

KR 1: Poster

Time: Wednesday 18:00–20:00

Location: Poster E

KR 1.1 Wed 18:00 Poster E

Mechanism of delafossite (CuFeO_2) formation in aqueous solution — ●MELANIE JOHN¹, ALADIN ULLRICH², and SORAYA HEUSS-ASSBICHLER¹ — ¹Ludwig-Maximilians-Universität München, München, Deutschland — ²Universität Augsburg, Augsburg, Deutschland

Recently we successfully synthesized delafossite (CuFeO_2) nanoparticles at 70°C by a facile precipitation and ageing process for the first time. In literature, there are only very few references on the formation mechanism of delafossite in aqueous solution. However, for further optimization of the synthesis processes and the transferability to other ABO_2 structures, it is necessary to get a better understanding of the formation mechanisms in this system. Our results show that green rust II (GR- SO_4 , a Fe(II-III) layered double hydroxysulphate) and Cu_2O precipitate first. During further OH-supply GR- SO_4 oxidizes and forms $\text{Fe}_{10}\text{O}_{14}(\text{OH})_2$, Cu_2O and CuFeO_2 crystals. Due to an alkaline pH further CuFeO_2 crystals grow at the cost of the unstable intermediate products. The reaction rate increases with increasing ageing temperature, reaction pH and, in particular, NaOH concentration in the solution. As a result, high crystalline CuFeO_2 nanoparticles showing hexagonal, platy morphology form. The precipitation residues were analyzed using ICP-OES, FTIR, XRD, SEM and TEM.

KR 1.2 Wed 18:00 Poster E

Compositional influence on the pyroelectric coefficient of $(1-x)\text{PMN}-x\text{PT}$ — ●SVEN JACHALKE, ERIK MEHNER, HARTMUT STÖCKER, ERIK SCHLEICHER, TILMANN LEISEGANG, and DIRK C. MEYER — TU Bergakademie Freiberg, Institut für Experimentelle Physik, Leipziger Str. 23, 09596 Freiberg

Solid solutions of lead magnesium niobate – $\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3$, PMN – and lead titanate – PbTiO_3 , PT – in different compositions – $(1-x)\text{PMN}-x\text{PT}$ – attract a large scientific interest due to their superb electromechanical and electrothermal properties, especially near

the morphotropic phase boundary around $x = 0.30$. The present study focuses on the pyroelectric properties, i.e. the change of spontaneous polarization due to temperature fluctuations. Pyroelectric coefficients $p(T)$ of single crystals are determined systematically with respect to different compositions ($x = 0.25$ to $x = 0.32$) and crystallographic orientations ($\langle 111 \rangle$, $\langle 011 \rangle$ and $\langle 001 \rangle$), including ferroelectric-to-ferroelectric and ferroelectric-to-dielectric phase transitions (at the Curie temperature T_C), in the temperature range of 273 K to 423 K. Data acquisition and analysis using the Sharp-Garn-method [1] allow separating the pyroelectric from disturbing non-pyroelectric current signals and yield temperature dependent pyroelectric coefficients (accuracy 1–5 %) and polarization.

[1] L. E. Garn and E. J. Sharp, “Use of low-frequency sinusoidal temperature waves to separate pyroelectric currents from nonpyroelectric currents”, J. Appl. Phys., Vol. 53, No. 12, p. 8974, 1982.

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Theoretical Exploration of Phase Diagrams using Monte-Carlo Site Swapping — ●KATHRYN BRADLEY, MATTHEW DYER, JOHN CLARIDGE, GEORGE DARLING, and MATTHEW ROSSEINSKY — Department of Chemistry, University of Liverpool, Crown Street, Liverpool, L69 7ZD, United Kingdom

A method has been developed for investigating the phase diagrams of structures with similar structural motifs, using a combination of structural prediction, forcefield calculations and density functional theory (DFT). Li_3PO_4 and Li_4SiO_4 can be described in terms of close-packed oxide lattices with cations present in the interstitial sites. It is therefore possible to generate a superlattice with a mixed composition. The structure is first evaluated using forcefield optimisation with Monte-Carlo site swapping, and the stability of the suggested composition is then assessed using DFT energies. This new approach will help with the exploration of phase diagrams to assist in the field of materials discovery.