Atomic Structure Refinement of Pbnm-type Perovskite Oxide Films

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Complex ABO$_3$ oxide heterostructures are of interest due to their wide variety of electronic, optical, and magnetic properties. One of the controlling factors to these functionalities is the distortions and rotations of the corner-connected BO$_6$ octahedral network. This BO$_6$ octahedra network directly couples to the electronic bandwidth of these materials, but the inability to determine the full atomic structure in thin films has inhibited quantitative understanding of how factors such as epitaxial strain alter the octahedral rotations in this broad class of materials. Earlier work of has demonstrate that half-order diffraction peaks can be used to quantify octahedral rotations in thin strained films. Here, we build on this approach to solve for both the oxygen and A-site positions in films of the commonly occurring Pbnm structure type. We present on epitaxial RFeO$_3$ heterostructures, where R is a rare earth element, to demonstrate the feasibility of quantifying oxygen and A-site displacements in films using synchrotron diffraction. This work is supported by the National Science Foundation (DMR-1151649).