

MM 2: Topical Session TEM I

Time: Monday 11:00–13:00

Location: IFW A

Topical Talk

MM 2.1 Mon 11:00 IFW A
Study at picometres precision of structure and properties of oxide ferroelectrics — ●CHUN-LIN JIA — Institute of Solid State Research and Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons (ER-C) Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany

Epitaxial thin films of ferroelectric oxides have attracted increasingly intensive research both for fundamental and application issues. The physical properties of these film systems depend strongly on the particular microstructure and configuration of lattice defects.

By means of a spherical aberration corrector in a transmission electron microscope the value of the spherical aberration Cs can be tuned to negative values resulting in a novel imaging technique: The negative Cs imaging (NCSI) technique. The images obtained with the NCSI technique are superior to positive Cs images in the magnitude of the contrast and the image intensity of atom columns. The image signal obtained with the NCSI technique is significantly more robust against noise, resulting in measurement of atomic positions with a precision of a few picometres.

In this talk, we present the results of a study using NCSI technique of the epitaxial thin-film system of PbZr_{0.2}Ti_{0.8}O₃. The positions of all the atomic species are measured, unit cell by unit cell, with a precision of a few picometres. On this basis the relative ion displacements in the individual unit cells are calculated. These displacements depict the details of electric dipole moments in domains, at domain walls, as well as at defect area.

Topical Talk

MM 2.2 Mon 11:30 IFW A
In-situ TEM as a nanolab for studying electrical and electrochemical transport mechanisms in perovskites — ●CHRISTIAN JOOSS¹, JONAS NORPOTH¹, STEPHANIE RAABE¹, MALTE SCHERFF¹, JOERG HOFFMANN¹, JAMES CISTON², DONG SU², LIJUN WU², and YIMEI ZHU² — ¹Institute of Materials Physics, University of Goettingen, Germany — ²Brookhaven National Laboratory, Upton NY, USA

Perovskite oxide materials with strong electronic or electron-lattice correlations exhibit a rich variety of properties ranging from colossal resistance effects over remanent resistance switching to multi-electron transfer in catalytic reactions. Intrinsic inhomogeneities such as electronic phase separation on the nanoscale and extreme sensitivity to defect structure make atomic resolution studies of properties and behavior in external fields highly desirable, in order to understand underlying mechanisms. In this talk, we will show through two examples, the opportunities of in-situ TEM for a detailed understanding of electrical transport properties in doped manganites. In one example, a piezo-controlled STM tip (Nanofactory) has been used to electrically stimulate a hole-doped manganites and metal-manganites heterostructures. The induced resistance change was correlated to the locally induced structural and electronic changes. In the second example, in-situ studies of water splitting using CaMnO₃ based catalysts have been performed in a FEI Titan microscope with an environmental chamber. Catalytic activity was observed at specific crystalline sites and related changes in the oxidation state of the Mn cations during the reaction were recorded via Electron Energy Loss Spectroscopy.

MM 2.3 Mon 12:00 IFW A
Direct evidence for cation non-stoichiometry and Cottrell atmospheres around dislocation cores in functional perovskite oxide interfaces — ●MIRYAM ARREDONDO¹, QUENTIN RAMASSE², MATTHEW WEYLAND³, IONELA VREJOU¹, DIETRICH HESSE¹, NIGEL BROWNING⁵, and VALANOOR NAGARAJAN⁴ — ¹MPI of Microstructure Physics, Halle, Germany — ²LBNL NCEM, Berkeley, CA, USA. — ³MCEM, Monash Uni., Victoria, Australia — ⁴SMSE, UNSW, Australia — ⁵Chem. Eng. & Mater. Sci., UC Davis, USA.

Exploiting the electronic properties of oxides in functional devices requires their deposition on an underlying substrate, often with an unavoidable lattice mismatch. We consider the chemical implications in the accommodation of this mismatch by misfit dislocations, by the characterization of the lattice mismatched system: a PbZr_{0.52}Ti_{0.48}O₃ ferroelectric film deposited on a SrRuO₃ electrode-buffered SrTiO₃ substrate. Cs-corrected Z-contrast imaging and chemical analysis techniques are exploited to yield evidence for cation excess within dislocation cores at the interface. Multislice image simulations

reproduces fairly well the observed image contrast. EDX maps reveal Pb and Sr interdiffusion and EELS scans at the core reveal that it is oxygen-deficient compared to the defect-free lattice. Geometric phase and theoretical elastic modeling reveal that the local strain around the dislocation core is sufficient to create stress-assisted diffusion of cations. This study provides insights into the link between the local chemistry, physical structure and observed functional behavior in the ferroelectric at the proximity of a dislocation core.

MM 2.4 Mon 12:15 IFW A
Scandate/Titanate Interfaces: Structure and Composition on the Atomic Scale — ●MARTINA LUYBERG¹, JÜRGEN SCHUBERT², KOUROSH RAHMANIZADEH³, GUSTAV BIHLMAYER³, LENA FITTING KOURKOUTIS⁴, and DAVID A MULLER⁴ — ¹Institute of Solid State Research IFF-8 and Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons, Research Centre Jülich, D-52425 Jülich, Germany — ²Institute of Bio- and Nanosystems and JARA-FIT, Research Centre Jülich, D-52425 Jülich, Germany — ³Institute of Solid State Research IFF-1, Research Centre Jülich, D-52425 Jülich, Germany — ⁴Applied and Engineering Physics, Cornell University, Ithaca, NY 14853, USA

When scandates and titanates are joint at an interface, a polar discontinuity occurs. Unlike the polar interface between LaAlO₃ and SrTiO₃, where a conducting interface has been discovered, the scandate-titanate heterojunctions remain electrical insulating. Recently we reported on an intermixing of the cations across the interface of DyScO₃ and SrTiO₃. This intermixing of ions of different valency counteracts the interface dipoles arising from the polar discontinuity, making the interface insulating. In the paper presented here we focus on an additional property of the interface: an ordered interface structure. High resolution electron microscopy and electron energy loss spectroscopy on individual atomic columns will be shown, which reveal an ordering on the Sr/RE (RE=Gd or Dy) sublattice. These results will be discussed in conjunction with ab-initio calculations.

MM 2.5 Mon 12:30 IFW A
Electron beam induced surface diffusion on metallic nanoparticles — ●ALEXANDER SURREY¹, DARIUS POHL¹, ULRICH WIESENHÜTTER², LUDWIG SCHULTZ¹, and BERND RELLINGHAUS¹ — ¹IFW Dresden, Helmholtzstr. 20, D-011156 Dresden, Germany — ²FZ Dresden, Postfach 510119, D-01314 Dresden, Germany.

The predominant mass transport mechanism during the coalescence of adjacent metallic nanoparticles is assumed to be surface diffusion. Upon exposure to an electron beam in a transmission electron microscope (TEM) the diffusion of surface atoms towards the sintering neck is stimulated thereby reducing the particles's surface free energy. This electron beam induced inter-particle coalescence is investigated in FePt and Au nanoparticles with icosahedral or truncated octahedral structure by means of aberration-corrected TEM. The particles are prepared by inert gas condensation which provides for free and uncovered surfaces. Aberration-corrected TEM is employed to monitor and analyze quantitatively temporal changes of the surface atom configurations on particle facets oriented parallel to the electron beam. It is observed that the path of the surface atoms towards the sintering neck is chosen to always optimize the local coordination. The influence of the electron energy (which can be chosen by adjusting the acceleration voltage) on the beam-induced surface diffusion is discussed.

MM 2.6 Mon 12:45 IFW A
Soot formation in a diesel engine — ●MIRZA MAČKOVIĆ^{1,2}, SEBASTIAN PFLAUM³, GERHARD FRANK², ERDMANN SPIECKER¹, GEORG WACHTMEISTER³, and MATHIAS GÖKEN^{1,4} — ¹Center for Nanoanalysis and Electron Microscopy (CENEM), Cauerstraße 6, 91058 Erlangen, Germany — ²Institute of Biomaterials, Cauerstraße 6, 91058 Erlangen, Germany — ³Institute of Combustion Engines, Schragenhofstraße 31, 80992 Munich, Germany — ⁴Department of Materials Science and Engineering, General Materials Properties, Martensstraße 5, 91058 Erlangen, Germany

Diesel engine soot is known as one of the main environmental pollutants and has become an important environmental and scientific topic. Diesel soot is a product of pyrolysis or incomplete combustion of hydrocarbons. Especially, the formation mechanism of soot particles is one of the central themes of research activities in the area of combustion

and pyrolysis of fossil fuels. It is known that soot particles from the exhaust of diesel engines appear as chain-like agglomerates and consist of several tens to hundreds of primary soot particles. In this study soot particles are collected from nearly the centre of the combustion chamber of a diesel engine, using a newly developed technique, and analyzed by means of transmission electron microscopy and electron

energy loss spectroscopy. Thus the development of the soot nanostructure could be shown as a function of crank angle and time after the combustion of the diesel fuel begins. The early formation, growth and oxidation of the soot particles are observed and some aspects regarding the complex process of soot formation are proposed.