Poster Presentation

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Defect separation in strontium titanate: Formation of a polar phase

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Stoichiometric perovskite-type strontium titanate acts as an insulator because of its wide electronic band gap and has therefore great potential as high-k dielectric and storage material in memory applications. Degradation phenomena of insulating properties of transition metal oxides occur during long time voltage application. From the defect chemistry point of view the question arises how mobile species react on an external electric field and which impact the redistribution has on the stability of the crystal structure. Here, we discuss near-surface reversible structural changes in SrTiO3 single crystals caused by oxygen vacancy redistribution in an external electric field. We present in-situ X-ray diffraction during and after electroformation. Several reflections are monitored and show a tetragonal elongation of the cubic unit cell. Raman investigations were carried out to verify that the expansion involves a transition from the centrosymmetric to a less symmetric structure. Regarding a whole formation cycle, two different time scales occur: a slow one during the increase of the lattice constant and a fast one after switching off the electric field. Based on the experimental data we suggest a model containing the formation of a polar SrTiO3 unit cell stabilized by the electric field, which is referred to as migration-induced field-stabilized polar phase [1] at room temperature. As expected by a non-centrosymmetric crystal structure, pyroelectric properties will be presented in conjunction with temperature modulated electroformation cycles. Furthermore, we show that intrinsic defect separation establishes a non-equilibrium accompanied by an electromotive force. A comprehensive thermodynamic deduction in terms of theoretical energy and entropy calculations indicates an exergonic electrochemical reaction after the electric field is switched off. Based on that driving force the experimental and theoretical proof of concept of a solid-state SrTiO3 battery is reported.

[1] *J. Hanzig et al, Physical Review B, 88, 024104 (2013)*

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