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HRTEM CHARACTERIZATION OF INTERFACE BETWEEN ISO-STRUCTURAL THIN SOLID FILM AND SUBSTRATE

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α-Fe_2O_3 and *c*-CeO_2 thin films have been epitaxially grown on α-Al_2O_3 and yttria-stabilized *c*-ZrO_2 substrates, respectively, by oxygen plasma assisted molecular beam epitaxy (OPA-MBE). The interface structural features between the films and the substrates were characterized by high resolution transmission electron microscopy (HRTEM), electron energy-loss spectroscopy (EELS), Rutherford backscattering spectrometry (RBS), and x-ray diffraction (XRD). For the two systems studied, the interfaces are similarly characterized by coherent regions that are separated by misfit dislocations periodically distributed along the interface. These results will be presented along with the results from molecular dynamics (MD) simulations of these interfaces.

Thin solid films have a wide range of applications as both functional and structural materials[1-3]. In most cases, defects in a thin film are initiated from the interface between the film and the substrate. Defects and their spatial distribution within a film may be controlled by carefully tailoring the factors which determine the interface structure. These factors include the in-plane lattice mismatch, substrate surface termination and relaxation, crystallographic orientation and phase compatability between the film and the substrate, deposition temperature, and growth rate. In this paper, we discuss our recent HRTEM, EELS, RBS and XRD investigation of the interface structural features between α-Fe_2O_3 and α-Al_2O_3 and that between *c*-CeO_2 and *c*-ZrO_2. These two systems of film-substrate pairs were commonly featured by the fact that the film and the substrate possess the same crystallographic structure.

For the α-Fe_2O_3/α-Al_2O_3 pair, two films were analyzed, one with a film thickness of ~ 7 nm and the other with a film thickness of ~ 70 nm. In order to analyze the dislocation core structure for the 7 nm sample, two cross sectional thin foils were prepared for TEM observation of the interface. One specimen was imaged along the $[\bar{2}110]$ zone axis and the other was viewed along the $[01\bar{1}0]$ zone axis. For the 70 nm specimen, one cross sectional thin foil was prepared such that the HRTEM image was taken along the $[\bar{2}110]$ zone axis. For the *c*-CeO_2/ *c*-ZrO_2 system, the film has a thickness of 58 nm and the HRTEM images were taken along the [100] zone axis, which is common to the film and the substrate [4,5].

Figure 1(a) is a low magnification TEM picture showing the general feature of the thin *c*-CeO_2 film on the *c*-ZrO_2 substrate, which possess an orientation relationship as $[100]_{CeO_2} \parallel [100]_{ZrO_2}$ and $(001)_{CeO_2} \parallel (001)_{ZrO_2}$. Figure 1(b) shows a HRTEM image of the interface between cubic ZrO_2 and cubic CeO_2, revealing that the in-plane lattice mismatch between the *c*-CeO_2 film and the *c*-ZrO_2 substrate is fully accommodated in the interface region by interface misfit dislocations. These dislocations are periodically distributed along the interface with a dislocation spacing ~3.3 ± 0.5 nm when observed from the [100] direction. This result is consistent with that calculated using the lattice mismatch measured by selected area electron diffraction.

The in-plane lattice mismatch between the α-Fe_2O_3 film and the α-Al_2O_3 substrate is also similarly accommodated in the interface region by interface misfit dislocations with a dislocation spacing ~ 7 nm when observed from the $[\bar{2}110]$ direction and a dislocation spacing of ~ 4.5 nm when observed from the $[01\bar{1}0]$ direction. It is clearly demonstrated that for this iso-structural film/substrate pair, interface misfit dislocations are the primary mechanism for accommodating the lattice mismatch.

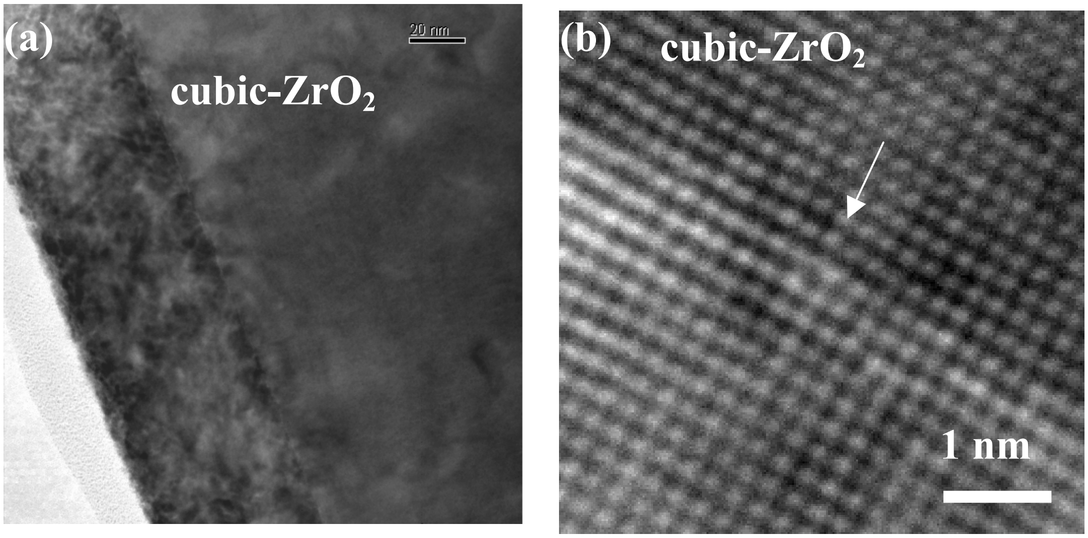

Figure1. (a) TEM image of c-CeO_2 film on c-ZrO_2 and (b) HRTEM image revealing the interface misfit dislocation (arrowed).

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