Abstract

A wide array of techniques were applied in this research to investigate the perovskite materials $SrTiO_3$ and $LaAlO_3$ with the goal of furthering the understanding of oxide surfaces. Specifically, a combination of transmission electron diffraction, direct methods and density functional theory was used to determine the structure of the $SrTiO_3$ (001) $(\sqrt{13}\times\sqrt{13})R33.7^{\circ}$ surface reconstruction. It has a TiO_2-rich surface with a 2D tiling of edge or corner-sharing TiO_5 octahedra. By tiling these units and forming network surface structures ranging from ordered like the 2x1 and c(4x2), to pseudo-ordered, like the c(6x2), to a disordered glass-like surface layer made up of TiO_x units, dictated by local bond valence sums.

The $LaAlO_3$ (110) 3x1 surface reconstruction, here reported for the first time, was found to have a hydroxylated Al-rich surface with X-ray photoelectron spectroscopy. Transmission electron diffraction data and direct methods revealed a high resemblance to the previously solved $SrTiO_3$ (110) 3x1 reconstruction leading to a hydrated version of this for $LaAlO_3$ 3x1 structure. The hydroxyl groups are necessary to balance the surface polarity, an issue arising from the difference in cationic valences between La/Sr and Al/Ti.

Also reported and investigated here for the first time is a $LaAlO_3$ (100) 5x2 reconstruction. An EDM analysis was done for several sets of recorded diffraction pattern; however the results have yet to lead to an atomic surface structure solution. X-ray photoelectron spectra were collected over a range of detector-to-surface-normal angles elucidating an Al-rich surface layer. X-ray photoelectron intensities were calculated for a model of alternating Al and La layers over a range

of grazing angles and varying amounts of Al in the top surface layer. An Al concentration of 0.5 was found to give the best fit to experimental results.