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


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α-Fe₂O₃ and c-CeO₂ thin films have been epitaxially grown on α-Al₂O₃ and yttria-stabilized c-ZrO₂ 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 compatibility 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-Fe₂O₃ and α-Al₂O₃ and that between c-CeO₂ and c-ZrO₂. 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-Fe₂O₃/α-Al₂O₃ 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 [2110] zone axis and the other was viewed along the [0110] zone axis. For the 70 nm specimen, one cross sectional thin foil was prepared such that the HRTEM image was taken along the [2110] zone axis. For the c-CeO₂/ c-ZrO₂ 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-CeO₂ film on the c-ZrO₂ substrate, which possess an orientation relationship as [100]CeO₂ || [100]ZrO₂ and (001)CeO₂ || (001)ZrO₂. Figure 1(b) shows a HRTEM image of the interface between cubic ZrO₂ and cubic CeO₂, revealing that the in-plane lattice mismatch between the c-CeO₂ film and the c-ZrO₂ 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-Fe₂O₃ film and the α-Al₂O₃ substrate is also similarly accommodated in the interface region by interface misfit dislocations with a dislocation spacing ~ 7 nm when observed from the [2110] direction and a dislocation spacing of ~ 4.5 nm when observed from the [0110] 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.

Acknowledgements: Partial support for this work was provided by the US Department of Energy (DOE), Office of Basic Energy Sciences, Division of Chemical Sciences. The experiments were carried out at the Environmental Molecular Sciences Laboratory (EMSL), a National Scientific User Facility located at Pacific Northwest National Laboratory (PNNL) and supported by the US DOE Office of Biological and Environmental Research. PNNL is operated by Battelle Memorial Institute for the US DOE under Contract DE-AC-06-76RLO 1830. The authors gratefully acknowledge helpful suggestions from W. J. Weber (PNNL) and Y. J. Kim of Dept. of Chemical Technology, Taejon National University of Technology, Taejon, Korea.

References