test the "universal law" of dielectric response; parameters n and m were estimated.

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PS11.05.43 NEUTRON DIFFRACTION STUDY OF THE MARTENSITIC PHASE TRANSFORMATION IN In-Tl ALLOYS. H.G. Smith and J.L. Robertson, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA, T. R. Finlayson, Monash University, Clayton, Australia M. Wuttig, University of Maryland, College Park, Maryland, USA

InTl binary solid solutions with Tl concentrations between 15.5 and 31.0 atomic percent are know to undergo a martensitic phase transition from face-centered cubic, fcc, to face centered tetragonal, fct, upon cooling below the transformation temperature, Tm. Tm depends strongly on the Tl concentration dropping from 425K at 15.5 atomic percent Tl to nearly zero Kelvins at 31.0 atomic percent Tl. Appreciable phonon softening has been predicted from the theoretical calculation of the phonon dispersion relations and because the elastic stiffness modulus, c' = (c11 - c12)/2, approaches zero near Tm. A careful measurement of the phonon dispersion curves using inelastic neutron scattering, however, shows no phonon softening within the accessible Q range, but rather a slight hardening as would be expected for a metal. The discrepancy between the temperature dependence of c' and the complicated behavior of the phonon dispersion has yet to be resolved.

The intent of the present study is to examine more closely the structural changes that take place when the alloy transforms. High resolution neutron diffraction patterns were collected at several temperatures starting at 300K and decreasing to 9K on a In(23at%)Tl(77at%) polycrystalline sample. The martensitic transformation is observed to begin around 250K when the peaks associated with the face-centered cubic phase develop small shoulders. The structure continued to change continuously as the temperature was decreased even though the sample had completely transformed to the fct phase at around 200K. Upon warming the fcc phase reappeared 15K above where it vanished when cooling and the lattice parameters showed very little histeriesis. The sample had completely transformed back into the fcc phase by 260K. From these results we conclude that this martensitic transformation is weakly first order in the sense that the c/a ratio on the fct phase continues to increase as the temperature is lowered all the way down to 9K. It is important to remember, however, that this is a polycrystalline sample and any strains present could have a large affect on these observations. Further single crystal work is necessary in order to determine with more certainty the details of this transformation.

PS11.05.44 RAMAN SPECTRA INVESTIGATION OF TEMPERATURE PHASE TRANSITIONS IN ALKALI METAL PERCHLORATES. V.I. Snejkov, North Caucasus Scientific Center, 140, Pushkinskaya, Rostov-on-Don, 344006, Russia

It was discribed the obtained Raman spectra for wide temperature region (at room temperature to metling one). The degeneration of internal moleculer frequences is increased with growth of temperature and differ from as room - temperature data so ones predicted by symmetrical analysis. For example the Y2 mode of $LiClO_4$ contains two line for both solid phases. This fact indicates the higher temperature phase has a noncubic distorsion. For (K, Rb, Cs)ClO_4 the Y1 mode consist of only one line. The other mode (Y3) contains two lines for low teperature state which go out after phase transition. Such behaviour does not coincide with generally admitted interpretation of nature of these frequences. On the base of the obtained data it was proposed the new interpretation main modes (Y1, Y2, Y3) and elobarated the teoretical model explaining in frame work of slow symmetry the temperature behaviour of Raman spectra. This model connects the significances of frequance splittiny with the temperature stracture distorsin. In particuler the higher phase is pseudocubic (the tetragonal type) for $NaClO_4$ and it is cubic for (K, Rb, Cs)ClO_4. The last have tetragonal low temperature phase turning into ortorombic one under the room temperature.

PS11.05.45 AMMONIUM FLUOROBERYLLATE; NEUTRON STRUCTURE IN TWO PHASES. By R. C. Srivastava*, Department of Physics, Indian Institute of Technology, Kanpur 208016, India; W. T. Klooster and T. F. Koetzle, Chemistry Department, Brookhaven National Laboratory, Upton, NY 11973-5000, USA

Ammonium fluoroberyllate [$(NH_4)_2BeF_4$] undergoes a ferroelectric transition at 175 K (Pepinsky & Jona, Phys. Rev., 1957, 105, 344-345) and a non-ferroelectric transition at 182 K (Makita & Yamauchi, Phys. Soc. Jpn., 1974, 37, 1470). The phases are orthorhombic. The ferroelectric phase has a superlattice with the superlattice a-axis double that of the room-temperature phase. The intermediate phase also has a similar superlattice but is incommensurate along the a-axis (Iizumi & Gesi, Solid State Comm., 1977, 22, 37). The room-temperature x-ray structure has been reported by Garg & Srivastava (Acta Cryst., 1979, 335, 1432) and the ferroelectric phase x-ray structure by Srivastava & Craven (abstract PJ23, ACA Annual Meeting, 1991).

To obtain more accurate hydrogen positions the crystal structures at 200 K, 163 K and 20 K have been determined from neutron diffraction. The slight tilts of BeF_4^- and NH_4^+ ions from the mirror planes present in the paraelectric phase result in stronger hydrogen bonds in the ferroelectric phase. Two NH_4^+ ions reorient parallel to the polar b-axis. These will have some dipole moment and appear to be primarily responsible for ferroelectricity in the low temperature phase. Details of the neutron diffraction results will be presented.

The neutron diffraction study was carried out at Brookhaven National Laboratory under contract DE-AC02-76CH00016 with the U.S. Department of Energy and supported by its Office of Basic Energy Sciences.

PS11.05.46 THE STRUCTURE OF $Cs_5(HSO_4)_3(H_2PO_4)_2$. G. Staneff, P. Calkins, S. Fu and S.M. Haile, Department of Materials Science and Engineering, University of Washington, Seattle, WA 98195

The new compound $Cs_5(HSO_4)_3(H_2PO_4)_2$ was synthesized as part of an ongoing study to examine the relationship between hydrogen bonding and phase transitions in solid acid compounds. The compound crystallizes in space group C2/c and has lattice constants a = 34.07(2), b = 7.661(4), c = 9.158(6) Å and b = 90.44(2)°. The structure of $Cs_5(HSO_4)_3(H_2PO_4)_2$ contains both layers and chains of hydrogen-bonded XO_4 groups (where X = P or S). Phosphate groups form corrugated layers that are perpendicular to b, whereas sulfate groups form branched chains, located between the phosphate layers. These chains extend along c. The compound is unusual in that the two crystallographically distinct SO_4 sites have different numbers of hydrogen-bonded oxygen atoms: S(1) has only one oxygen nearest neighbor that is hydrogen bonded whereas all 4 oxygen atoms bonded to S(2) are additionally hydrogen-bonded to neighboring oxygen atoms. Similarly, all oxygen atoms participating the PO_4 tetrahedra are hydrogen bonded.

The presence of both hydrogen-bonded and non-hydrogen-bonded oxygen atoms suggests that the material will undergo a superprotonic phase transition at elevated temperatures. Indeed, a transition is observed at 391K by differential scanning calorimetry. Furthermore, the presence of locally disordered hydrogen bonds suggest the material will undergo a ferroelectric material at low temperatures.