Domain Ordering of a Highly Strained 5 ML $SrTiO_3$ Film grown on Si(001).

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Introduction

The ability to suppress the growth of amorphous SiO_2 at the initial formation of ordered oxide growth on Si is tantamount to creating an ordered interface. Highly ordered and strained (-1.66%) films with a high degree of lattice matching between the $SrTiO_3$ films and Si (001) substrate were studied. The films are rotated 45˚ in the film plane with respect to the Si (001) substrate, $(001)_{Si}$ // $(001)_{STO}$: $(100)_{Si}$ // $(110)_{STO}$.

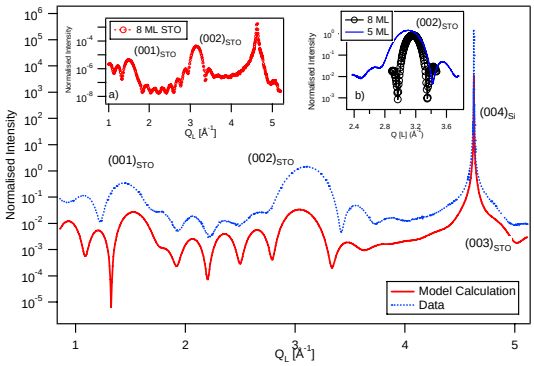

Figure 1; shows the specular rod scans for a 5ML and 8ML STO film. A modeled calculation is compared with the 5ML data.

Results & Discussion

Figure 1 presents the (00L) 'out of plane' rod scans of both 5ML and 8ML samples of STO grown on Si (001). Out of plane lattice expansion occurs for both films 4.038Å at 5ML to 3.963Å at 8ML, with bulk STO measuring 3.905Å.The modeled (00L) rod scan of the 5ML sample comparison assumes the Si (001) to be a semi-infinite substrate. The STO structure was independently described layer by layer, beginning with a half monolayer of Sr followed by a full layer of SrO, the separation between the two was 1.5Å, the 5 units of STO terminates with a layer of SrO. The complete overlayer film was then added to the substrate with a phase factor determining the separation between the substrate and film, this was measured at 0.3Å. This separation coupled with the ½ ML Sr–SrO distance strongly effected the modeled scan around the Si(004) which overlaps with the STO(003) Bragg reflection. This vertical arrangement agrees favourably with the ½ ML Sr sitting low, equidistant from two pairs of Si dimmers. The strong asymmetric shape of the STO Bragg peaks and the beat of the fringes between STO (002) and (004), were replicated by adding an identical but separate STO film vertically offset by the height of a single Si layer of 1.358Å.

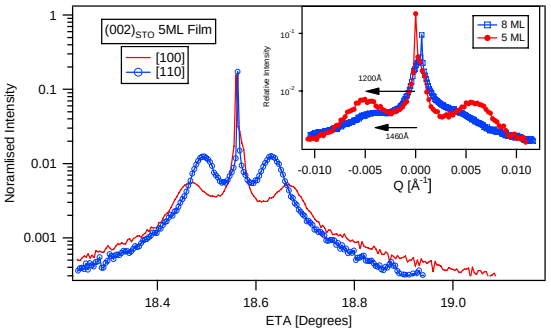

Figure 2; presents Omega scans along the [100] and [110] through the (002) STO for the 5ML film. Inset compares the [100] direction for both 5 and 8ML films.

Strong in-plane (HK) satellite features were identified around the STO Bragg reflections as shown in figure 2, where Omega scans across the STO (002) are presented. The scans shown are two different azimuthal orientations 45˚ apart, indicating 4-fold symmetry whereby the wings are elongated along the H_{Si} and K_{Si} to form a square. The edge length of the square shaped coherent domains measured ~1200Å. Omega scans across the STO (002) reflection for both films are presented in figure 2 inset. The 8ML system measures ~1460Å. With azimuthal rotation of the 8ML sample there is no change in the position or intensity of the satellite features, the wings are broader and of lower intensity at all angles. The satellites form a ring in the HK plane around the STO(002) reflection at a separation indicating an averaged correlation distance roughly half way between 1200Å and 1700Å, which form the side and diagonal length of the square domains.

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