

05.1-68 SOME HIGH PRESSURE X-RAY DIFFRACTION STUDIES USING BERYLLIUM GASKETING TECHNIQUE ON A DIFFRACTOMETER WITH ROTATING ANODE X-RAY SOURCE. By Y.K. Vohra, V. Vijaya Kumar, B.K. Gowal, S.K. Sikka and R. Chidambaram, Neutron Physics Division, Bhabha Atomic Research Centre, Trombay, Bombay 400085, India.

The use of beryllium (Be) gasketing technique for high pressure studies on a tungsten carbide anvil powder diffractometer has been investigated through measurements of equation of state (EOS) of alkaline earth metal strontium (Sr) and the phase transformations in group III element gallium (Ga) and the rare earth alloy $Ce_{0.92}La_{0.08}$. A high brilliance rotating anode X-ray source was employed. The Be-gasketing allows the use of a liquid pressure transmitting medium (4:1 methanol: ethanol) thereby ensuring the hydrostatic pressure conditions up to 10 GPa. In addition, for low Z-samples, $CuK\alpha$ radiation can be used for high resolution studies of interplanar spacings at high pressures. The Be-gasket was calibrated using known compression of NaCl at high pressures. The Sr-metal EOS was measured in both the low pressure (fcc) and high pressure (bcc) phases. This metal exhibits unusual compressibility in the high pressure phase indicating strong electron transfer from sp to d-bands. In Ga-metal a new phase transition from body-centered tetragonal phase (Ga-III) to a hcp phase was observed around 4.5 GPa at ambient temperature. The $V \rightarrow \alpha$ valence transition in $Ce_{0.92}La_{0.08}$ alloy was observed around 0.7 GPa but the transition was smeared out compared to the pure cerium-metal. The EOS of this alloy was measured up to 7 GPa.

05.1-69 TEMPERATURE INDUCED PHASE TRANSITIONS IN LIPID BILAYER MODELS. By G. Chapuis and K. Schenk, Institut de Cristallographie, Université de Lausanne, CH - 1015 Lausanne, Switzerland

Various types of compounds containing n-alkylammonium ions will be presented, notably $(C_nH_{2n+1}NH_3)_2MCl_4$ (short CnM, M = Cu, Zn and Cd) and $C_nH_{2n+1}NH_3Cl$ (CnCl). In these substances layers of n-alkylammonium ions alternate with layers of counter ions. The n-alkylammonium chains in the organic layer may be intercalated or not, depending on the length of the chains, on the nature of the adjacent layers or even on the temperature. These layer compounds are of particular interest as they mimic smectic liquid crystals and lipid bilayers as found in biomembranes.

All these compounds display various structural phase transitions which are due mainly to changes in the chain conformations at the interface with the counter ions. In the phases stable at the lowest temperature, the structure of the chains is such as to optimize the packing density. As a consequence, the central part of the layer consists always of chains in the all-trans conformation. Depending on the constraints imposed by the adjacent layers, the chains may introduce kinks (C-C torsion angles of $\pm 60^\circ$) near the ammonium end of the chains. Cl3Zn represents an interesting case in which the transitions preceding the melting of the chains could be structurally analyzed step by step. A characteristic of the room temperature phase is the existence of zones of different

packing densities. The first transition above room temperature features the complete disappearance of all kinks found in the room temperature phase. Instead a slight curvature of the zig-zag plane near the ammonium end was observed. In subsequent transitions, torsion angles are reintroduced at different locations, the number of independent chains varies and the disorder increases.

The p-cell, defined as the unit cell of the idealized periodic array of aliphatic carbon atoms, often varies according to the parity of the number of carbon atoms contained in the chain. In CnZn for example, the number of transitions observed up to the melting point depends on the p-cell type, whereas in CnCd no such regularity can be observed.

The series CnCl represents a novel type of reconstructive transitions from intercalated to non-intercalated chains. The driving force of the mechanism consists in an increase of the effective chain diameter (Kind et al., Phys. Rev. A26, 1816 (1982)) due to partial melting of the chains and a rearrangement of the network of hydrogen bonds in the nitrogen-chlorine layer.

Other examples of transition mechanisms involving aliphatic chains will be presented.

05.1-70 THE DEHYDRATION OF $CuSr_2(HCOO)_6 \cdot 8H_2O$: A CRYSTALLOGRAPHIC STUDY. By R.F. Baggio, M.A.R. de Benyacar, P.K. de Perazzo & G. Polla, Departamento de Física, Comisión Nacional de Energía Atómica, Buenos Aires, Argentina.

The dehydration of $CuSr_2(HCOO)_6 \cdot 8H_2O$ (CSFH) has been studied and the resulting products identified. The process seems to be one of internal dissolution, with further recrystallization of the stable phases at the working temperature. One of these, $CuSr(HCOO)_4$ (CSFA), has not been reported so far in the literature, and a thorough crystallographic characterization is given:

$CuSr(HCOO)_4$; monoclinic; Pc; Z=2;
 $a=7.35(1) \text{ \AA}$, $b=8.69(1) \text{ \AA}$, $c=6.70(1) \text{ \AA}$, $\beta=97.25(5)^\circ$
 $d_o=2.60(1) \text{ g/cm}^3$ (pycnometric); $d_c=2.591 \text{ g/cm}^3$.

When the dehydration takes place near room temperature, the remaining product, $Sr(HCOO)_2$ (SFA), bears a topotactical relationship to the parent structure:

$(hk0)_{CSFH} // (hk0)_{SFA}$ and $\langle 0k0 \rangle_{CSFH} // \langle 0k0 \rangle_{SFA}$.

As no structural motives seem to be preserved in the transformation, an alternative explanation is given to account for the topotactical relationship found.