Materials Research, FZ Dresden-Rossendorf, 01328 Dresden, Germany. [b]Institute of Structural Physics, TU-Dresden, 01062 Dresden, Germany.
E-mail: m.zschornak@fzd.de

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

FA2-MS06-P07

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.*
E-mail: paufler@physik.tu-dresden.de

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

FA2-MS06-P08

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.*
E-mail: hasse@incoatec.de

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

assisted biaxially textured substrates) [1], epitaxially grown ceramic buffer layers and also textured ceramic buffer layers like YSZ (yttria stabilized zirconia), which were deposited with the so-called IBAD technology (ion-beam assisted deposition) [2]. Our measurements will be compared to the results using conventional sealed-tube setups.

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Keywords: texture studies; two-dimensional diffraction; thin films

FA2-MS06-P09

Effect of Sn Dopant on the Crystalline Structure of Sol-Gel Coated ZnO Film. Yasemin Caglar[a], Mujdat Caglar[a], Saliha Ilican[a]. [a]*Anadolu University, Department of Physics, Eskisehir, Turkey.*
E-mail: yasemincaglar@anadolu.edu.tr

Undoped and Tin doped zinc oxide (ZnO and ZnO:Sn5%) films have been prepared by sol-gel process using spin coating method. Zinc acetate dehydrate was used as starting materials. 2-methoxyethanol and monoethanolamine were used as a solvent and stabilizer, respectively. The dopant source is tin cloride. The coating solution was dropped into glass substrate, which was rotated at 3000 rpm for 30 s using a spin coater. After the spin coating, the film was dried at 300 oC for 10 min in a furnace to evaporate the solvent and to remove organic residuals. This coating/drying procedure was repeated for ten times before the film was inserted into a tube furnace and annealed at 450 oC in air for 1 h. The crystal structure and orientation of the films have been investigated by X-ray diffraction method. The films have the polycrystalline structure and (002) as the preferred orientation. The information on strain and crystallite size was obtained from the fullwidths-at-half-maximum (FWHM) of the diffraction peaks. The texture coefficient and lattice parameters of the films were also calculated. The deformation in crystalline structure of the ZnO film was observed due to Sn incorporation.

Keywords: metal oxides; sol-gel method; X-ray diffraction and structure

FA2-MS06-P10

XRD Study of Indium Oxide Film Deposited by Sol-Gel Spin Coating. Mujdat Caglar[a], Saliha Ilican[a], Yasemin Caglar[a], Fahrettin Yakuphanoglu[b]. [a]*Anadolu University, Department of Physics, Eskisehir, Turkey.* [b]*Firat University, Department of Physics, Elazig, Turkey.*
E-mail: mcaglar@anadolu.edu.tr

Transparent-conducting oxide (TCO) film coatings are important in a number of optoelectronics devices including photovoltaic cells. In this study, Indium oxide film has been prepared by sol-gel process using spin coating method. Indium III chloride, 2-methoxyethanol and monoethanolamine were used as a starting materials, solvent and stabilizer, respectively. A liquid film on glass substrate was formed in a spinning-coater at a spinning speed 2000 rpm for 30s. After the spin coating, the film was dried at 120 °C for 10 min in a furnace to evaporate the solvent and to remove organic residuals. This coating/drying procedure was repeated for ten times before the film was inserted into a tube furnace and annealed at 300 °C in air for 45 min. The heat treatment temperature was selected 400 °C and 500 °C (in air for 1 h). The crystal structure and orientation of the films have been investigated by X-ray diffraction method. Indium oxide film has polycrystalline structure. Some structural parameters such as texture coefficient, lattice parameters, grain size of the film were calculated. Surface morphology of the film has been also analyzed by a scanning electron microscope (SEM). The enhanced in crystalline structure of the Indium oxide film was observed due to heat treatment.

Keywords: metal oxides; sol-gel method; X-ray diffraction and structure

FA2-MS06-P11

Effects of Plastic Deformation and Inhomogeneous Thermal Fields During Grinding and Milling on the Real Structure of Steels. Zdenek Pala[a], Nikolaj Ganev[a], Jan Drahokoupil[a,b]. [a]*Department of Solid State Engineering, Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague, Prague, Czech Republic.* [b]*Department of Metals, Institute of Physics,Academy of Sciences of the Czech Republic, Prague, Czech Republic.*
E-mail: zdenek.pala@fjfi.cvut.cz

Mechanical surface treatments like grinding and milling are often used as the last machining operations and have, therefore, pronounced impact on the resulting real structure of surface layers. Since the surface itself forms an interface between the bulk and its neighborhood, knowledge of its real structure represents information which is paramount for understanding various surface-related processes as well as for surface quality assessment. An effective source offering diverse array of real structure parameters can be found in analysis of data from suitably designed diffraction experiments. Both milling and grinding are accompanied by plastic deformation and thermal fields which are inherently inhomogeneous due to the anisotropy of directional movements of the used tool. In general, two dominant physical processes are under way. Firstly, energy of plastic deformation and friction between the tool and the machined object generate heat whose presence causes creation of inhomogeneous thermal fields. These fields dynamically evolve as the whole system strives to get into thermal equilibrium and as the tool goes back and forth. Secondly, the surface layers of machined object are being removed and plastic deformation is, thus, inherently inhomogeneous. Moreover, external forces and moments are present and as soon as they cease to be in action, the object proceeds to the state of mechanical equilibrium [1] while the unloading can be