Stabilization origin of α-Fe_2O_3 epitaxial thin films grown by Pulsed Laser Deposition on different substrates

Aida Serrano[1], Juan Rubio-Zuazo[1], Jesús Lopez-Sanchez[2], Eduardo Salas-Colera[1], Iciar Arnay[1], German R. Castro[1]

(1) Spanish CRG-Spline, The European Synchrotron (ESRF), 38000 Grenoble, France and Instituto de Ciencia de Materiales de Madrid, ICMM-CSIC, 28049 Madrid, Spain
(2) Departamento de Física de Materiales, Universidad Complutense de Madrid, 28040 Madrid, Spain and Unidad Asociada IQFR (CSIC)-UCM, 28040 Madrid, Spain

aida.serrano@icv.csic.es

Hematite (α-Fe_2O_3) is an antiferromagnetic material at room temperature, which presents a wide interest in diverse applications due to its low toxicity, abundance and easy control of morphology. Specifically, this iron oxide phase is a promising semiconductor for gas sensor and photocatalytic applications because its band gap is about 2.1 eV. However, the efficiency of bulk α-Fe_2O_3 is limited due to its low hole mobility and short carrier lifetimes. One possible approach to tailor the physical and chemical properties is using α-Fe_2O_3 thin films deposited on several substrates varying their crystallographic orientation and lattice parameter. In this work, we evaluate the growth factors of α-Fe_2O_3 single crystalline thin films deposited by Pulsed Laser Deposition (PLD) on three different substrates: $SrTiO_3$ (111), α-Al_2O_3 (0001) and $LaAlO_3$ (001). An exhaustive study of morphological and structural properties of thin films and the possible formation of other phases has been carried out. For that, several techniques has been employed: Grazing Incidence Surface X-Ray Diffraction (GIXRD), X-ray Absorption Spectroscopy (XAS), Atomic Force Microscopy (AFM), X-ray Photoelectron Spectroscopy (XPS) and Raman Spectroscopy. Hematite thin films exhibit a continuous surface with a similar grain size, and the lowest roughness is found for the film grown on the $SrTiO_3$(111) substrate. The crystallographic orientation and lattice parameter of substrate influence on the growth of hematite layer: α-Fe_2O_3(0001) grows with its crystallographic axes parallel and rotated 30 degrees with respect to those of α-Al2O_3(001) and $SrTiO_3$(111) substrate respectively, while α -Fe_2O_3(11$\bar{1}$2) along its r-plane is grown rotated 45 degrees on $LaAlO_3$(001) reducing the large lattice mismatch to be accommodated the layer. The structural characterization indicates the lowest crystalline disorder for hematite film deposited on α-Al2O_3(0001), increasing as the grain domain size decreases and being lower for hematite evaporated on $LaAlO_3$(001). Moreover, an Fe-O elongation and Fe-Fe contraction of first neighbors distances are originated to be stabilized the α-Fe_2O_3 crystalline structure as the lattice misfit strain decreases. Therefore, we demonstrate that a control of morphological and structural characteristics of epitaxial hematite can be conducted varying the lattice parameter and the crystallographic orientation of the oxide substrate, opening the possibility of designing the growth and properties of thin films for advanced applications.

This work has been supported by the Ministerio Español de Economia, Industria y Competitividad (MINECO) through the projects PIE-2010-OE-013-200014 and MAT2012-38045-C04-03. J. L-S thanks the FPI fellowship. The ESRF, MINECO and CSIC are acknowledged for the provision of synchrotron radiation facilities.