05. PHYSICAL PROPERTIES AND STRUCTURE

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. Godwal, S.K. Sikka and B.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 transitions in group III element gallium (Ga) and the rare earth alloy Ce 0.92 Eu 0.08. A high brilliance rotating anode X-ray source was employed. The Be-gasket allows the use of a liquid pressure transmitting medium (di: methanol: ethanol) thereby ensuring the hydrostatic pressure conditions up to 40 GPa. In addition, for low Z samples, CuKα 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 of 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-II) to a hop phase was observed around 4.5 GPa at ambient temperature. The 0.5-1% valence transition in Ge 0.92 Eu 0.08 alloy was observed around 0.7 GPa but the transition was smeared out compared to the pure cecium-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-alkyl-ammonium ions will be presented, notably (CH₃)₂N+(CH₃)₄NH₄ (short CH₃, M = Cu, Zn and Cd) and CH₃)₂N+(CH₃)₄Cl (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 in the inorganic layer 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 2.50°) near the ammonium end of the chains. C13Sn 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 CnSn 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 CnCd 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 CuSr₂(HCOO)₄·8H₂O: A CRYSTALLOGRAPHIC STUDY. By R.F. Baggio, M.A.R. de Bergara, P.K. de Perezzo & G. Polla, Departamento de Fisica, Comision Nacional de Energia Atomatica, Buenos Aires, Argentina.

The dehydration of CuSr₂(HCOO)₄·8H₂O (CnSn) has been studied and the resulting products identified. The process seems to be one of interval dissolution, with further recrystallization of the stable phases at the working temperature. One of these, CuSr(HCOO)₂ (CSFA), has not been reported so far in the literature, and a thorough crystallographic characterization is given:

CuSr(HCOO)₂; monoclinic; P2; Z = 2 ;
α = 7.35(1) Å, β = 8.69(1) Å, γ = 6.70(1) Å, β = 97.25(5)°
ρ = 2.60(1) g/cm³ (pycnometric); d = 2.5912 g/cm³.

When the dehydration takes place near room temperature, the remaining product, Sr(HCOO)₂ (SPA), bears a topotactical relationship to the parent structure:

<CHA(100)>/<O0K> SPA and <CHA(100)>/<O0K> SPA.

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