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Strontium titanate ($SrTiO_3$) is an oxide crystallizing with cubic perovskite-type of structure that exhibits a high tunability of dielectric, electric, mechanical and optical properties by means of defects. Apart from dopants, also intrinsic oxygen vacancies or ordered stacking faults, e.g. Ruddlesden-Popper (RP) phases $SrO(SrTiO_3)_n$, may influence these properties.
We have investigated the structural stability, electronic properties and surface energies of such RP phases up to n = 5 by means of density-functional theory. We find a significant gain of formation energy up to n = 3 and can approximate the interaction range of neighbouring stacking faults to 11.7 Å. From band structure and density of states calculations we see a quasi continuous evolution of the band gap in an interval of about 0.4 eV beginning at RP n = 1 and approaching the $SrTiO_3$ bulk value for higher ordered members which suggests tunability by selection of an appropriate RP phase. Surface calculations will be presented for <001> and <100> directions with all possible perfect crystal terminations and several more complex structures.
Further, we have theoretically verified a reversible elastic softening along an O-deficient <001> direction recently found in nano-indentation of $SrTiO_3$ under influence of an electric field. The results of an isotropic as well as an anisotropic modelling of oxygen vacancy distributions in a 2x2x2 $SrTiO_{3-\delta}$ super cell will be presented.

Keywords: DFT; defects in oxides; surface structure and relaxation

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The Benefit of Nanoindentation for the Evaluation of Near-Surface Properties. Peter Paufler[a], Irina P. Shakhverdova[a], Dirk C. Meyer[a]. [a]*FR Physik, TU Dresden, D-01062 Dresden, Germany.*
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Nanoindentation tests are probing elastic and plastic properties by applying normal loads F<10mN and penetration depths $h \leq 0.2$ µm depending on the material investigated. Most impor- tantly, the whole dependence $F(h)$ is recorded throughout the loading - deloading cycle. The major mechanical entities ob- tained are the (reduced) Young's modulus E_r and the nano-hardness H. The former $E_r = (dF/dh) /c\ Amax$ is derived from the slope of the initial portion of the unloading curve $F(h)$ and the projected area of contact A_{max} at maximum load, where c is of the order of 1 and depends on the shape of the indenter [1]. For the latter $H = F(h_{max})/A_{max}$ holds at the maximum penetration depth h_{max}. There are several benefits of the small volume activated mechanically: (1)The properties of thin films may be characterised separately. (2)Both lateral and in-depth resolution down to some nanometers enables composition gradients to be assessed. (3) E_r and H may be obtained directly from $F(h)$. When using the nanoindenter in conjunction with an atomic force microscope, the nanoindent may be imaged *in-situ*. (4)Thanks to the relationship $Y = H/3$ the yield stress Y of nanolayers or near-surface regions may be obtained, which is otherwise difficult to assess.(5) High pressures underneath the indenter enable phase transitions to be studied. (6) Confinement of the small indented volume by the surrounding material prevents the sample from global fracture. (7) Fracture toughness of thin films and near surface regions may be calculated from cracks. (8) Because the diameter of indents is generally smaller than the average spacing of dislocations in crystals, elementary mechanisms leading to permanent deformation of defect-free regions might be identified. In particular, the generation of mobile dislocations at the beginning of the deformation process may be revealed directly. - The following materials have been studied and above- mentioned parameters determined: crystalline S_rTiO_3 [2] and Li_3O_5 [3]; nanoporous borosilicate glass [4]; quasicrystalline i-YMgZn, i-AlPdMn and d-AlCoNi [5]; ultra-high carbon steel [6]; metallic glass Cu-Ti-Zr-Ni-Si-Sn [7], and VC/TiC multilayers on Si or Al_2O_3.

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Keywords: hardness; elastic properties; surface characterization

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Texture Measurements on Thin Films Using an X-ray Microfocus Source. Bernd Hasse[a], Jürgen Graf[a], Carsten Michaelsen[a]. [a]*Incoatec GmbH, Max-Planck-Straße 2, 21502 Geesthacht, Germany.*
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We will present texture measurements of components of high-temperature superconducting coated conductors. We used a state-of-the-art diffractometer which was equipped with a 2-dim detector and the new Incoatec Microfocus X-ray Source IµS. The IµS is a 30 W air-cooled sealed X-ray tube. It has all advantages of a sealed tube, it is maintenance free and it needs no cooling water. In the IµS the beam was collimated with the special multilayer optics for a two dimensional beam-shaping, the so-called Quazar Optics. The source was integrated in a Bruker D8 GADDS system with VÅNTEC-2000 detector. This setup for two dimensional diffractometry is especially useful for the investigation of powders as well as for materials characterization like thin films.
With our new equipment we analyzed the texture of metallic substrates produced by the RABiTS technology (rolling