

An important characteristic of the room temperature phase concerns the packing of the aliphatic chains. The periodic array of the C atoms within a single layer can be described by a monoclinic cell with $a=7.9$ $b=10.3$ $c=2.54$ and $\beta=99^\circ$ with space group symmetry $P2_1$. This type of packing is not mentioned in the list given by Segerman (Acta Cryst. 19, 789, 1965).

Three additional transitions appear in calorimetric studies when n =odd and larger than 4. The transition enthalpy of the first one by increasing temperature, is small and no changes could be observed on a powder diagram for $C5Zn$. In the next transition, important structural transformations occur such as an abrupt increase of the c lattice constant, characteristic for the reorientation of the chains. The corresponding phases of $C5Zn$ and $C14Zn$ are orthorhombic with lattice constants $a=10.19(2)$ $b=7.09(1)$ $c=27.9(1)$ and $a=10.3(1)$ $b=7.6(1)$ $c=57.5(1)$ respectively.

In this series of compounds, the transition from an ordered monoclinic phase to a quasi-liquid high temperature phase occurs in successive steps, including an intermediate orthorhombic phase with space group symmetry $Pnma$. In this state, the disordered chains oscillate between two equilibrium positions related by a plane of symmetry.

05.1-17 DUPLEX CHARACTER OF DEFECT ZINC BLENDE

STRUCTURE OF α AND γ Ga_2Se_3 . By S.Z. Ali, National Physical Laboratory, New Delhi 110012 and M.Y. Khan, Jamia Millia Islamia, New Delhi 110025, INDIA.

X-ray powder patterns of α and γ Ga_2Se_3 , both belonging to cubic defect zinc blende structure, give lattice parameters:

$$a_{\alpha} = 5.433(1) \text{ \AA} \text{ from sharp lines with } h+k+l=4n,$$

$$\left\{ \begin{array}{l} = 5.445(4) \text{ \AA} \text{ from reflections } hkl \text{ all odd,} \\ a_{\gamma} = 5.463(1) \text{ \AA} \text{ from all } hkl \text{ reflections.} \end{array} \right.$$

However, the powder pattern information for both phases is grossly inadequate as regards structure delineation. Our single crystal work shows that both structures are duplex in character. All strong, sharp reflections of α phase with $h+k+l=4n$ have diffuse components on the low angle side of θ Bragg with corresponding lattice parameter ~ 5.445 \AA . Weak reflections with hkl even and $h+k+l=2(2n+1)$ are diffuse with lattice parameter again 5.445 \AA , same as for the strong, diffuse, hkl all odd, spots each of which has a remarkable set of streaks extending to all neighbouring reciprocal lattice nodes with $h+k+l=4n$ or $2(2n+1)$. In the case of γ Ga_2Se_3 all reciprocal lattice nodes of high intensity have diffuse, broad spots on the high angle side of θ Bragg with lattice parameter ~ 5.41 \AA , smaller than that of the sharp spots. The unique set of streaks however is missing in the γ phase. The duplex character of both phases is similar to that of neutron-irradiated BeO (Austerman, S.B. and Miller, K.T., phys. stat. sol. (1965), 11, 241).

05.1-18 HIGH-TEMPERATURE INVESTIGATIONS OF MAGNETITE (Fe_3O_4). By N. Tzafaras, W. Adlhart, H. Jagodzinski, Institut für Kristallographie und Mineralogie der Universität München, München, Federal Republic of Germany.

The cation distribution of magnetite (spinel structure) has been investigated with a high-temperature X-ray camera. At temperatures above 1273K the NaCl-structure of $Fe_{1-y}O$ develops. The reversible transformation $Fe_3O_4 \rightleftharpoons Fe_{1-y}O$ can be performed by a slight variation of the oxygen partial pressure without destroying the single crystal. The kinetics of this transformation can be explained by diffusion of the iron-cations to the octahedral vacancies.

The lattice constant of magnetite was measured as a function of the temperature ($a_0=8.396$ \AA at 298K, $a_0=8.545$ \AA at 1273K expansion coefficient $\alpha_0=14.9 \cdot 10^{-6}/K$ at 1273K).

Structural refinements at 573K and 1073K yield an increase of the oxygen parameter X , indicating an increase of the O-Fe distance. We assume that this effect stems from anharmonic motions which may also explain the R-factor rising from 4.6% at 573K to 8.5% at 1073K.

05.1-19 CRITICAL NEUTRON SCATTERING IN THE 3-d ISING METAMAGNET $DyPO_4$ ^{a)}. By A.H. Millhouse H. Dachs, and M. Steiner, Hahn-Meitner-Institut, Glienicke Strasse 100, D-1000 Berlin 39, Germany.

The critical neutron scattering near the critical line of $DyPO_4$ has been investigated as a function of temperature, magnetic field, and hydrostatic pressure. At atmospheric pressure and at T_N the behaviour of the critical scattering is in agreement with theoretical predictions for the 3-d Ising model. As one moves along the critical line to lower temperatures the critical scattering peak weakens and disappears below 1.85 K. This indicates a change over from second- to first-order behaviour below this temperature. Magnetic domain effects do not vanish above this temperature in agreement with light-scattering measurements (Jahn, I.R., et al. Solid State Commun. 28, 421 (1978)). That strains are important in this system was confirmed by measurements under hydrostatic pressure. T_N is not sensitive to pressure up to 5 kbar but the transition at T_N becomes anomalous. It appears to be second-order for increasing temperature and first-order for decreasing temperature. This cannot be understood in terms of present theory.

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