

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

#### FA2-MS14-P11

**Kinetic and magnetic studies of the phase behaviour in LiFePO<sub>4</sub>-FePO<sub>4</sub> mixed crystals.** J. Davaasambu<sup>a</sup>, N. Tuvjargal<sup>b</sup>, F. Güthoff<sup>a</sup>, P. Axmann<sup>c</sup>, S. Demeshko<sup>d</sup>, G. Eckold<sup>a</sup>. <sup>a</sup>*Institute of Physical Chemistry, University of Göttingen, Germany.* <sup>b</sup>*Department of Physics, National University of Mongolia, Mongolia.* <sup>c</sup>*Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg, Ulm, Germany.* <sup>d</sup>*Institute of Inorganic Chemistry, University of Göttingen, Germany.*  
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In the last years, the development of novel materials for battery applications on lithium-basis has achieved great progress. Among them, LiFePO<sub>4</sub> is one of the most prominent and promising compounds[1]. The phase behaviour of the mixed system LiFePO<sub>4</sub> - FePO<sub>4</sub> 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<sub>x</sub>FePO<sub>4</sub> samples which were quenched from the homogeneous phase to lower temperatures. LiFePO<sub>4</sub> 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<sub>4</sub> and orthorhombic FePO<sub>4</sub>, 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<sub>4</sub>) and 50K (LiFePO<sub>4</sub>). 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.

[1] Padhi A.K., Nanjundaswamy K.S., Goodenough J.B., *J. Electrochem. Soc.*, 1997, 144, 1188. [2] Delacourt C., Poizot P., Tarascon J.-M., Masquelier C., *Nature Materials*, 2005, 4, 254. [3] Dodd J.L., Yazami R., Fultz B., *Electrochemical & Solid-State Letters*, 2006, 9, A151. [4] Lee J., Teja A.S., *Materials Letters*, 2006, 60, 2105.

**Keywords:** battery materials, phase behaviour, magnetic properties

#### FA2-MS14-P12

**Magnetic and Electrical Properties of InSe<sub>1-x</sub>Fe<sub>x</sub>(Co<sub>x</sub>) in Relation to Nano- Structure.** Karimat El-Sayed<sup>a</sup>, Z.K. Heiba<sup>a</sup>, K. Sedeek<sup>b</sup>, Z.K. Heiba<sup>a</sup>, H.H. Hantour<sup>b</sup>.

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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 remanance magnetization in case of Fe and antiferromagnetic in case of Co. From the (magnetic susceptibility - Temperature relation) the Curie temperature and the Blocking temperature were calculated for InSe<sub>0.9</sub>Fe<sub>0.1</sub> 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<sub>0.9</sub>Fe<sub>0.1</sub>. On the other hand InSe<sub>0.9</sub>Co<sub>0.1</sub> 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<sub>4</sub>Se<sub>3</sub> 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<sub>0.9</sub>Fe<sub>0.1</sub> 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<sub>RT</sub> of InSe<sub>0.9</sub>Fe<sub>0.1</sub> was nearly hundred times that of the InSe. Correlation with the ferromagnetic and antiferromagnetic character of InSe<sub>0.9</sub>Fe<sub>0.1</sub> and InSe<sub>0.9</sub>Co<sub>0.1</sub> with each other and with nano structure was considered in discussing the magnetic and conductivity data.

**Keywords:** Diluted Simiconductor, Spintronic semiconductor, Nano materials

#### FA2-MS14-P13

**The Thermoresponsive Phase Behaviour of CuSICON: CuM<sub>2</sub>P<sub>3</sub>O<sub>12</sub> [M = Ti, Zr, Sn & Hf].** Roy P. Forbes<sup>a</sup>, David G. Billing<sup>a</sup>. <sup>a</sup>*National Research Foundation Centre of Excellence in Strong Materials. School of Chemistry University of the Witwatersrand Johannesburg, South Africa.*  
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The NaSICON (Na Super Ionic Conductor) structural family with formula A<sub>x</sub>M<sub>y</sub>P<sub>3</sub>O<sub>12</sub> [0≤x≤1; 1≤y≤3] crystallize with rhombohedral symmetry [space group R-3c (No. 167)] and are composed of a three dimensional corner sharing framework of PO<sub>4</sub> tetrahedra and MO<sub>6</sub> 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 possess. CuSICON (Cu super ionic conductor), with general formula CuZr<sub>2</sub>P<sub>3</sub>O<sub>12</sub> is an example of a material that is isostructural with the NaSICON parent structure [2]. TGA and EPR studies