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 heptamolybdates (where R=La,Nd) and mixed (La-Nd) is achieved using the system R $(NO_3)_3$ - MoO_3-NH_4 OH - HNO_3-Na_2SiO_3 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 10^3 Hz for $T<T_o$ (T_o being the transition temperature) is attributed to the contribution to a major contribution from space charge polarization. The functional relationship between the dielectric constant (ε) and conductivity (σ) and temperature T is theoretically linked to analytical expressions of the type $\varepsilon = a_0 + a_1T^2$ and $-\ln \sigma = a+b(T-T_o)^2$ for $T<T_o$. The indications of these materials being ferroelectric are suggested by the non-linearities and anamolous behaviour of dielectric constant near the transition temperature and further supplemented by the results of preliminary hystereses experiments.

PS10.07.09 X-RAY DIFFRACTION STUDIES OF THE STRUCTURAL ORIGIN OF SOME OPTICAL EMISSION BANDS IN ION-DOPED NaCl CRYSTALS. A. E. Cordero-Borboa, Instituto de Fisica, UNAM. A.P. 20-364, D.A. Obregon Mexico D.F. 01000, Mexico.

X-ray diffraction studies were carried out together with luminescence measurements for NaCl:Sr^{+2}:Eu^{+2}, NaCl:Eu^{+2} and NaCl:Pb^{+2} single crystals under thermal annealing treatments at 200°C. The weak diffracted beams, coming out from the precipitation of secondary phases into the NaCl matrixes, were enhanced by using a simple pneumatic grinder designed and built to obtain small single-cristal 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 $SrCl_2$ phase and a fluorite-type $EuCl_2$ phase into the NaCl matrixes are responsible for the presence of emission bands peaking at 407 and 410 nm in the optical fluorescence spetra of specimens annealed for long periods.

PS10.07.10 THE CRYSTAL STRUCTURE OF Cd_4GeSe_6, A II_4 IV VI_6 SEMICONDUCTING MATERIAL. J.M. Delgado*, J.A. Henao*, A.E. Mora** and M. Quintero**. *Departamento de Química and **Departamento de Física, Facultad de Ciencias, Universidad de Los Andes, Mérida 5101, Venezuela

X-ray quality single crystal fragments of Cd_4GeSe_6 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 Cd_2GeSe_4, a II_2 IV VI_4 semiconductor, instead of the II_4 IV VI_6 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, =109.85(1) and Z=4. Its structure can be described as a superstructure based upon a $MgCu_2$-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-cystal x-ray diffractometer.

A detailed discussion of the different structure types reported for the II_4 IV VI_6 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 crystalline diffraction experiments for the salts based on bis(ethylenedithio)tetrathiafulvalene (ET) and 5,6-dihydro-1,4-dithiin-2,3-dithiol (DDDT), which are potential electronic materials. As a subject for crystallochemical analysis were chosen the family of molecular conductors $(ET)_8[Hg_4X_{12}(PhY)_2]$ (X=Y=Cl, metal down to 1.3 K; X=Cl, Y=Br, T_{MI}=10 K; X=Br, Y=Cl, T_{MI}=90 K; X=Y=Br, T_{MI}= 125 K), the first stable down to 1.3 K molecular metals, $[Ni(DDDT)_2]_3(AuBr_2)_2$ and $[Pd(DDDT)_2]Ag_{1.54}Br_{3.50}$, in the $M(DDDT)_2$ family of conducting complexes, as well as such relative compounds as molecular semiconductors $(ET)_8[Hg_4Br_{12}(MeC_6H_4Cl)_2]$, $(ET)_8[Hg_4Cl_{12}]\cdot 2C_6H_6$, $(ET)_4[Hg_2I_6]$ and investigated recently new organic metals $(BEDO)_4Pt(CN)_4H_2O$ and $(BEDO)_2Cl2H_2O$. In order to understand the structure-property problem in this case, we have performed a multistage crystallochemical analysis of the investigated salts by the scheme: Composition → Anion 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 (T_{MI}) 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 $KTiOPO_4$ 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 $KTiOPO_4$ (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 made to image the mosaic blocks, and energy-dispersive x-ray analysis has been performed to determine if dopant levels are homogeneous throughout the sample.