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Determining oxygen octahedral rotations in strained perovskite films using x-ray diffraction[1] STEVEN MAY, Drexel University, JONG WOO KIM, Argonne National Laboratory, JAMES RONDINELLI, NICOLA SPALDIN, University of California, Santa Barbara, JENIA KARAPETROVA, ANAND BHATTACHARYA, PHILIP RYAN, Argonne National Laboratory — While strain is known to alter the octahedral distortions and rotations in perovskite films, the details of how the local atomic structure accommodates strain are poorly understood due to the difficulty of measuring oxygen positions in thin films. Using epitaxial $LaNiO_3$ as a model system, we present a general strategy for determining the atomic structure of strained perovskites via x-ray diffraction. The oxygen positions have been determined by comparing the intensities of half-order Bragg peaks, arising from the two unit cell periodicity of the octahedral rotations, with calculated structure factors. The bond angles and lengths have been determined for $LaNiO_3$ films grown on $SrTiO_3$ (tensile strain) and $LaAlO_3$ (compressive strain), respectively, and are found to depend strongly on the strain state. These diffraction-based results are in excellent agreement with *ab initio* density functional calculations.

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