High-quality Nano-thickness Single Crystal Sc2O3 Film Grown on Si (111)

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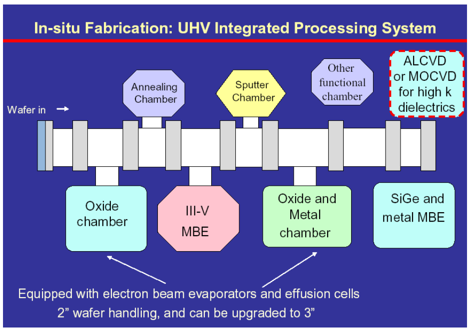
High-quality single-crystal Sc2O3 films a few nanometer thick have been grown epitaxially on Si (111) despite a huge lattice mismatch. The films were electron beam evaporated from a Sc2O3 target. Structural and morphological studies were carried out by x-ray diffraction and reflectivity in a synchrotron radiation source, AFM, HRTEM, and MEIS, with the initial epitaxial growth monitored by in-situ RHEED. The films have the cubic bixbyite phase with a remarkably uniform thickness and high structural perfection. The film surfaces are very smooth and the oxide/Si interfaces are atomically sharp. The films are well aligned with the Si substrate, with a normal orientation relationship of Si (111) // Sc2O3 (111), and an in-plane expitaxy of Si $[\bar{1}10]$ // Sc2O3 $[\bar{1}01]$.



Synchrotron X-ray normal scans (Fig.4) display substrate peaks (111) and (222), and also (222) and (444) peaks of the bixbyite phase of the Sc2O3 epitaxial film. Peak positions of the film along the surface normal agree well with the bulk lattice constant of Sc2O3, indicating that the epitaxial film is fully relaxed. The well defined fringe patterns about the Bragg peaks of the film confirm a highly uniform film thickness compared with XRR(Fig.5). The x-ray scans (Fig.6) carried out in other parts of the reciprocal space found that, while the <111> axes of the silicon substrate and the Sc2O3 film are well aligned, the two cubic cells are in-plane rotated by 60° with respect to each other.

The rocking scans (Fig.7) shapes are not symmetric about the center as would have been expected from fully strain relaxed film growth.

Cubic Sc2O3 and Si have significantly different crystal structures, different bonding, and lattice constants. The bulk lattice constants of Si (5.43 Å) and Sc2O3 (9.86 Å) are mismatched by 9.2 % (relative to the doubled Si unit cell dimension). It is intriguing that a highly ordered epitaxial growth was obtained with this unusually large mismatch.

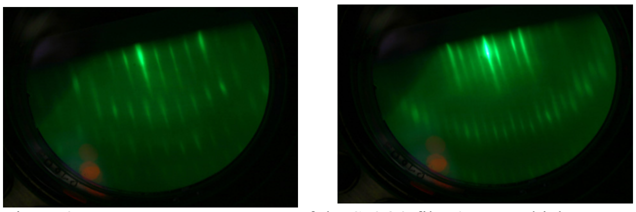
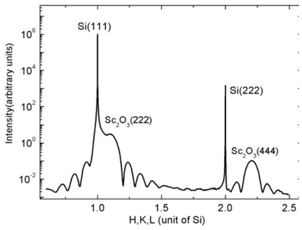


Figure 3. *In-situ* RHEED patterns of the Sc2O3 film 0.5 nm thick showing a (4x4) reconstruction. (a) along [110] axis (b) along [112] axis



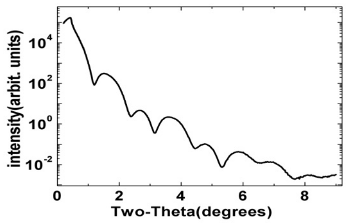


Figure 4. Single crystal scans along the surface normal Fig. 5 XRR

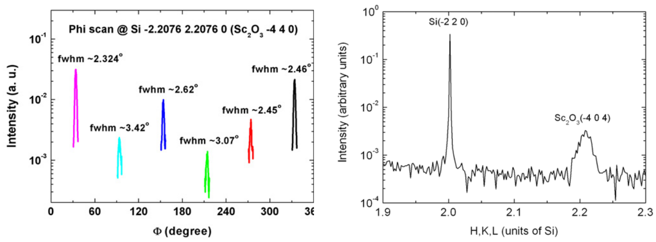


Figure 6. (a.) Phi cone scan of Si {220} and Sc2O3{440}; (b.) A radial scan in the in-plane surface

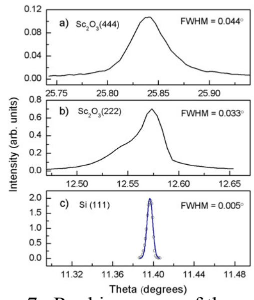


Figure 7. Rocking scans of the substrate and the epitaxial film peaks

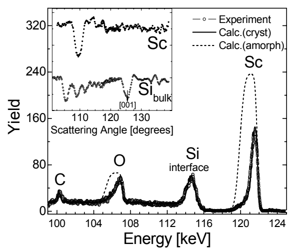


Figure 8. Backscattering energy spectrum (130 keV H+) of a Sc2O3 film on Si(111) in a normal incidence and substrate blocking geometry.