Contribution ID: **46** Type: **Invited**

Advanced functional oxides

Tuesday, 6 December 2011 09:00 (30 minutes)

Ionic and electronic transport in functional oxide materials is of great relevance for applications in the field of energy and data storage, e.g. solid oxide fuel cells (oxygen ion conductivity), oxygen permeation membranes (ambipolar diffusion of oxygen), or data storage materials (electronic and/or ionic conductivity). In this contribution our recent work on the influence of defect inter-actions, grain structure and space charge effects, and electronic structure will be discussed for highly non-stoichiometric crystalline and amorphous oxides.
The general phenomenon of a maximum in the oxygen ion conductivity against dopant fraction will be analyzed in terms of defect interactions [1] and using density functional theory and kinetic Monte Carlo simulations [2]. In nanocrystalline oxide ion conductors, space charge effects at grain boundaries and surfaces hinder oxygen ion transport [3]; on the other hand, the grain boundaries are conductive for protons, even at room temperature [4].
Highly non-stoichiometric and amorphous oxides exhibit fascinating electronic properties. Internal disproportionation reactions can induce an insulator-metal transition [5] and may have an immediate impact on applications such as electronic devices and permanent data storage. This novel mechanism and its implications will be discussed considering experimental and theoretical results for amorphous and highly non-stoichiometric gallium oxide.

1. M. Martin, J. Electroceram. 17 (2006) 765.
2. M. Nakayama, M. Martin, Phys. Chem. Chem. Phys. 11 (2009) 3241.
3. R.A. De Souza et al., Phys. Chem. Chem. Phys. 10 (2008) 2067.
4. S. Kim et al., Phys. Chem. Chem. Phys. 11 (2009) 3035.
5. L. Nagarajan et al., Nature Mater. 6 (2008) 391.

Primary author: Prof. MARTIN, Manfred (Institute of Physical Chemistry, RWTH Aachen University; WCU Hybrid Materials Program, Seoul National University)

Presenter: Prof. MARTIN, Manfred (Institute of Physical Chemistry, RWTH Aachen University; WCU Hybrid Materials Program, Seoul National University)

Session Classification: Solid State and Bio Physics I