polycrystalline fcc, bcc and hcp metals and alloys. Plastic flow regularities are found to occur from yield limit to failure as macro-localization patterns.

It is found that active localized plasticity nuclei would emerge and evolve on the macro-scale level over the entire flow process. These nuclei can be regarded as meso-scale defects responsible for plastic flow development on the macro-scale level. Their salient feature is that the spatial distributions of elongation, shear and rotation increments within a nucleus are interrelated. Each active localization nucleus corresponds with a set of shears or deformation twins over the glide plane of the acting glide or twinning system, which have maximal Schmidt factor values. A space-time localization pattern results from dislocation self-organization; this has wave features, i.e. length $5 < \lambda < 10$ mm and rate $10^{-5} \le V \le 10^{-4}$ m/s. A two-component model of plastic flow self-organization is proposed, which is based on the interaction of the crystal's phonon and dislocation sub-systems. This reconciles commonly known dislocation mechanisms acting at the various deformation hardening stages in single crystals and accounts for the above regularities of wave generation. The basic assumptions of the model are as follows. Relaxation-type plasticity involves dislocation acts that generate acoustic emission pulses causing elastic energy re-distribution among the stress concentrators (dislocations). As a result, the stresses at the concentrators grow to initiate their relaxation by dislocation shears. The sequence of events is repeated. For relaxation events to be activated, stress concentrators of the same type and size must be initiated, which is provided by acoustic pulses of strictly specified shape and spectrum, their amplitude being less significant. The concepts of defect self-organization and of energy re-distribution among stress concentrators involved successively in relaxation acts, might help account for the low values of localization wave rate and for the large-scale correlations of localization domains occurring in a deforming system that only contains micro-scale defects (dislocations). Thus, use of the above model allows one to explain the most important features of plastic deformation localization and transition to necking and failure in solids.

[1] Zuev L.B., Ann. Phys. 2007, 16, 286.

Keywords: plasticity; wavelength; localisation

FA3-MS04-P06

Reversible Structural Changes by Electrostatic Fields in Strontium Titanate at Room Temperature. Hartmut Stöcker^a, Tilmann Leisegang^a, Matthias Zschornak^{a,b}, Alexandr A. Levin^a, Emanuel Gutmann^a, Torsten Weißbach^a, Sibylle Gemming^b, Dirk C. Meyer^a. ^aInstitut für Strukturphysik, Technische Universität Dresden, 01062 Dresden, Germany. ^bInstitut für Ionenstrahlphysik und Materialforschung, FZ Dresden-Rossendorf, 01314 Dresden, Germany. E-mail: stoecker@physik.tu-dresden.de

While strontium titanate (SrTiO₃) is mainly used as substrate material, its high dielectric permittivity makes it an interesting material for electronic and other applications. Its

properties strongly depend on the defects in its perovskitetype of structure, even at room temperature. Mobile oxygen can cause the formation of non-stoichiometric regions when an electric field of sufficient strength (~1000 V/mm) is applied. Our *in-situ* investigations revealed reversible structural changes at room temperature caused by a systematic field-induced redistribution of oxygen.

The structural changes are highlighted by means of wideangle X-ray scattering, X-ray absorption spectroscopy, nanoindentation and time-resolved measurements of the electric current. We found a reversible conversion of the perovskite structure to a long-range ordered variant with changed lattice parameter. The temporal change of the structure of SrTiO₂ at near-surface regions (depth in the order of 10 µm) can be described by a model assuming solid-state electrolysis at room temperature driven by the electric field applied. Local changes of the refraction index caused by stress birefringence were discovered by optical polarization microscopy. These local stress fields may be attributed to dislocation cores acting as paths for the oxygen transport to the anode. From spectroscopic measurements showing a change of titanium valence in near-surface regions, we can prove the oxygen diffusion model. Effects on the mechanical properties, i. e. hardness and elasticity were measured and compared to ab-initio simulations.

Our results reveal the possibility of structurally modifying the technologically relevant perovskite oxides using electrostatic fields. The tunable lattice spacings observed might be used in the field of adaptive X-ray optics. Also, substrates with tunable dielectric properties at constant basal lattice parameters could be realized.

Keywords: crystals in electric fields; solid-state structural changes; structure-properties relationships

FA3-MS04-P07

Temperature-dependent X-ray Diffraction Studies of Mullite-type $(Bi_{1,x}Sr_{x})_2M_4O_9$ Phases. Reinhard X. Fischer^a, Hartmut Schneider^a, <u>Thorsten M. Gesing</u>^{a,b}. *^aFB05 Kristallographie*, Universität Bremen, Klagenfurter Straße, 28359 Bremen (Germany). ^bInstitut für Mineralogie, Universität Hannover, Callinstraße 3, 30167 Hannover (Germany). E-mail: gesing@uni-bremen.de

The temperature-dependent behavior of $Bi_2M_4O_9$ compounds, known to have potential as electrolytes in solid oxide fuel cells (SOFC) [1], was investigated by X-ray powder diffraction methods using a Paar HTK1200N heating chamber. Data were recorded at 298 K and between 323 K and 1273 K in steps of 50 K in heating and cooling cycles. Three compositions were used for these investigations: $Bi_2Fe_4O_9$, $Bi_2Al_4O_9$ and $(Bi_{0.8}Sr_{0.2})_2Al_4O_9$ were synthesized using the glycerin method as described in [2] and finely ground in acetone.

For Bi₂Al₄O₉, a similar heating and cooling behavior of the metric parameters was observed showing thermal expansions of $5.5 \cdot 10^{-6}$, $9.4 \cdot 10^{-6}$, $7.8 \cdot 10^{-6}$ and $2.3 \cdot 10^{-5}$ for the lattice parameters *a*, *b*, *c*, and for the unit cell volume *V*, respectively. No phase transitions or unexpected structural changes are observed. From TG/DTA measurements the phase stability up to 1429 K can be derived. For the

^{25&}lt;sup>th</sup> European Crystallographic Meeting, ECM 25, İstanbul, 2009 *Acta Cryst.* (2009). A**65**, s 232