

X-ray spectroscopy analysis of the chemical and electronic structure of BaTiO₃ ultrathin films

S. Gonzalez¹, P. Rojo-Romeo², M. Bugnet³, P. Schöffmann⁴, E. Otero⁴, B. Vilquin², N. Baboux¹, B. Gautier¹, G. Herrera⁵, O. Boisron⁵, D. Le Roy⁵, F. Tournus⁵, P. Ohresser⁴, V. Dupuis⁵, I. C. Infante¹

¹Univ. Lyon, INSA Lyon, CNRS, ECL, UCBL, CPE Lyon, Institut des Nanotechnologies de Lyon, UMR5270, 69621 Villeurbanne, France - sara.gonzalez@insa-lyon.fr

²Univ. Lyon, ECL, CNRS, CPE Lyon, Institut des Nanotechnologies de Lyon, UMR5270, Ecully, France

³Univ. Lyon, CNRS, INSA Lyon, UCBL, MATEIS, UMR 5510, 69621 Villeurbanne, France

⁴Synchrotron SOLEIL, CNRS-CEA, L'Orme des Merisiers, Saint-Aubin, 91192 Gif-sur-Yvette, France

⁵Univ Lyon, Université Claude Bernard Lyon 1, Institut Lumière Matière, CNRS UMR 5306, France

Nano ferroelectricity has promising technological applications as energy-saving, low-sized electronic devices. Tunnel junctions and transistors using ferroelectric gates are examples of potential applications [1]. BaTiO₃ (BTO) is a lead-free ferroelectric showing fascinating properties when connected to an electrode, in particular a “positive dead-layer” [2] or interface ionic relaxation [3], making BTO a promising candidate for integration in multifunctional structures with ultimate nanoscale dimensions. For this purpose, the physical and chemical properties of interfaces and ultrathin layers based on BTO have to be understood and means to control their properties must be sought out. In this work, we propose to study ultrathin BTO films grown by industrially scalable magnetron sputtering on conductive Nb-doped SrTiO₃ substrates and on structurally compatible conductive layers of SrRuO₃, with capping electrodes defining BTO-capacitors, to explore the effect of the conduction and chemical reconstruction phenomena within the films and at the different interfaces.

The average structure and strain of BTO films from 2 to 16 nm were investigated using X-ray diffraction. A thorough spectroscopic analysis of the films was carried out to study the relationship between strain and materials and processing parameters. Combining synchrotron X-ray absorption spectroscopy in capacitors and laboratory X-ray photoelectron spectroscopy, we probed the electronic structure under the influence of different UHV annealing conditions, studied the promotion of electronic and ionic defects, *e.g.* oxygen vacancies. Structural and polarization states of differently strained BTO films were analyzed through X-ray natural linear dichroism at the Ti-L_{2,3} edges along with multiplet calculations supporting the experimental evidence of the contribution of the strain to the polarization of the films. Scanning transmission electron microscopy and electron energy loss electron spectroscopy provided the atomic scale evidences of the electronic structure through the films and at the interfaces. Combined with piezoresponse force microscopy and electrical characterizations to probe ferroelectric and electrical properties under electric field, these results are crucial to understand and master the underlying physical mechanisms leading to the ferroelectric properties of operating BTO-based devices.

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