PS10.07.08 DIELECTRIC CHARACTERISTICS OF PURE & MIXED RARE EARTH (La,Nd) HEPTAMOLYBDATE CRYSTALS GROWN BY GEL ENCAPSULATION TECHNIQUE. Sushma Bhat, S.K. Khosa, P.N. Kotru, R.P. Tandon*, Department of Physics, University of Jammu, Jammu-180004 (India)*, National Physical Laboratory, New Delhi, India

Single crystal growth of single rare earth heptamolybdate (where R=La,Nd) and mixed (La-Nd) is achieved using the system R (NO3)3 - MoO3·NH4 OH - HNO3·Na2SO3 by gel encapsulation technique. The crystals are characterized using X-ray and electron diffraction, IR spectroscopy, SEM and optical microscopy. Dependence of dielectric constant, dielectric loss and conductivity of the samples subjected to different frequencies of the applied a-c fields at different temperatures is studied. The dielectric constant of the materials increase sharply, attains a peak value then decreases rapidly, as the temperature is raised. Dielectric loss and conductivity are strongly temperature and frequency dependent. The sharp rise of dielectric constant with temperature at 103 Hz for T<Tc (Tc being the transition temperature) is attributed to the contribution to a major contribution from space charge polarization. The functional relationships between the dielectric constant (ε) and conductivity (σ) and temperature (T) is theoretically linked to analytical expressions of the type ε = a + b (T - T0) for T<Tc. The indications of these materials being ferroelectric are suggested by the non-linearities and anomalous behaviour of dielectric constant near the transition temperature and further supplemented by the results of preliminary hysteresis experiments.


X-ray diffraction studies were carried out together with luminescence measurements for NaCl:Sr2:Eu2+,2%, NaCl:Er2+ and NaCl:Pb2+ single crystals under thermal annealing treatments at 200-400°C. The weak diffracted beams, coming out from the precipitation of secondary phases into the NaCl matrices, were enhanced by using a simple pneumatic grinder designed and built to obtain small single-crystal spheres of optimum size for minimize the absorption effects. This device offers an advantage over previous grinder systems in that it allows the selection in advance of the final diameters of the crystal spheres by means of pneumatic expulsion through a standard brass gauze. It was found that the precipitation of a secondary SrCl2 phase and a fluoride-type EuCl3 phase into the NaCl matrices are responsible for the presence of emission bands peaking at 407 and 410 nm in the optical fluorescence spectra of specimens annealed for long periods.

PS10.07.10 THE CRYSTAL STRUCTURE OF CdGeSe4, A III4 IV VI4 SEMICONDUCTING MATERIAL. J.M. Delgado*, J.A. Henao*, A.E. Mora** and M. Quintero**, *Departamento de Quimica and **Departamento de Fisica, Facultad de Ciencias, Universidad de Los Andes, Mérida 5101, Venezuela

X-ray quality single crystal fragments of CdGeSe4 were isolated from polycrystalline samples prepared by direct fusion of the elements in sealed, evacuated quartz ampoules. The stoichiometric proportion Cd:Ge:Se=2:1:4 was used because it was originally intended to prepare Cd2GeSe4, a III2 IV V111 semiconductor, instead of the IIIC4 IV VI4 finally obtained. The chemical composition of this phase was established using a KeveX EDX equipped Hitachi S-1250 SEM. The structural study carried out using single crystal diffraction techniques showed that this material crystallizes in the monoclinic space group Cc, with a=12.843(2), b=7.411(1), c=12.855(2)Å, β=109.85(1) and Z=4. Its structure can be described as a superstructure based upon a MgCu2-type of structure. The superstructure nature of this material was deduced from Buerger precession photographs and confirmed in the structural analysis using the intensity data collected with a four-circle single-crystal x-ray diffractometer.

A detailed discussion of the different space groups types reported for the IIIC4 IV VI4 family of semiconductors is presented. This work was supported by CONICIT, Programa de Nuevas Tecnologías, Grant NM-18. JAH thanks UIS, Bucaramanga, Colombia for a fellowship.

PS10.07.11 MOLECULAR METALS: STRUCTURE AND PROPERTIES. O.A. Dyachenko, V.V. Gritsenko, S.V. Konovalikhin, R.N. Lyubovskaya, E.B. Yagubskii, R.B. Lyubovskii, Institute of Chemical Physics, RAS, Chernogolovka MD 142432 Russia, and E.Canadell, ICMAB, Campus de la UAB, 08193 Bellaterra, Spain

The structure-conductivity relationships were derived from crystal-line diffraction experiments for the salts based on bis(ethylenedinitro)tetrafluorvalene (ET) and 5,6-dihydro-1,4-dithin-2,3-dithiol (DDDT), which are potential electronic materials. As a subject for crystallochemical analysis were chosen the family of molecular conductors (ET)2[Hg2X2(P3)2] (X=Cl, Br, XeCl3 metal down to 1.3 K; XeBr, Y=Cl, Tm=90 K; XeBr, Y=Br, Tm=125 K), the first stable down to 1.3 K molecular metals, [Ni(DDDT)2]2(AlBr3) and [P(DDDT)2]2Ag0.80Bi0.20, in the M(DDDT)2 family of conducting complexes, as well as such relative compounds as molecular semiconductors (ET)2[Hg2Br2]2(Mg2H2O)4, (ET)2[Hg2Cl2]2(CdHg)2, (ET2)2[Ge2P2] and investigated recently new organic metals (BEDO)P(CN)2H2O and (BEDO)2C2H2O. In order to understand the structure-property problem in this case, we have performed a multisite crystallochemical analysis of the investigated salts by the scheme: Composition → Amion and anionic layer structure → Conducting layer structure (packing and overlapping types, shortened intermolecular contacts) → Conductivity. On the basis of this analysis it has been established, that: i) the packing type of a conducting layer determines the conductivity type (superconductor, metal, semiconductor), and ii) there is an inverse dependence between the temperatures of metal-insulator transitions (Tm) and the densities of conducting layers. Tight-binding band structure calculations have been carried out for comparison of the electronic structures of relative molecular metals.

PS10.07.12 COMPARATIVE INVESTIGATIONS OF Nb AND Ta DOPED KTOPO MATERIALS BY HIGH-RESOLUTION X-RAY DIFFRACTION. C.J.Eaton, P.A.Thomas, Department of Physics, University of Warwick, Coventry, CV4 7AL, UK K. B. Hutton, R.C.C. Ward, University of Oxford, Clarendon Laboratory, Parks Road, Oxford, OX1 3PU, UK

Doping of the KTOPO (KTP) family of materials with ions such as Ta and Nb yields promising non-linear optical materials with increased birefringence but modified physical properties, such as mechanical strength. In this work, 10% niobium doped KTP, and 1% tantalum doped KTP have been studied using high-resolution x-ray diffraction to investigate the crystal quality compared with that of pure KTP. Topographs and reciprocal-space maps are shown and indicate that there is a degree of mosaicity within the material, with both similar and differing d-spacings in the mosaic blocks. These microstructural features are discussed in relationship to the crystal growth and quality of doped KTP and the suppression of growth along the [100] direction in particular.

In addition, second-harmonic generation studies have been conducted to image the mosaic blocks, and energy-dispersive x-ray analysis has been performed to determine if dopant levels are homogeneous throughout the sample.