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Composition of Epitaxial ZrO_2:Y_2O_3/$SrTiO_3$ Heterostructures.

Frank J. Scheltens[1], Daniel E. Huber[1], Robert E. A. Williams[1] and David W. McComb[1]

[1.] Center for Electron Microscopy and Analysis, Department of Materials Science and Engineering, The Ohio State University, Columbus OH 43212, United States

Thermally activated oxygen ion conductivity in the electrolyte of a solid oxide fuel cell (SOFC) device is critical to its successful operation. The current generation of bulk solid oxide electrolytes requires temperatures in the range of 700 to 1000 ˚C in order to achieve the required level of oxygen conductivity, which leads to longevity issues due to thermal stress and fatigue and the requirement for more costly materials [1]. The search for SOFC materials with enhanced ion conductivity at low temperatures has lead researchers to the arena of strained epitaxial heterostructures. Reports of ion conductivity increases of several orders of magnitude in highly strained multilayers consisting of alternating layers of yttria stabilized zirconia (YSZ) and $SrTiO_3$ (STO) [2] have created a great deal of excitement in the field SOFC development.

A SOFC heterostructure device consisting of STO and YSZ layers (10 nm and 2.5 nm nominal thicknesses, respectively) was grown on a <100> oriented STO substrate with four repetitions using a high O_2 pressure RF sputtering system (2.8 mbar pure O_2) at 900ºC. A capping layer of 40 nm of STO was grown on the top of the sample [3]. Cross sectional transmission electron microscopy samples were prepared by dual beam focused ion beam (DB-FIB) such that the either the <100> or <110> type crystallographic orientation was normal to the foil surface. These samples were examined by high angle annular dark field (HAADF) high resolution scanning transmission electron microscopy (HRSTEM) and energy dispersive x-ray spectroscopy spectrum imaging (EDS SI) using an aberration-corrected Titan G2 instrument operating at an accelerating voltage of 200 kV and equipped with a Super-X system containing four silicon drift detectors. Quantitative compositional images and line profiles were calculated using the Cliff-Lorimer k-factor method as implemented in the Esprit software package using experimentally determined values for K_α k_{ZrY} and K_α k_{SrTi}

HAADF STEM images and quantitative compositional maps in Figures 1 (a) through (f) clearly show the presence of YSZ layers that are several nanometers thick along with intervening STO layers of approximately 10 nm. Although the YSZ layers appear to be continuous, there seems to be substantial variation in thickness along the length of the YSZ layer, as evidenced by intensity variations in the yttrium and zirconium compositional maps. Quantitative compositional line profiles taken along the growth direction, displayed in Figure 1 (g), demonstrate an asymmetry in the yttrium composition profile across the YSZ layer that creates a variation in the yttria molar percent in the growth direction. At the leading growth edge of the YSZ layer the yttria content is approximately 30 mol% Y_2O_3:ZrO_2 while at the trailing edge it fall to about 8 mol% Y_2O_3:ZrO_2. In addition, the titanium and strontium quantitative compositional line profiles provide evidence of a non-stoichiometric, titanium (B-site) deficient STO composition in the intervening STO growth layers.

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[3] SOFC device grown by Alberto Rivera, Carlos León, Jacobo Santamaría of Universidad Complutense Madrid, Departamento de Física Aplicada III, GFMC, E-28040 Madrid, Spain

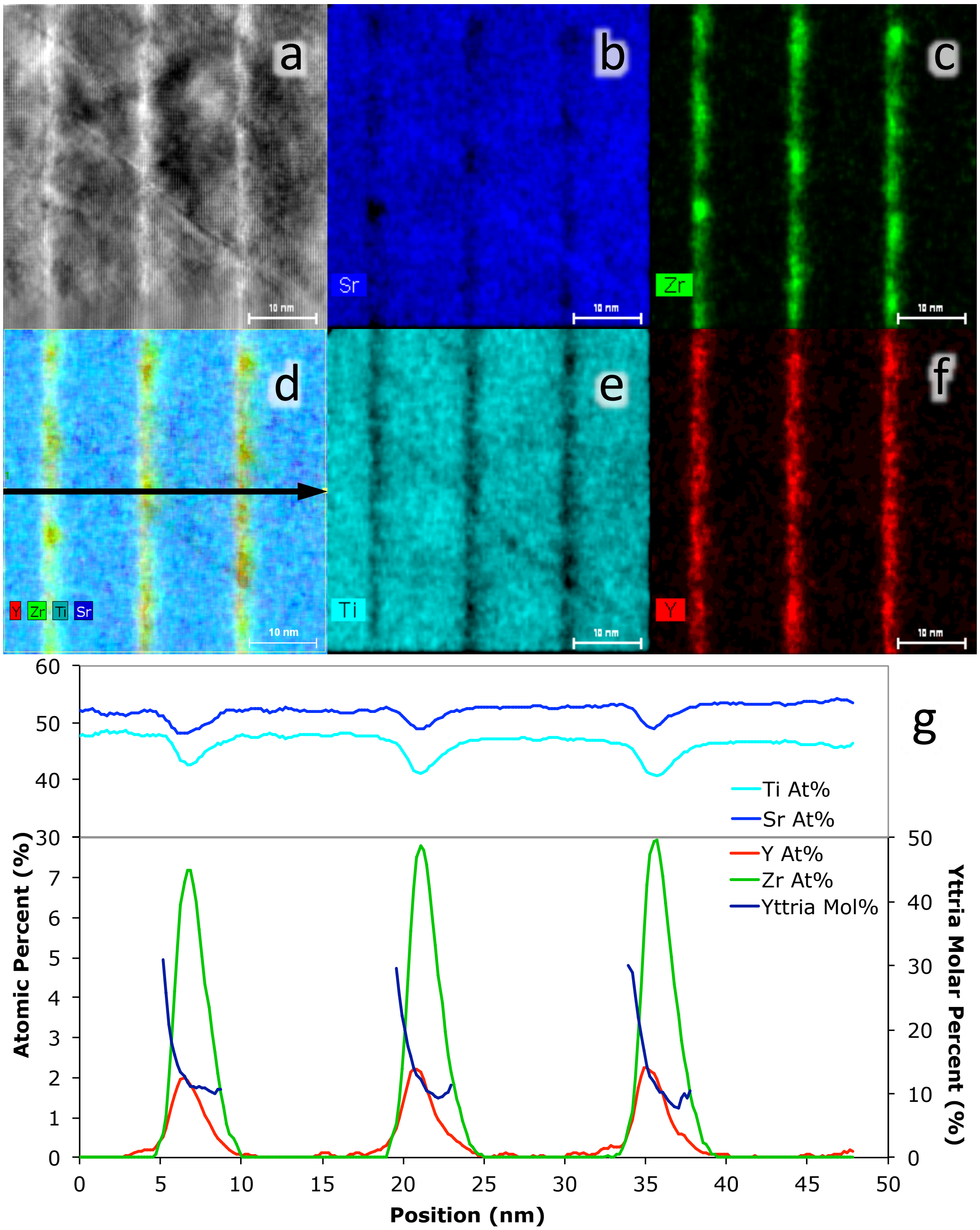

Figure 1. HAADF STEM image (a), quantitative compositional spectrum images (b-f) and extracted quantitative compositional line profiles (g) taken along the growth direction of three adjacent YSZ layers with intervening STO layers.

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