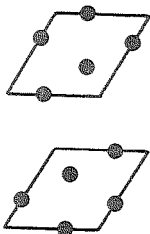


3 atoms being placed on each layer with the rotation of  $60^\circ$  in successive layers as shown in the figure. These sublayers contain 90 atoms altogether in the unit cell. The other 38 atom positions as well as the configuration in the sublayers were refined by Fourier synthesis and full-matrix least-squares to  $R(F)=0.095$ , based on 1337 observed reflections. The  $\zeta$ -phase structure comes out as the following: Ge atoms occupy every fifth layer in the 30 sublayers, and the other



layers are occupied by Mn atoms. Remaining 38 atoms are located on the three fold axes of  $00z$ ,  $\frac{1}{3}\frac{2}{3}z$  and  $\frac{2}{3}\frac{1}{3}z$ . Positions of Mn atoms

on these axes are above and below the Ge sublayers, and Ge atoms on the axes are settled in between these Ge sublayers.

Coordination numbers for the atoms on three fold axes are mainly 10 and 11, and the atoms on sublayers have coordinations from 11 to 13. Interatomic distances range from 2.43 to 3.20Å except for a few shorter distances of 2.21Å. The structure has similarity with the ones of  $Mn_5Ge_3(D8_8)$  and  $MnGeNi(B8_2)$  with respect to the layer structure and the atomic arrangements in the sublayers.

#### 08.3-11 IS THE SPHERE-PACKING MODEL APPROPRIATE FOR THE SIGMA PHASE?

By Clara Brink Shoemaker and David P. Shoemaker, Oregon State University, Corvallis, OR 97331, USA.

C. G. Wilson and F. J. Spooner [Acta Cryst. (1973). A29, 342] have used a sphere-packing model of the sigma phase to predict the cell dimensions by averaging three estimates for  $a$  and  $c$  derived from different "panels" of atoms in the structure. The sphere radii are derived from the occupancy and the CN12 radii of the atoms. Their individual estimates from different panels in the same structure differ (in the case of random order,  $\bar{r} = 1.35 \text{ \AA}$ ) by as much as 0.72 Å in  $c$  and 1.27 Å in  $a$ , although the averages, perhaps fortuitously, agree well with the observed values. This model has been discussed recently by L. M. Alte da Veiga *et al.* [Acta Cryst. (1981), to be published.]

In our study of 14 sigma-phase related "tcp" phases we have found that atoms with coordinations higher than 12 are much better represented by "dimpled spheres" having two radii rather than one. With such radii we obtain estimates for  $a$  and  $c$  for the different panels that are in much better agreement. Even more reliable predictions can be made by using all the distances, calculated from these radii by our 1969 procedure (C. B. Shoemaker and D. P. Shoemaker in: Developments in the structural chemistry of alloy phases. B. C. Giessen, Ed., Plenum Press, p. 135). In view of our finding that radii for a given CN type in a given compound are insensitive to occupancy, and in view of the crudeness of the sphere model, we regard the latter's predictions of ordering as unreliable.

#### 08.3-12 INTERMETALLIC PHASES ON THE Ga RICH SIDE OF THE R-Ga SYSTEMS (R=RARE EARTH METAL).

By G. Kimmel, J. Pelleg and L. S. Zevin, Materials Engineering Department, Ben Gurion University of the Negev, Beer Sheva, Israel.

The existence of intermetallic compounds hitherto unidentified, on the Ga-rich side of the R-Ga systems, such as for example Nd-Ga, has already been reported and later confirmed by the present authors (J. Less-Common Met. (1978) 61, 293; J. Less Common Met. (1980) 75, 133). One of these compounds, the  $RGa_6$ , has a tetragonal symmetry,

$PuGa_6$  type, and it is a common feature of all R-Ga systems. Nd-Ga<sub>6</sub>, one of such compounds, is formed by a peritectic reaction at 617°C. It undergoes a transition at 463°C probably of an allotropic nature. Details of this transition will be discussed.

$RGa_2$  type compounds show a wide homogeneity range of about 10-15 at.% Ga in some R-Ga systems investigated. The systems belong to the light lanthanides. The lattice parameters of the hexagonal  $RGa_2$  compounds (AlB<sub>2</sub> type) increase on addition of Ga. A model is presented to explain the increase in lattice parameters.

#### 08.3-13 STRUCTURAL PRINCIPLES OF LITHIUM-GROUP III-COMPOUNDS.

By J. Stöhr, W. Müller and H. Schäfer, Abt. II für Anorganische Chemie der Technischen Hochschule Darmstadt, West-Germany.

Single crystals of the following Li-Group III-compounds were prepared and the structures determined.  $Li_5Ga_4$ : trigonal,  $P\bar{3}m1$ ,  $a=437.5 \text{ pm}$ ,  $c=825.7 \text{ pm}$ . The Ga-atoms form undulating hexagonal double sheets, which are separated by layers of Li-atoms.  $Li_3Ga_2$ : trigonal,  $R\bar{3}m$ ,  $a=436.7 \text{ pm}$ ,  $c=1389.6 \text{ pm}$ . The simple undulating hexagonal sheets of Ga-atoms are separated by layers of Li-atoms.  $Li_2Ga$ : orthorhombic,  $Cmcm$ ,  $a=456.2 \text{ pm}$ ,  $b=954.2 \text{ pm}$ ,  $c=436.4 \text{ pm}$ . The Ga-atoms form zig-zag-chains.  $Li_5In_4$ : trigonal,  $P\bar{3}m1$ ,  $a=478 \text{ pm}$ ,  $c=888 \text{ pm}$ , isostructural to  $Li_5Ga_4$ .  $Li_3In_2$ : trigonal,  $R\bar{3}m$ ,  $a=474.8 \text{ pm}$ ,  $c=1474.0 \text{ pm}$ , isostructural to  $Li_3Ga_2$ .  $Li_2In$ : orthorhombic,  $Cmcm$ ,  $a=476.3 \text{ pm}$ ,  $b=1001.7 \text{ pm}$ ,  $c=473.5 \text{ pm}$ , isostructural to  $Li_2Ga$ .  $Li_3In_3$ : cubic,  $Fd\bar{3}m$ ,  $a=1355.6 \text{ pm}$ . Isolated In-atoms are observed, i.e. they have only Li-atoms as neighbours.  $Li_2Tl$ : orthorhombic,  $Cmcm$ ,  $a=474.1 \text{ pm}$ ,  $b=1002.3 \text{ pm}$ ,  $c=478.6 \text{ pm}$ , isostructural to  $Li_2Ga$ .  $Li_5Tl_2$ : trigonal,  $R\bar{3}m$ ,  $a=471.6 \text{ pm}$ ,  $c=2039.9 \text{ pm}$ . This structure, which is isostructural to  $Li_5Sn_2$ , is characterized by  $Tl_2$ -units.  $Li_3Tl$ : cubic,  $Fm\bar{3}m$ ,  $a=667.1 \text{ pm}$ . Isolated Tl-atoms are observed, isostructural to  $Li_3Bi$ .  $Li_2Tl_5$ : cubic,  $F\bar{4}3m$ ,  $a=2000.3 \text{ pm}$ . Isolated Tl-atoms, isostructural to  $Li_2Pb$ .  $Li_5InTl$ : trigonal,  $R\bar{3}m$ ,  $a=472.2 \text{ pm}$ ,  $c=2029.5 \text{ pm}$ , isostructural to  $Li_5Tl_2$ .

These compounds are interpreted as Tungsten variants and their structural relationship to the Li-Al-compounds are discussed.