## TUT 3: Tutorial: Functional (oxide) single crystals and epitaxial films - from growth to function

Time: Sunday 16:00-18:15

## Tutorial

TUT 3.1 Sun 16:00 H4 Influence of ferroelectric phase transitions on the melt growth of bulk oxide crystals — •MANFRED MÜHLBERG and MANFRED BURIANEK — Universität zu Köln, Institut für Kristallographie, Zülpicher Str. 49 b, 50674 Köln

Various applications in electronics, linear and nonlinear optics and other fields are connected with components taken from bulk single crystals. Also the determination of several fundamental physical properties like dielectric constants, piezo- or pyroelectric tensor components requires single crystalline samples. To meet these requirements one is primarily concerned with obtaining crystals of predetermined size with a high degree of structural perfection and a well-determined chemical composition.

In this introductory lecture, the most important growth methods from the melt and from high temperature solutions will be presented focusing on examples of selected ferroelectric perovskites and tetragonal tungsten bronzes. The chemical and thermophysical properties of the multi-component materials also represented by phase diagrams determine the synthesis steps and the details of the growth process.

A short overview of the defect types depending on the material properties and growth parameters will be given. Some options for reducing the defect content and improving the crystalline quality are reported for potassium lithium niobate and calcium barium niobate. Finally, a special attention is focused on the types and the influence of ferroelectric phase transitions being occuring between the growth temperature and the crystalline state at room temperature.

Tutorial TUT 3.2 Sun 16:45 H4 Electromechanical properties of crystals — •Eiken Haussühl Institut für Geowissenschaften / Abt. Kristallographie, Goethe Universität Frankfurt

The knowledge of physical properties of crystals as bulk materials is rather limited in comparison to the huge number of known crystal structures. In this introductory tutorial fundamental aspects of crystal physics will be presented. The lecture is intended to provide the basics for the understanding of the distinctiveness of crystalline compounds and to bring closer the phenomenological aspects under the influence of symmetry. It is also intended to highlight practical considerations for the measurement of selected tensorial properties. The main part will be focused on the mechanical properties of the bulk material like thermal expansion, elasticity and on electrical properties like piezoelectricity. Different effects arising from phase transition of selected organic and inorganic materials like oxides will be discussed.

Tutorial TUT 3.3 Sun 17:30 H4 Epitaxial ferroelectric oxide thin films, nanostructures, and superlattices — •DIETRICH HESSE, IONELA VREJOIU, and MARIN ALEXE — Max Planck Institute of Microstructure Physics, Halle, Germany

Epitaxial ferroelectric thin films, nanostructures and superlattices represent a particularly interesting part of functional materials. In this tutorial, fundamental terms of epitaxial growth will be presented, along with a detailed characterization of growth-structure-property relations of a number of examples of perovskite-type ferroelectric structures. E.g., it will be shown how remanent polarization and switchability of pulsed-laser deposited Pb(Zr,Ti)O<sub>3</sub> (PZT) epitaxial thin films depend on the defect content (threading dislocations, stacking faults), and how the properties of antiferroelectric/ferroelectric PbZrO<sub>3</sub>/PZT superlattices depend on the thickness of the individual layers via strain. The properties of epitaxial, ferroelectric (Bi,La)<sub>4</sub>Ti<sub>3</sub>O<sub>12</sub> nanostructures and Pt/PZT/Pt nanocapacitors of sub-100 nm size are shown to be determined by crystallographic orientation, crystal perfection, and size. The role of 2D defects will be highlighted, viz. ferroelectric 90 degree domain boundaries in epitaxial PZT films serving as nucleation centers for 180 degree switching, and the atomic structure of 180 degree boundaries influencing the switching process. Overall the interesting physical properties of epitaxial functional perovskite structures are discussed in terms of growth, crystal orientation, defect type, defect content, and strain.

## Location: H4