MS17-O2 Analysis of complex phase transitions using time resolved XRPD data

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Due to recent upgrades of synchrotron- and laboratory sources and the parallel development of new position sensitive detectors and reaction cells, it is now possible to collect a vast amount of powder diffraction patterns *in situ* in dependence on external variables (i.e. temperature or pressure) with a time resolution in the second or even sub-second regime thus allowing to track many complex structural changes in detail [1-6]. The real challenge is to get the maximum amount of information from these high quality data. In principal, the information content of a powder pattern is huge, but much effort is needed to reveal the often hidden information. In the last decade, many new ideas have been successfully applied to powder diffraction, like the method of maximum entropy (MEM), fundamental parameters, global optimization in direct space, parametric Rietveld refinement, kinetics, distortion mode amplitudes, to name just a few. It is the intention of this talk to discuss some hot topics in powder diffraction concerning methodology and application to various problems in solid state research. [1] Tomislav, F., Halasz, I. Beldon, P.J., Belenguer, A.M., Adams, F., Kimber, S.A.J., Honkimäki, V., Dinnebier, R.E., *Nature Chem.*, **2013**, *5*, 66–73. [2] Magdysyuk, O.V., Denysenko, D., Weinrauch, I., Volkmer, D., Hirscher, M., Dinnebier, R. E., *Chem. Commun.*, **2015**, *51*, 714-717. [3] Magdysyuk, O.V., Müller, M., Dinnebier, R.E., Lipp, C., Schleid, T. *J., Appl. Crystalogr.*, **2014**, *47*, 701-711. [4] Panda, M.K., Runcevski, T., Chandra, Sahoo, S., Belik, A.A., Nath, N.K., Dinnebier, R.E., Naumov, P., *Nat. Commun.*, **2014**, *5*, 4811-4818. [5] Runcevski, T., Petrusevski, G., Makreski, P., Ugarkovic, S., Dinnebier, R.E., *Chem. Commun.*, **2014**, *50* , 6970—6972. [6] Runčevski, T., Blanco-Lomas, M., Marazzi, M., Cejuela, M., Sampedro, D., Dinnebier, R.E., *Angew. Chem. Int. Ed.*, **2014**, *53*, 6738-6742.

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MS17-O3 Kinetics of strain mechanisms in functional materials: Stroboscopic powder diffraction on piezoceramics

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Piezoelectric ceramics exhibit the remarkable property to couple elastic strain and polarization under the influence of an applied electric field. Among the various types of ferroelectric devices only actuators rely on high electric fields to generate high strains and forces. Prominent examples for actuators are multilayer stack actuators used for nanopositioning or in modern combustion engines for automobiles to control injection cycles. Despite extensive studies and elaborated measurement techniques, the correlation between macroscopic strain and structural response is still not fully understood. Most of the relevant systems found up to now are compositions close to phase boundaries linking highly correlated phases. This results in major challenges for structural analyses due to overlapping reflections. Apart from the well-known field induced structural responses such as domain switching and the piezoelectric effect we recently identified field induced phase transitions in different systems as an additional poling mechanism [1,2]. In order to resolve all three involved poling mechanisms within only one experiment we developed a structural analysis technique with *in situ* X-ray and neutron powder diffraction data [3]. The results not only separately reveal the contributions of each poling mechanism to the macroscopic strain, but also different behaviours of the individual phases. In several studies on lead containing as well as lead free systems we found significant changes while crossing the phase boundaries. Additionally, the calculation of the elastic strain perfectly matches the macroscopic observations, confirming the accuracy of the applied models. With specially designed pump-probe stroboscopic data acquisition routines we recently were able to investigate these effects on time scales down to the microsecond regime. In this contribution we present the latest research on the elucidation of strain mechanisms in piezoceramics of different solid solution systems with perovskite structure. [1] M. Hinterstein, M. Knapp, M. Hoelzel, W. Jo, A. Cervellino, H. Ehrenberg and H. Fuess, *J. Appl. Phys.* **43**, 1314 (2010). [2] M. Hinterstein, J. Rouquette, J. Haines, Ph. Papet, M. Knapp, J. Glaum and H. Fuess, *Phys. Rev. Lett.* **107**, 077602 (2011). [3] M. Hinterstein, M. Hoelzel, J. Rouquette, J. Haines, J. Glaum, H. Kungl, M. Hoffman, *Acta Mater.* in revision (2015).

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