Atomic structure of Pt/$SrTiO_3$(001) interface probed by x-ray standing waves

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Introduction

A key aspect of investigating the electrical behavior of complex oxide films is an understanding of the electrode/oxide interface, which may easily dominate the electrical response for insulating films thinner than a few hundred nanometers. Band alignment and charge transfer at such interfaces typically fall between the extremes of the simple Schottky and Bardeen models, necessitating the use of more complex calculations with, if possible, the true atomistic structure as an input. However, little precise information has been experimentally obtained on the structure of such metal/crystalline oxide interfaces. This interface is very difficult to investigate nondestructively at the atomic scale level using conventional analytical methods. The x-ray standing wave (XSW) technique [1] can provide unique structural information related to interfaces, as demonstrated in studies of semiconductor/metal and semiconductor/semiconductor interfaces [2]. As a model system, we studied a submonolayer of Pt on the $SrTiO_3$(001) surface.

Experimental

The *in situ* XSW experiments were performed at the BESSRC undulator 12-ID-D beamline. The $SrTiO_3$ substrates were etched in buffered HF [3] and annealed by oxygen at 1050° C to obtain a Ti-terminated surface. The crystals were loaded into the XSW-MBE (molecular beam epitaxy) system and annealed in an ultra high vacuum (UHV) at 950° C. The Auger electron spectroscopy (AES) showed a clean surface with negligible carbon contamination, and the low-energy electron diffraction (LEED) pattern revealed a two-domain 2 x 1 structure. A submonolayer amount of Pt in the range of 0.1 to 1.0 ML (monolayer) was deposited from an e-beam evaporator in the MBE chamber with a base pressure of 10^{-10} mbar. The sample was then transferred into the x-ray chamber for the UHV XSW measurements.

The degree of perfection of the oxide crystals is the main obstacle in applying the XSW technique. We demonstrated that this problem could be partially solved by using the high brightness of the x-ray undulator source. The x-ray optics we used in our experiments included an up-stream Si(111) liquid-nitrogen-cooled double-crystal monochromator, followed by a Si(004) channel-cut crystal and a 20 x 100 μm^2 slit. Using highly collimated, quasi-plane-wave, monochromatic, and very narrow x-ray beam, we were able to find near-perfect regions on the $SrTiO_3$ crystal yielding a rocking curve close in width and shape to theory (Figure1, dashed lines). The Pt-Lα fluorescence yield was measured as a function of the incident angle while scanning the crystal through the (002) reflection.

Results and Discussion

We studied the temperature dependence of the Pt position along the [001] direction for coverages of 0.1 and 0.5 ML. Interestingly, for both coverages we found one occupation site at a low (550–700° C) temperature and another at a high (800–910° C) annealing temperature. The transition from the low-temperature surface structure into the high-temperature structure happens within a temperature range of 100° C. The experimental data and analysis for the 0.1 ML coverage are shown in Figure1 for 700° C (a) and 910° C (b). The thermally induced change in the coherent position corresponds to an inward displacement of the Pt atoms by $0.72 \bullet d_{002} = 1.40$ Å from the position located at 1.07 Å above the top TiO_2 layer to the position slightly (by 0.33 Å) below the TiO_2 atomic plane.

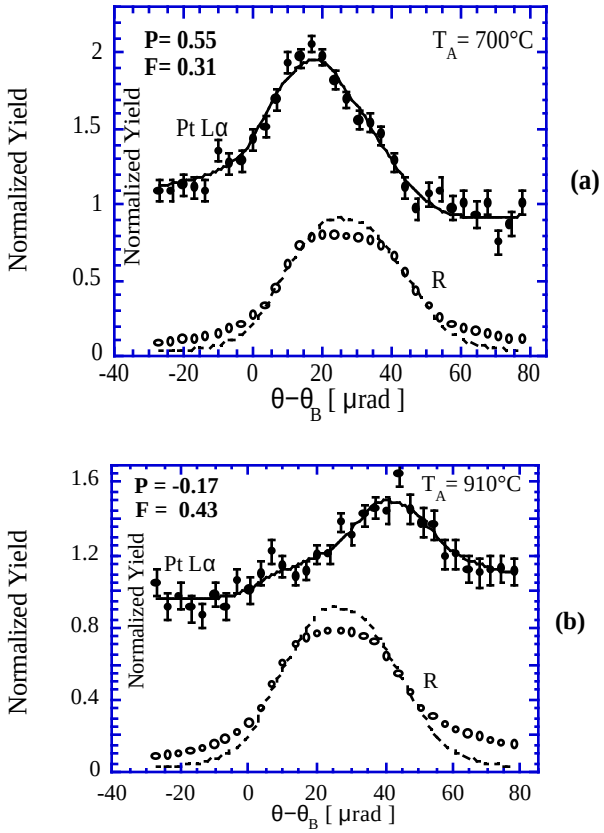

Figure 1: The $SrTiO_3$(002) Pt-L experimental XSW curves measured for 0.1 ML of Pt after annealing at 700° C (a) and 910° C (b) (solid circles) and the corresponding rocking curves (open circles). The results of the fit (solid lines = XSW yield, dashed lines = reflectivity) reveal two different sites with coherent positions of P = 0.55 for 700° C and P = -0.17 for 910° C. The transition from one site into another corresponds to an inward displacement of Pt atom by 1.42 Å.

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