Quantification of Octahedral Rotations in Strained $LaAlO_3$ Films via Synchrotron X-ray Diffraction

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Abstract: In recent years, there has been an increased interest in octahedral rotations in perovskite materials, particularly on their response to strain in epitaxial thin films. The current theoretical framework assumes that rotations are affected primarily through the change in in-plane lattice parameters imposed by coherent heteroepitaxy on a substrate of different lattice constant. This model, which permits prediction of the thin-film rotational pattern using first-principles density functional theory, has not been tested quantitatively over a range of strain states. To assess the validity of this picture, coherent $LaAlO_3$ thin films were grown on $SrTiO_3$, $NdGaO_3$, $LaSrAlO_4$, $NdAlO_3$, and $YAlO_3$ substrates to achieve strain states ranging from +3.03% to -2.35%. The out-of-plane and in-plane octahedral rotation angles were extracted from the intensity of superlattice reflections measured using synchrotron x-ray diffraction. Density functional calculations show that no measurable change in intrinsic defect concentration should occur throughout the range of accessible strain states. Thus, the measured rotation angles were compared with those calculated previously for defect-free films. [Hatt and Spaldin, Phys. Rev. B 82, 195402 (2010)]. Good agreement between theory and experiment was found, suggesting that the current framework correctly captures the appropriate physics in $LaAlO_3$.