known: $Gly_3 \cdot ZnCl_2$ (space group $Pbn2_1$), $Gly_2 \cdot ZnCl_2 \cdot 2H_2O$ (space group $C2/c$), $Gly \cdot ZnCl_2 \cdot H_2O$ (space group $P2_1/a$) and $Gly \cdot ZnCl_2$ (space group $P2_1$), (gly = abbreviation of glycine) [1-5]. In recent studies crystals of the polar compound $Gly_3 \cdot ZnCl_2$ turned out to be attractive optical materials, that show both, phase-matchable second harmonic generation (SHG) and efficient frequency conversion by stimulated Raman scattering (SRS) with a rather large Raman shift of about 3000 cm^{-1} [2, 6]. Motivated by these results we focused our interest on the further glycine compounds listed above. In the present contribution we report on crystal growth of $Gly_2 \cdot ZnCl_2 \cdot 2H_2O$ and of $Gly \cdot ZnCl_2$, together with their basic linear optical properties. Large single crystals of $Gly_2 \cdot ZnCl_2 \cdot 2H_2O$ were grown from aqueous solution at 38°C by controlled slow evaporation of the solvent. Within three months crystals with dimensions up to 5 x 4 x 3 cm were obtained. Crystal growth of $Gly \cdot ZnCl_2$ was performed at 50°C and resulted in crystals of dimensions up to 2.5 x 1 x 0.7 cm after a growth period of six months. Refractive indices and their dispersion were determined by the prism method in the wavelength range of 0.365 – 1.083 μm. These results establish the essential prerequisites for further nonlinear optical investigations. In the centrosymmetric crystals of $Gly_2 \cdot ZnCl_2 \cdot 2H_2O$ SRS will be unaffected by $\chi^{(2)}$-based nonlinear optical processes such as SHG and sum frequency generation (SFG), while the polar crystals of $Gly \cdot ZnCl_2$ are expected to allow the study of both, SHG and cascaded $\chi^{(2)} + \chi^{(3)}$ nonlinear processes.

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Keywords: glycine zinc chloride, crystal growth, optical properties

FA2-MS14-P09

Synthesis and structural properties of ZnO films grown by spray pyrolysis of zinc acetate solution.

Nancy Castillo[a], Rodrigo Esparza[b] Jesus Velazquez[b], Agustin Conde Gallardo[a] Miguel Jose Yacaman[b]. [a]*FISICA, Centro de Investigacion y de estudios Avanzados del IPN, D:F: Mexico.* [b]*2International Center for Nanotechnology and Advanced Materials, Department of Physics & Astronomy, University of Texas, San Antonio USA.*
E-mail: necastillo@yahoo.com

Crystalline ZnO films have a wide variety of applications in the manufacturing of devices such as gas sensors, flat panel displays, transparent electrode materials, solar cells, electroluminescent diodes, etc. The films used have a range of crystal structures and morphologies, and many different methods such as sputtering[1], vacuum evaporation[2] thermal oxidation of Zn films, atomic layer epitaxy and spray pyrolysis. This last technique can be distinguished from the others due to its simplicity, low cost and efficiency, and it provides a powerful tool for creating diverse film structures (from the point of view of grain habits and their associations) with significant differences in morphology, by varying the of pyrolysis conditions.

The morphology and some principal details of the crystallographic grain structure of zinc oxide thin (50–300 nm) films obtained from acetate $Zn(CH_3CO_2).2H_2O$ solution by spray pyrolysis deposition were studied using X-ray diffraction (XRD), extreme high-resolution scanning electron microscopy (XHR SEM) and Transmission Electron microscopy (TEM) methods. Direct correlation between the pyrolysis temperature and several fundamental nanoscale grain shapes and crystallographic features successively replacing each other with *T*pyr was shown.

The X ray diffraction patterns of the films were recorded using a diffractometer with monochromatic Cu K radiation. XRD and TEM results show that these nanoparticles are composed of ZnO with hexagonal structure The parameters of the hexagonal elementary cell are as follows: a = 3.2539(1) Å, c = 5.2098(3) Å, c/a = 1.6011, V = 47.77 Å^3. The microstructure of the film was studied with the electron microscope. From these studies it was observed that the orientation of the grains was uniform and the crystallites were very small in size. The morphology qualitatively remained the same and variation in film thickness

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Keywords: nanoparticles, TEM, ZnO, thin film

FA2-MS14-P10

Effects on the physical properties of cation substitution in (La, Sr) CoO_3 perovskite system.

A. Cheikhrouhou[a-b], M. Koubaa[a], N. Mahfoudh[a], W. Cheikhrouhou-Koubaa[a]. [a]*Faculté des Sciences de Sfax, B.P.1171, 3000, Sfax, Tunisie.* [b]*Institut NEEL, B.P.166, 38042 Grenoble-France.*
E-mail abdcheikhrouhou@yahoo.fr

Cobaltites with general formula $Ln_{1-x}M_xCoO_3$ (Ln is a rare earth element and M is a divalent alkali earth element) have received recently considerable interest due to their potential technological applications. Several studies have been reported on strontium doped $LaCoO_3$ compounds because of its complex phase diagram. At low Sr doping a spin glass (SG) and/or cluster glass (CG) behavior is observed at low temperature, whereas larger Sr doping leads to ferromagnetic ordering. In this work, we present the effects of both (La,Sr)-site and Co-site substitutions on the physical properties in the $(La,Sr)CoO_3$ powder system. Our samples have been elaborated using the solid state reaction method at high temperatures. The Rietveld refinements of the X-ray diffraction patterns recorded at room temperature show that our compounds are single phase and crystallize in the rhombohedral structure with $R\bar{3}c$ space group. The zero field cooled (ZFC) and field cooled (FC) magnetization curves at 50mT show thermomagnetic irreversibility. The magnetic phase at low temperature is found to be correlated to the Co^{3+}/Co^{4+} ratio as well as the A-site average ionic radius. The magnetic entropy change, $|\Delta S_M|$, as a function of temperature and magnetic applied field has been determined from the isothermal magnetization measurements using the Maxwell relations.

Keywords: Cobalt compounds, X-ray diffraction, magnetic properties.

FA2-MS14-P11

Kinetic and magnetic studies of the phase behaviour in $LiFePO_4$-$FePO_4$ mixed crystals. J. Davaasambuu[a], N. Tuvjargal[b], F. Güthoff[a], P. Axmann[c], S. Demeshko[d], G. Eckold[a]. [a]*Institute of Physical Chemistry, University of Göttingen, Germany.* [b]*Department of Physics, National University of Mongolia, Mongolia.* [c]*Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg, Ulm, Germany.* [d]*Institute of Inorganic Chemistry, University of Göttingen, Germany.*
E-mail: jdavaas@gwdg.de

In the last years, the development of novel materials for battery applications on lithium-basis has achieved great progress. Among them, $LiFePO_4$ is one of the most prominent and promising compounds[1]. The phase behaviour of the mixed system $LiFePO_4$ - $FePO_4$ is controversially discussed in the literature. There are different phase diagrams reported by Delacourt et al.[2] and Dodd et al.[3].
Time-resolved X-ray diffraction was used to investigate the kinetics of phase separation in polycrystalline Li_xFePO_4 samples which were quenched from the homogeneous phase to lower temperatures. $LiFePO_4$ was synthesized via solid-state reactions according to Lee et al.[4]. For the preparation of mixed crystals with different concentrations of lithium we used the chemical delithiation route proposed by Dodd et al.[3]. On quenching from 380°C (homogeneous phase) to ageing temperatures around 100°C, we observed that the structural features of the formation of the two product phases $LiFePO_4$ and orthorhombic $FePO_4$, i.e. the splitting of selected Bragg reflections, appear on a time-scale of hours. But the demixing process does not complete within 24h. The kinetic behaviour seems to vary strongly with the ageing temperatures. In the case of quenching to temperatures lower than 50°C, no significant splitting of Bragg reflections is observed. Hence, the homogeneous phase may be stabilised by quenching to sufficiently low temperatures.
We have studied the magnetic properties of the samples by SQUID-magnetometry. The partially delithiated samples show the known temperature dependence of the magnetic susceptibility with ordering temperatures of about 122K ($FePO_4$) and 50K ($LiFePO_4$). In order to create a single phase, the samples were quenched from the homogeneous phase to room temperature. Obviously, Néel temperatures of these samples were observed in between the values of pure compounds and depend on the overall composition.

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Keywords: battery materials, phase behaviour, magnetic properties

FA2-MS14-P12

Magnetic and Electrical Properties of $InSe_{1-x}Fe_x(Co_x)$ in Relation to Nano- Structure. Karimat El-Sayed[a], Z.K. Heiba[a], K. Sedeek[b], Z.K. Heiba[a], H.H. Hantour[b]. [a]X-ray Dffraction unit, Physics Department, Faculty of *Science, Ain Shams University.* [b]*Physics Department Faculty of Science Girls Branch Al-Azhar Uniersity.*
E-mail: elkarimat@yahoo.com

Introducing few magnetic elements such as (Fe,Co) into the non-magnetic semiconductor InSe changes the materials to ferromagnetic with very low coercivity and very low reminance magnetization in case of Fe and antiferromagnetic in case of Co. From the (magnetic susceptibility - Temperature relation) the Curiee temperature and the Blocking temperature were caculated for $InSe_{0.9}Fe_{0.1}$ to be 873K and 733K respectively , a property that will allow this system to be used in spintronic devices operated at room temperature and above.
The cluster model was applied to explain the origin of ferromagnetism in the nanosize diluted magnetic semiconducting (DMS) sample $InSe_{0.9}Fe_{0.1}$. On the other hand $InSe_{0.9}Co_{0.1}$ sample indicated that more than one antiferromagnetic transition states takes place with paramagnetic state in between and with two different Neel temperatures. The XRD indicates the presence of a non-magnetic second minor phase In_4Se_3 in InSe and confirm the presence of nano size particle of different ranges. Transmission electron microscope (TEM) confirms that the particle size ranges between the quantum dot and the bigger nano size.The scanning electron microscope (SEM) images demonstrate the presence of stacking faults in all samples. For $InSe_{0.9}Fe_{0.1}$ sample, the relation between logσ and 1/T is a straight line which argues the exhaustion of the center of the forbidden gap of the InSe of localized states. Only one band of localized states situated at the top of the extended states was suggested (ΔE=0.43eV) . The conductivity data argue that the incorporation of Fe or Co creates new band configuration and hence modification of the electronic density of states of InSe.The increase in σ_{RT} of $InSe_{0.9}Fe_{0.1}$ was nearly hundred times that of the InSe. .Correlation with the ferromagnetic and antiferromagnetic character of $InSe_{0.9}Fe_{0.1}$ and $InSe_{0.9}Co_{0.1}$ with each other and with nano structure was considered in discussing the mgnetic and conductivity data..

Keywords:Diluted Simicoductor, Spintronic semicoductor, Nano materials

FA2-MS14-P13

The Thermoresponsive Phase Behaviour of CuSICON: $CuM_2P_3O_{12}$ [M = Ti, Zr, Sn & Hf]. Roy P. Forbes[a], David G. Billing[a]. [a]*National Research Foundation Centre of Excellence in Strong Materials.* [a]*School of Chemistry University of the Witwatersrand Johannesburg, South Africa.*
E-mail: roy.forbes@students.wits.ac.za

The NaSICON (Na Super Ionic Conductor) structural family with formula $A_xM_yP_3O_{12}$ [$0 \leq x \leq 1$; $1 \leq y \leq 3$] crystallize with rhombohedral symmetry [space group *R-3c* (No. 167)] and are composed of a three dimensional corner sharing framework of PO_4 tetrahedra and MO_6 octahedra connected to form a chain like structure with two dimensional channels extending throughout the structure **[1]**. Owing to the flexibility of this structure towards ionic substitutions at various lattice sites, these materials have enjoyed consistent scientific interest due to the various useful physical properties that they posses. CuSICON (Cu super ionic conductor), with general formula $CuZr_2P_3O_{12}$ is an example of a material that is isostructural with the NaSICON parent structure **[2]**. TGA and EPR studies