

## DS 25: Focus Session: Resistive Switching by Redox and Phase Change Phenomena II (Valence and phase change in oxides)

Time: Wednesday 11:15–12:45

Location: CHE 89

**Invited Talk** DS 25.1 Wed 11:15 CHE 89

**Nanoscale redox-processes in resistive switching oxide devices** — ●REGINA DITTMANN — Peter Gruenberg Institut (PGI-7), Forschungszentrum Juelich GmbH, 5425 Juelich

Although there exists a general consensus that bipolar resistive switching in transition metal oxides is in most cases connected with a redox-process, the details of the underlying physical mechanism are only poorly understood up to now. One of the obstacles for its further elucidation is that the net changes of structure, stoichiometry and valence state during electroforming and switching are very small and occur primarily at the electrode interface or within nanoscale filaments. Besides electron microscopy and spectroscopy, different Synchrotron radiation based spectroscopy and scattering techniques have been employed so far in order to detect local redox-processes and/or filament formation caused by the electrical treatment of resistive switching oxide devices. This talk will give an overview over electrically-induced structural and stoichiometric changes detected in different types of oxide thin film devices and will discuss their implications on device scaling and stability.

DS 25.2 Wed 11:45 CHE 89

**First principles investigation of Sr-rich phases in SrTiO<sub>3</sub>** — ●IVETTA SLIPUKHINA, STEFAN BLÜGEL, and MARJANA LEŽAIĆ — Peter Grünberg Institut, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Perovskite-type oxides exhibit a whole variety of functionalities, among which resistive switching is one of the most interesting due to the potential use in non-volatile random access memory. In many of these materials the unintentionally formed secondary phases are known to be responsible for the observed resistive switching phenomena. Recently, Sr-rich secondary phases were observed during electroforming in SrTiO<sub>3</sub> thin films grown by pulsed laser deposition [A. Köhl, PhD thesis]. The structure and composition of these phases are unknown so far. By means of ab initio calculations, we have considered possible mechanisms for the formation of Sr-rich phases in SrTiO<sub>3</sub> and compared the calculated electronic structures with the existing experimental XPS and XAS data.

This work was supported by the SFB917-Nanoswitches.

DS 25.3 Wed 12:00 CHE 89

**Correlation of Local Conductivity and Imaging X-ray Photoelectron Spectroscopy in Resistively Switching SrTiO Thin Films** — ●CHRISTOPH BAEUMER<sup>1</sup>, ANNEMARIE KOEHL<sup>1</sup>, MARCO MOORS<sup>1</sup>, MARTEN PATT<sup>1</sup>, VITALIY FEYER<sup>1</sup>, CARSTEN WIEMANN<sup>1</sup>, CLAUD MICHAEL SCHNEIDER<sup>1</sup>, RAINER WASER<sup>1,2</sup>, and REGINA DITTMANN<sup>1</sup> — <sup>1</sup>Peter Grünberg Institut, Forschungszentrum Juelich GmbH, Germany — <sup>2</sup>Institut für Werkstoffe der Elektrotechnik (IWE-2), RWTH Aachen, Germany

Resistively switching oxides are investigated extensively as a possible route towards future non-volatile memory or as basis for the design of novel neuromorphic circuits. Despite the existing strong experimental evidence that resistive switching in transition metal oxides is caused by nanoscale redox reactions, many fundamental details are not yet understood. In particular, the electronic and chemical structure of the resistively switching regions after electroforming and after each switching event remains elusive.

Here we will present a direct correlation of localized chemical com-

position alterations in SrTiO<sub>3</sub> thin films with local conductivity measurements. Imaging X-ray photoelectron spectroscopy after *in-situ* top electrode delamination revealed sub-micrometer regions characterized by an altered cation stoichiometry and increased surface potential, which form after electrical treatments. UHV-LC-AFM measurements showed that these regions possess strongly increased electrical conductivity. This observation hints at a non-negligible contribution of cation diffusion in the formation of conducting channels.

DS 25.4 Wed 12:15 CHE 89

**Vacancy-vacancy interaction in SrTiO<sub>3</sub> bulk and surfaces** — ●ALI AL-ZUBI, GUSTAV BIHLMAYER, and STEFAN BLÜGEL — Peter Grünberg Institut (PGI) & Institute for Advanced Simulation (IAS), Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

We employ the density functional theory (DFT) to model point defects, in particular oxygen vacancies, in the perovskite SrTiO<sub>3</sub>. We use a bulk super-cell model to calculate the formation energy of single and double O-vacancies for different arrangements in the unit cell. Our results indicate a clear trend of the defects to form one-dimensional extended structures in the ground state.

We extend the study to surfaces and calculate the interaction energy of homogeneously distributed O-vacancies on SrO- and TiO<sub>2</sub>-terminated (001) surfaces. To compare to the bulk, we investigate clustering effects, in particular on the TiO<sub>2</sub>-terminated surface. For an analysis of the results, we study the role of structural relaxations and estimate the importance of electronic effects by comparison to DFT+*U* calculations that simulate correlation effects via a Hubbard-*U* parameter. Furthermore, interaction energies on the SrO-terminated surface are compared to results for O-vacancies in the SrO plane in the Ruddlesden-Popper phases, exhibiting the importance of screening effects in the bulk matrix.

We acknowledge the DFG, SFB 917 project A4, for financial support.

DS 25.5 Wed 12:30 CHE 89

**Resistive switching in SrTiO<sub>3</sub>:Nb single crystals related to phase transformations** — ●CHRISTIAN RODENBÜCHER, GUSTAV BIHLMAYER, RAINER WASER, and KRISTOF SZOT — Peter-Grünberg-Institut 1 + 7, Forschungszentrum Jülich, 52425 Jülich, Germany

The understanding of the nanoscale origin of resistive switching is of particular importance for the development of non-volatile memories. While investigations of the model material SrTiO<sub>3</sub> using LC-AFM revealed a filamentary type of switching, the switching type changes upon doping with the donor Nb to a cluster-like switching mechanism related to Nb segregation effects in Verneuil-grown single crystals. We show that the switching itself takes place in the surface layer that can change its properties under the influence of external gradients easily. In particular, we demonstrate that during electrodegradation, which can be used as an emulation of switching, fundamental chemical and crystallographic phase transformations from SrTiO<sub>3</sub> towards different substoichiometric TiO<sub>x</sub> phases take place in the surface layer under electrical gradients. Based on ab-initio calculations and analyses by various surface-sensitive methods such as XPS, LEED, EBSD and LC-AFM with atomic resolution, we present a potential nanoscale model of the cluster-like resistive switching assuming a phase transformation mechanism inside a nano-filament acting as a switch between the conducting clusters.