XSW Study of Sr Adsorption on the Si(001) Surface

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Introduction

Identification of adsorption sites and surface-phase atomic structure of metals on semiconductors is important for both modeling and fabrication of many different metal- and oxide-semiconductor interfaces. Recent interest in the integration of ferroelectric perovskites such as $SrTiO_3$ on Si[1,2] has highlighted the technological importance of Sr adsorption on the Si(001)-(2 x 1) surface. Low energy electron diffraction (LEED) and scanning tunneling microscopy (STM) studies[3,4,5] have suggested probable Sr adsorption sites and provided qualitative descriptions of some phases of Sr on Si(001). The present study utilizes the x-ray standing wave (XSW) technique[6,7] to quantitatively characterize structures of sub-monolayer coverages of Sr on Si(001).

Methods and Materials

Si(001)-(2 x 1) surfaces were prepared using standard ultra-high-vacuum (UHV) techniques in the UHV XSW molecular beam epitaxy (MBE) system at the BESSRC undulator 12-ID-D beamline. 2/3 ML Sr was deposited at a rate of 0.06 ML/min onto room-temperature substrates. Sr coverages were measured with Rutherford backscattering (RBS), Auger electron spectroscopy (AES), and X-ray fluorescence (XRF). LEED images of the as-deposited surface showed a weak (3 x 1) reconstruction with high background. Post-deposition anneals for 10 min at 700 and 800 ºC caused Sr to desorb to coverages of 0.31 and 0.09 ML respectively. LEED images taken after the 700ºC anneal showed a (2 x 1) pattern, while those taken after the 800ºC anneal indicated a (3 x 2) surface reconstruction.

In situ XSW measurements conducted after each anneal involved monitoring Sr-Ka fluorescence yield as a function of incident angle while scanning through the Si (004) and (022) reflections at an incident enrgy of 18.50 keV. The X-ray optics used in these experiments consisted of an up-stream Si(111) liquid-nitrogen cooled double-crystal monochromator followed by two Si(004) channel-cut crystals.

Results and Discussion

Our (004) XSW data (Fig. 1) indicates that as the Sr/Si surface structure changes from the (2 x 1) to the (3 x 2) phase, the primary Sr atomic height shifts outward by approximately $0.16d_{004} = 0.22$ Å . The relationship between our experimentally measured coherent positions P_{004} and P_{022} for both phases is nearly identical to $P_{022} = P_{004}/2$. By symmetry, this indicates that Sr atoms occupy either the cave or bridge sites on the Si(001)-(2 x 1) surface. (See Fig. 2 for the location of these two sites.) We rule out the bridge site based on steric hindrance with the two Si atoms in the underlying Si dimer. This is in agreement with STM studies[4,5], which show that the Si dimers and dimer rows are still intact at these Sr coverages and also suggest that Sr atoms are located at cave sites.

FIG. 1: Sr/Si(001) XSW Si(004)

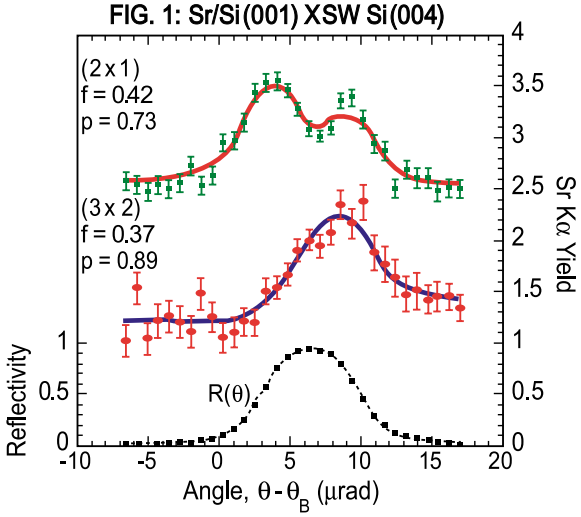

FIG. 1. The Si(004) Sr-Kα experimental XSW normalized fluorescence yield curves (solid circles and diamonds) after annealing 10 min at 700ºC (2 x 1), 10 min at 800ºC (3 x 2) and the corresponding Si(004) rocking curve (open circles). The dynamical diffraction theory fit results (solid lines = XSW yield, dashed lines = reflectivity) reveal coherent positions of $P_{004} = 0.73$ for the (2 x 1) surface, and $P_{004} = 0.89$ for the (3 x 2) surface. The (2 x 1) Sr yield is vertically offset by 1.5 for purposes of clarity.

FIG. 2: Sr on Si(001) (3 x 2) unit cell

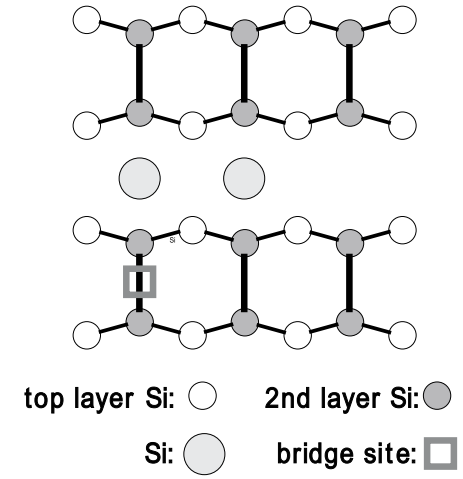

FIG. 2. The (3 x 2) Sr/Si(001) surface structure with Sr located on cave sites of the (1 x 2) dimerized Si(001) surface. The position of a bridge site (unoccupied) is also shown.

Acknowledgments

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