
Y_4GaCo_4	Y_4GaCo_4	B2/m	10,233	8,811	4,115
				$\gamma=109,15^\circ$	
Y_3GaCo_3	W_3CoB_3	Cmcm	4,098	10,11	13,01
Y_2GaCo_2	Mo_2NiB_2	Immm	5,382	8,457	4,105
			(10,024*)	$(\gamma=122,47^\circ)$ *	

* The orientation corresponds to one in the previous structures.

The atomic coordination numbers are: Y-17, Ga-12, Co-9,10. Their corresponding polyhedra in the structures studied are similar for Y and are the same for Ga and Co. The latter possesses a trigonal-prismatic coordination. The shortest interatomic distances lie in the range: Y-Y - 3,46-3,56, Y-Ga - 3,19-3,21, Y-Co - 2,84-2,95, Ga-Co - 2,47-2,49, Co-Co - 2,31-2,41 Å. Close coordination characteristics of the atoms indicate the structural relationship of the obtained compounds. They belong to the series of non-homogeneous linear structures of the $Y_{2m+2n}Ga_{2n}Co_{2m+2n}$ composition, where m and n are the quantities of more primitive structure fragments such as α -JT1 and UPT₂, from which the unit cells of the phases investigated consist of. For YCo - m=2, n=0; Y_5GaCo_5 - m=8, n=2; Y_4GaCo_4 - m=3, n=1; Y_3GaCo_3 - m=4, n=2; Y_2GaCo_2 - m=1, n=1. The YGaCo compound formally belongs to the same series with m=0 and n=2, however, the atomic distribution at the trigonal prism apices differs from that in the origin structure UPT₂. The shortest unit cell parameter is determined by an Y atom size and practically is the same for all structures of the series (4,098-4,123 Å). The next in value parameter (~10 Å) decreases regularly with the gallium content increase.

08.3-18 NEUTRON DIFFRACTION STUDY OF THE CRYSTALLOGRAPHIC AND MAGNETIC STRUCTURES OF THE $Mn_{58}Ga_{42}$ ALLOY. By Y.Abbas and H.Abou-Helal, Atomic Energy Est., Neutron Physics Dept., Atomic Energy Post, Cairo, Egypt, and E.Kren, Central Research Institute for Physics, Budapest, Hungary.

Neutron powder diffraction investigations show that Mn-Ga alloy with 58 at % Mn has a primitive unit cell with space group P43m. The structure is a gamma brass-like one built of two non-identical clusters A and B. In both clusters, 26 atoms are distributed on sites, inner tetrahedra (IT), outer tetrahedra (OT), octahedra (OH) and cubo-octahedra (CO). The twelve (OH) and eight (OT) positions are occupied by Ga atoms only. The rest of Ga atoms are distributed among the (IT) and (CO) positions with occupation numbers which are determined together with the atomic parameters.

Neutron diffraction measurements showed that the compound undergoes a magnetic transition to an antiferromagnetic state at a Neel temperature $T_N = 245 \pm 5$ K. The magnetic unit cell is doubled along the three crystallographic axes. The effective magnetic moment carried by the Mn atom was $(1.08 \pm 0.05) \mu_B$.

08.4-1 SPONTANEOUS STRAIN AND DOMAIN BOUNDARIES IN FELDSPARS. By B. Kuscholke and E.Salje, Institut für Kristallographie und Petrographie, Universität Hannover, Welfengarten 1, 3000 Hannover 1, Federal Republic of Germany. The triclinic feldspar structure as compared with the monoclinic modification contains two components of the spontaneous strain: $x_4 = \frac{c}{c_0} \cos \alpha$ and $x_0 = \frac{b}{b_0} \cos \gamma$. The structural state is best described by the spontaneous strain $e_s = \frac{1}{\sqrt{2}} \sqrt{x_4^2 + x_0^2}$. Its temperature dependence is induced either by elastic instabilities related to critical acoustic phonons or by Al/Si ordering or by a combination of both effects. The induced structural deformations of the Al - Si - O network give rise to the formation of domain boundaries. The shape and orientation of these boundaries reveal directly the structural strain. In case of twin formation, the dominant effects are: a) intersections of albite and pericline twin wall are always rounded, b) non - intersecting boundaries close to such intersections are bent in a S - shape and c) narrow twin domains tend to become needle - shaped close to the intersection with twin walls perpendicular to these domains. The ferroelastic character of the albite and anorthoclase structure is established from the results of Raman spectroscopy and diffuse X - ray scattering and is in agreement with electron microscopic investigations of Brown and Parsons (Phys.Chem.Min.,(1983) 10, 55)