Universität Basel

Research Project

SINERGIA Impact of composition and nanometer scale DISorder in transparent Conductive Oxides: a new route to design materials with enhanced transport properties (DisCO)

Third-party funded project

Project title SINERGIA Impact of composition and nanometer scale DISorder in transparent Conductive Oxides: a new route to design materials with enhanced transport properties (DisCO)
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In the past 10 years we have experienced a revolution in optoelectronic devices, which are becoming more efficient, lighter, in some cases wearable or even fully transparent. This includes ubiquitous flat-panels displays, solar cells, x-ray detectors. This trend demands a rapid development of new Transparent Conductive Oxide (TCOs) materials (which are used as transparent electrode in most optoelectronic devices) with not only the basic requirements of transparency and conductivity, but also properties like homogeneity (e.g to avoid grain boundaries when used in transistors) and mechanical robustness or flexibility when used in bendable devices. The extensive application of TCOs also requires the use of earth-abundant materials for their production, and therefore the replacement of, for example the rather rare metal indium (In). With the ultimate goal of designing and discovering new TCO materials, this collaborative project aims at bridging the gap between material processing, material simulation and material characterization, to understand the factors affecting the charge transport in disordered or "amorphous" TCOs. This will make possible the design and synthesize of new earth-abundant TCO materials with superior electrical, optical and mechanical properties. Disordered TCO materials are of great interest because of their ease of fabrication, and because of the variety of composition and atomic structure achieved ranging from quasi-polycrystalline to fully amorphous. However, disordered TCO materials are complex systems and, their electronic properties cannot be fully understood from sole experimental methods or material simulations, slowing down the development of new materials. To address this problem, we combine three strongly complementary fields in material science research, one theoretical (structural and electronic properties modeling) and two experimental ones (thin-film growth and nano-scale microscopy). The goal is to unravel the missing link between measured and simulated microstructural and electronic properties, to understand the factors affecting electron transport in disordered TCOs. This will be done by local nano-scale characterization of microstructure using unique ex and in situ advanced electron microscopy techniques; material structure and electronic properties prediction using high-end modeling algorythms; and material synthesis using superior thin-film TCO fabrication facilities. The gathered knowledge will be exploited to propose novel TCO coating processes allowing the design of new earth-abundant TCO materials with optimized electrical and optical properties. Due to the complex structure of disordered materials, both experimental and numerical studies will be highly challenging, but the complementary nature of the techniques constitutes the originality and strength of this project.

Keywords in situ TEM, Transparent conductive oxide, Charge transport modelling, Macroelectronics
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