Large interface conductivity as a consequence of the regular network of misfit dislocations in $BaZr_{0.8}Y_{0.2}O_{3-x}/NdGaO_3$ heteroepitaxial structure

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The last decade has witnessed an exponential growth of research on oxide films and heterostructures field, mainly driven by unique properties, such as the presence of high-mobility electron gas, superconductivity, metal-insulator transition, enhanced ionic conductivity, etc., arising at the interfaces between different oxides [1]. This incredible variety of functional properties results from one or, in the most cases, from the combination of different interface mechanisms like epitaxial strain, strain relaxation, polar discontinuity, space-charge regions etc. [2]. In recent years, progress has been achieved in exploring and making use of the fundamental properties of such interfaces, and it has become clear that these electron systems offer the potential for possible future devices concerning ionics and electronics.
Among the several compounds candidate as electrolyte in solid oxide fuel cells (SOFCs), the excellent chemical stability of $BaZr_{0.8}Y_{0.2}O_{3-\delta}$ makes it one of the most promising [3]. In order to investigate the protonic conductivity, the structure and transport properties of highly ordered, epitaxially oriented, $BaZr_{0.8}Y_{0.2}O_{2.9}$ (BZY) thin films grown on a (110) $NdGaO_3$ (NGO) substrate were intensively studied.
Previous transport measurements have shown an increase of the in-plane conductivity as the sample thickness decreases. Moreover, a strong increase of conductivity under wet H_2 atmosphere, relative to dry H_2 and dry N_2, supported the idea that the electrical transport is related to the localization of protons at the interface. The high values of conductivity were possibly related to the high densities of defects, mostly dislocations, at the film/substrate interface [4].
In this system, the lattice mismatch between the BZY film and the substrate is large (~ 8%) and lattice relaxation occurs by misfit dislocations (MDs) at the interface between the deposited film and the substrate. Surface x-ray diffraction (SXRD) measurements show the presence of MDs network that self-organizes in a regular square network at the interface with a large in-plane coherence length. The sample is then subjected to a thermal annealing in Ar saturated with H_2O and hydroxyl groups and protons are generated by water dissociation. The x-ray intensities of the MD peaks increase strongly after annealing of the sample in wet conditions and the effect is reversible upon annealing in O_2 dry atmosphere. This phenomenon can be explained by incorporation of hydroxyl groups in the MDs that change the local strain field and consequently the intensity of the diffraction peaks from the MDs network. This picture, obtained to explain the intensity variation of the x-ray diffraction MD peaks, may also well explain the reported high in-plane conductivity [4]. Namely, dislocation lines can act as fast paths for diffusing protons. Further studies are already scheduled in order to investigate the role of the MDs network on other interface conduction mechanisms in the present system as well as in different oxide interface systems.

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