Standard Project

Experimental Report template

Proposal title: Polarity compensation of oxide surfaces during Pt deposition				**Proposal number:** HC-623
Beamline: ID03	**Date(s) of experiment:** from: 19/07/2014		to: 23/07/2014	**Date of report:** 21/10/2014
Shifts: 12	**Local contact(s):** Roberto Felici			*Date of submission:* 22/10/2014

Objective & expected results (less than 10 lines):

It was noted in an earlier studies that polar oxide surfaces require charge compensation to minimize their surface free energies. How this occurs is directly relevant to the catalytic activity of oxides as well as to the morphology of nanostructures grown on such surfaces. Since compensation can be accomplished by a variety of mechanisms (*e.g.*, surface reconstructions, charged adsorbates, point defects, and free carriers), a longstanding point of contention has been whether or not the particular compensation mechanism can change during adsorption. To address this fundamental challenge, we have carried out systematic X-ray studies of the polar oxide surfaces LaAlO3(001) and SrTiO3(111), as well as on the non-polar SrTiO3(001) surface. We utilized the ultrahigh vacuum deposition system at ID03 to study the structure of such surfaces both before and after the deposition of one monolayer of Pt. We will use coherent Bragg rod analysis (COBRA) to retrieve 3D electron density maps from the collected crystal truncation rod data and look for changes in the surface structure upon Pt adsorption.

Results and the conclusions of the study (main part):

The three-unit-cell thick LaAlO3/SrTiO3(001), SrTiO3(111), and SrTiO3(001) surfaces were prepared at the University of Wisconsin-Madison, using pulsed laser deposition to grow the LaAlO3 epitaxial film. All of the surfaces should be B-site terminated. Three-unit-cell LaAlO3 films grown under similar conditions show no evidence of 2D electron gas formation, as expected for films below the critical thickness of four unit cells. This indicates that a polar field should span across the LaAlO3 material, and related experiments carried out at the Advanced Photon Source have shown evidence of both cation/anion displacements and electrostriction in response due to the internal field.

For each of the three samples, we collected a set of crystal truncation rods (CTRs) both before and after deposition of approximately one monolayer of Pt. The Pt was evaporated onto the samples at 700°C at a growth rate of approximately 0.07 Å per minute. As seen by the in-plane *HK* map in Fig. 1, the Pt grows pseudomorphically onto the different perovskites (presumably chemisorbed), and this should help charge compensate the polar surfaces. For the LaAlO3 sample, this should reduce and perhaps even eliminate the cation/anion displacements; a study by Xie *et al*., Nature Comm. **2,** 494 (2011) found that polar adsorbates could drive the buried interface into a conducting state.

Very high quality scattering data was taken during this beamtime. The data from the three different samples are currently under analysis. We anticipate that the results will be very high impact given the level of current interest in polar oxide surfaces.

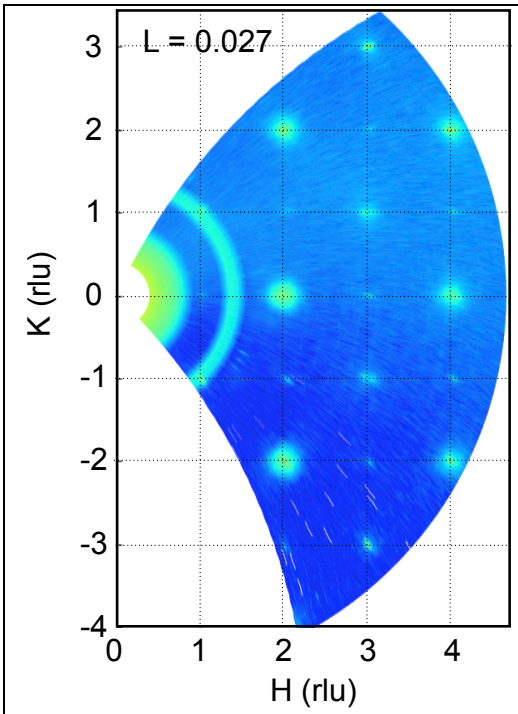

FIG 1: In-plane reciprocal space map of a 1 ML Pt / 3 unit cell LaAlO3 / SrTiO3(001) heterostructure, illustrating that Pt grows pseudomorphically on this polar surface. This is reflected in the broad peaks observed at the even-order reflections. Reflections from the substrate appear at all integer indices. The rings of scattering near the origin stem from the glue used to mount the sample.

Justification and comments about the use of beam time (5 lines max.):

The success of our experiment relied on both use of a synchrotron beam to provide the scattering data necessary for crystal truncation rod measurements, as well as the in-situ deposition capabilities at ID03. This is a unique beamline that has a UHV deposition chamber available for in-situ studies, and it is run very well by Dr Roberto Felici. Despite the complexity of the beamline equipment, he keeps the entire beamline and its components in excellent working order. Dr Felici's expertise was essential to the success of our experiment.

Publication(s):

- Publications will be forthcoming
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