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Electric Field Induced Structure and Resistance Modifications in Metal/$SrTiO_3$ Junctions. Hartmut Stöcker[a,b], Jörg Schulze[b], Juliane Seibt[a], Florian Hanzig[a], Matthias Zschornak[a,b], Susi Wintz[a], Barbara Abendroth[a], Jens Kortus[c], Dirk C. Meyer[a], [a]*TU Bergakademie Freiberg, Institut für Experimentelle Physik, Leipziger Straße 23, 09596 Freiberg, Germany* [b]*TU Dresden, Institut für Strukturphysik, Zellescher Weg 16, 01069 Dresden, Germany,* [c]*TU Bergakademie Freiberg, Institut für Theoretische Physik, Leipziger Straße 23, 09596 Freiberg, Germany*
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In oxides with perovskite-type of structure, oxygen can be a sufficiently mobile defect even at room temperature when an electric field of sufficient strength (~1000 V/mm) is applied. Our in-situ investigations of metal/$SrTiO_3$ junctions revealed reversible structural changes and the formation of non-stoichiometric regions during the application of external electric fields. This might be caused by a field-induced redistribution of oxygen vacancies. The investigations were carried out using wide-angle X-ray scattering, X-ray absorption spectroscopy, nanoindentation and time-dependent electric measurements.
Motivated by the successful use of $SrTiO_3$ with different doping metals for memory cells on the basis of resistive switching in combination with the findings on the major importance of oxygen vacancy redistribution, we want to show the possibility of realizing a resistance change memory based on vacancy-doped $SrTiO_3$. The formation of corresponding metal/$SrTiO_3$ junctions in an electric field will be discussed as well as the switching between ohmic and Schottky-type resistive properties. A notable hysteresis in the current-voltage characteristics can be used to carry out Write, Read and Erase operations to test the memory cell properties of such junctions. But whereas the electric field-induced formation of Schottky-type junctions may be explained by oxygen vacancy redistribution, the resistive switching is preferably discussed in terms of vacancies serving as electron trap states at the metal/oxide interface.

Keywords: structure-properties relationships, electrical properties of solids, perovskite oxides

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An AFM-study of the surface topography of anatase single crystals. Andreas Bürger[a], Uta Magdans[a], Hermann Gies[a], [a]*Department of Geology, Mineralogy and Geophysics, Ruhr-University of Bochum, Germany*
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Grazing Incidence X-ray diffraction (GIXRD) is a surface X-ray diffraction method for the analysis of mineral surfaces and interfaces on atomic scale [1,2]. This method requires very flat and large single crystal surfaces with a rms-roughness well below 10 nm. Therefore crystal surfaces used in GIXRD-experiments are analyzed for surface topography and roughness. Atomic force microscopy (AFM) provides a simple, inexpensive and fast technique to investigate the macroscopic surface structure and measure the surface roughness. TiO_2 is the most widely used photocatalytic material for heterogeneous photocatalytic oxidation (PCO) processes [3]. Photocatalytic thin films consist of a mixture of rutile and anatase nanocrystals, where the anatase surfaces are the most active part in the PCO process [4]. The structure and properties of the most abundant (101) and (001) anatase crystal faces are studied with a wide range of experimental and simulation techniques, however, to the best of our knowledge, exclusively in vacuum conditions. GIXRD experiments on anatase surfaces in environmental conditions will provide information about the surface and interface structure of natural anatase crystals, allowing to analyse the surface properties in more "real" conditions compared to UHV experiments. In preparation of these GIXRD experiments here the (101) and (001) surfaces of anatase single crystals from Hardangervidda, Norway, were characterized with atomic force microscopy (AFM). Four bipyramidally shaped crystals with (101) and (101) surfaces about 3 x 5 mm in size were scanned, whereas not all surfaces could be used, because of scratches or impurities. The surface topography consist mostly of wide terraces, with overall widths > 50 µm, sometimes spotted with small impurities. The roughness criteria for GIXRD experiments was met only by three out of the 22 faces analysed. The surface roughness of the samples is very high, with rms-roughnesses between 4 - 69 nm for the (101) faces and 14 – 59 nm for the (001) faces, respectively. The roughness could not be decreased by repeated tempering of the crystals at different temperatures between 300 – 700 °C during 1 and 7 days, alternately. The AFM analysis showed that no (001) face is suitable for GIXRD and only one (101) face of the antase crystals met the roughness criteria required for surface diffraction. This demonstrates that one of the major difficulties in performing surface X-ray diffraction experiments, especially with the GIXRD method, is finding suitable single crystal specimens.

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Keywords: atomic force microscopy, surface roughness, surface X-ray scattering

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Neutron radiography study of the dehydration kinetics of smectites in moulding sands. Guntram Jordan, Constanze Eulenkamp, Wolfgang W. Schmahl
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Natural bentonites are an important material in the casting industry. The bentonites plasticize and stabilize quartz sand moulds for cast metals. Depending on the time-temperature history during casting, the initially moist smectites become partially or completely dehydrated. Although rehydration of the smectites should be a reversible process per se, the industrially dehydrated smectites lose their capability to reabsorb water. This limits the number of possible process cycles of the mould material. An open question in the casting process is the detailed behavior of the pore water within the moulding sand as well as the interlayer-water within the

smectites as a function of time, location and temperature. As the reusability of the moulding sand is critically related to the hydration and dehydration of smectite, we designed experiments to investigate of the dehydration kinetics in-situ. At the neutron radiography beamline ANTARES (FRM II, Germany) we simulated a casting process by dropping a special casting mould filled with moulding sand (12 wt% bentonite) on a hot copper plate (Figure 1). The design ensured an ideal heat transfer corresponding to the thermal shock-like heat induction during the real casting process. With this experimental set up, we were successful to in-situ visualize water fluxes within the moulding sand quantitatively with high temporal and spatial resolution. Thermocouples placed within the moulding sand simultaneously provided information on the temporal temperature gradients.
The experiments revealed a progressive movement of water in the sand and resolved a broad transitional zone from the pristine hydration state of the sand to a fully dehydrated state. At this transitional zone positions can be determined which on the one hand relate to the onset of pore water dehydration and on the other hand relate to the completion of interlayer dehydration. Thus, the experiments allowed us to successfully simulate the shock-heating of the mould material in a industrial casting process. The consequence of the shock-heating is a strongly non-linear temperature-time-position relation convoluted with the diffusion processes. A quantitative evaluation of the simulation data will be presented.

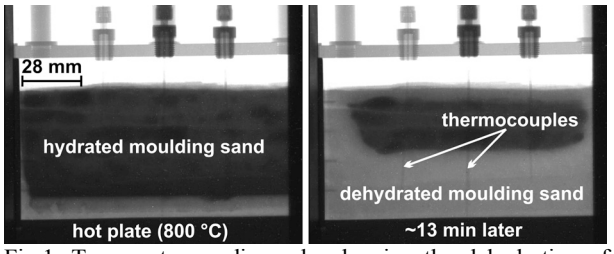

Fig.1. Two neutron radiographs showing the dehydration of the moulding sand. The process initiates at the hot bottom. The transitional zone between the pristine hydration state (top) and the fully dehydrated state (bottom) can be seen.

Keywords: smectites, interface processes, neutron radiography

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Surface and embedded 2-dim structures: a direct space approach to modelling.

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In the parameter space concept developed for the determination of 1-dimensional structures or structure projections without Fourier inversion, an arrangement of m equal scatterers is represented by a vector $\mathbf{t}(x_1, x_2, \ldots x_m)$ defined in space $\mathbf{P}^m$ [1,2]. Given a suitable number $n \geq m$ of observed intensities of reflections h, the principal objective of this approach is to find those test vectors $\mathbf{t}_t$ for which the best overall agreements between the observed $e(h)_{obs}$ and the model $e(h)_{calc}$ are obtained. The $e(h)$ are normalized structure amplitudes on absolute scale according to $e(h)^2 = n \cdot I(h)/\Sigma I(k)$, $k = 1,\ldots n$ [3], and the $\mathbf{t}_t$ proposed are fit to start a refinement procedure. Thus, it should be noted that (i) neither structure metrics nor any structure factor phases are needed, (ii) high spatial resolution is obtained from rather few experimental data, and (iii) homometric and quasi-homometric structures are automatically included. - The 1-dimensional approach was successfully tested in numerous examples with equal or nearly equal scatterers up to $m = 20$. In addition, we have shown that it is possible to reconstruct a 3-dimensional structure from the solutions obtained from up to 13 structure projections reflected in the central reciprocal lattice rows with low indices, *e.g.* $h00$, $0k0$, $00l$, $hh0$,…hhh *etc* [3]. - Encouraged by our experiences with the 1-dimensional structures we have started to apply the approach to simple acentric 2-dimensional structures or structure projections of symmetry ***p*1** with emphasis on exploring (a) the number(s) of scatterers m that can be handled in feasible PC computing times and (b) the numbers and kinds of reflections needed for finding test vectors $\mathbf{t}_t(x_1,y_1; \ldots x_m,y_m)$. - In ***p*1**, one scatterer (preferably the strongest) in (0,0) fixes the origin so that the problem is reduced to (m-1). In principle, there are two ways to generate $\mathbf{t}_t$'s, namely the systematic one by employing grid techniques (with the problem of finding the optimal spacing) and a random one (which is not necessarily inferior). Confining the discussion to the first technique we consider four basic strategies, *i.e.* the (i) exclusive use of a 2-dimensional grid and of general reflections hk, (ii) use of 1-dimensional x- or y-projection results based on reflections $h0$ or $0k$, respectively, with subsequent inspection of the corresponding rods at the proposed x_i or y_i to find the missing information from hk reflections, (iii) use of x- and y-projection results from $h0$ and $0k$ reflections, respectively, followed by finding correct (x,y) combinations from hk reflections, and finally, (iv) as (iii) but finding the correct (x,y) combinations with the aid of results obtained from reflections hh and $-h,h$, *i.e.* additional projections onto the directions [11] and [-1,1]. - Advantages and shortcomings of the different approaches with respect to structure sizes and computing times are compared, and including data errors examples of structure determinations are presented. Also addressed are possible extensions and applications, for instance in electron diffraction.

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Keywords: two-dimensional structures, phase problem eliminated, high resolution

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Dopant Effect on Surface Electronic State of TiO_2 estimated by First Principles Calculation.

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The surface electronic states of TiO_2 doped with various metallic elements on Ti site were estimated by the discrete variation X_α (DV-X_α) method, which is a sort of the first-principles molecular orbital method and uses the Hatre-Fock-Slater approximation.[1] The energy levels, the partial density of state and the charge densities were calculated by using cluster models for bulk and surface.