X-ray Standing Wave Studies of Sr/Si(001) Surface Phases

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Introduction

Strong factors are motivating the microelectronics community to find a high dielectric constant material that could replace SiO_2 as the gate dielectric in field effect transistors. Strontium titanate ($SrTiO_3$) is viewed as a likely candidate for future generations of gate dielectrics because of its high dielectric constant relative to SiO_2 and the small lattice mismatch between $SrTiO_3$(110) and Si(100) planes. Surface phases consisting of submonolayer amounts of ordered Sr on single-crystal Si(001) are believed to be important precursors to the growth of high-quality epitaxial thin films of $SrTiO_3$ on Si [1]. While these surface phases reportedly stabilize Si against oxidation during the growth of overlying oxide films, details of their atomic-scale structure are poorly understood.

Methods and Materials

Experiments were carried out in the Basic Energy Sciences Synchrotron Radiation Center Collaborative Access Team (BESSRC-CAT) experimental station 12-ID-D by using an ultrahigh vacuum (UHV) surface science chamber. An *ex-situ* RCA chemical treatment of single-crystal Si(001) followed by a 900°C UHV anneal was used to establish a clean Si(001)-(2×1) reconstructed surface observed by low-energy electron diffraction (LEED) and auger electron spectroscopy (AES). Sr flux from a Knudsen cell was used to deposit submonolayer amounts of Sr onto Si substrates. In some cases, Si substrates were held at room temperature during deposition of a disordered Sr layer and subsequently annealed at 700-800°C. In other cases, the substrate was held at 600°C during deposition, and no postdeposition anneal was performed. Sr coverage was determined by AES and x-ray fluorescence (XRF). Upon completion of deposition and heat treatment procedures, ordered surfaces of Sr/Si(001) showing (2×3) and (2×1) periodicities were observed by LEED.

In situ x-ray standing wave (XSW) measurements [2] were made on Sr/Si(001) surfaces by monitoring the Sir-Kα fluorescence yield while scanning in angle through the (004) and (022) Si rocking curves. The high-resolution optics used for the XSW measurements consisted of an upstream Si(111) monochromator followed by two Si channel-cut crystals. A nondispersive arrangement was maintained by using Si(004) and Si(022) channel cuts for the (004) and (022) XSW measurements, respectively.

Results

The reflectivity and normalized Sr-Kα fluorescence yield data from XSW experiments were fit to dynamical diffraction theory by using the Sr coherent fraction (f_H) and coherent position (p_H) as fitting parameters. XSW results for a (2×1) phase of 0.32-monolayer (ML) Sr on Si(001) prepared by depositing it onto heated Si, and results for a (2×1) phase of 0.54-ML Sr prepared by depositing it onto room-temperature Si and then annealing to 700°C, are shown in Fig. 1. The Sr coherent positions measured for both surfaces closely match the symmetry relationship $p_{022} = p_{004}/2$. These results are consistent with Sr atoms occupying either cave sites on dimerized Si (Fig. 2a) or bridge sites on a surface that is free of Si-Si dimers (Fig. 2b).

Discussion

It has been speculated that Sr/Si(001) surfaces prepared by depositing disordered Sr onto room-temperature Si and then inducing Sr ordering by annealing the substrate are fundamentally different from ordered phases prepared by depositing onto heated Si [1]. This proposed path dependence suggests that at least one of the two preparation routes leads to a metastable phase. Our experimental findings, however, indicate that thermally activated ordering of initially disordered Sr on Si(001) results in an atomic-scale structure that is very similar to that achieved when ordering and deposition occur simultaneously. The symmetry we have detected for the Sr positions on the Si(001) surface is consistent with first principles calculations [3] and with cross-sectional transmission electron microscopy (TEM) observations of interfacial Sr silicide layers located between Si substrates and overlying $SrTiO_3$ films [1, 4].

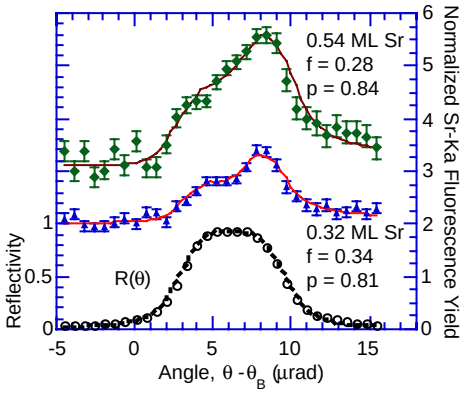

FIG. 1. The Si(004) Sr-Kα experimental XSW normalized fluorescence yield curves (solid diamonds and triangles) for a (2 ×1) surface of 0.54-ML Sr on Si(001) resulting from Sr deposition onto room-temperature Si followed by a 700℃ anneal, for a (2 ×1) surface of 0.32-ML Sr deposited onto Si(001) held at 600℃, and for the corresponding Si(004) rocking curves (open circles). The dynamical diffraction theory fit results (solid lines = XSW yield, dashed lines = reflectivity) exhibit coherent fractions and coherent positions as follows: f_{004} = 0.28 and p_{004} = 0.54 for the 0.54-ML surface, and f_{004} = 0.34 and p_{004} = 0.81 for the 0.32-ML surface.

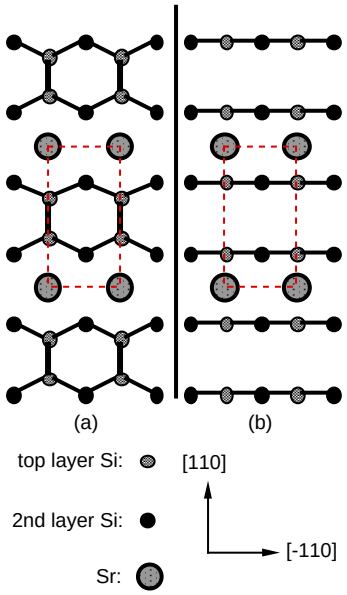

FIG. 2. (2 ×1) Sr/Si(001) surface unit cells (dashed lines) with local coverage of 0.5 ML showing Sr atoms located at (a) cave sites of a dimerized Si(001) surface and (b) bridge sites of an undimerized Si(001) surface.

Acknowledgments

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