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Influence of Symmetry on the Octahedral Rotations of Epitaxial $RNiO_3$ Thin Films I.C. TUNG, Department of Materials Science and Engineering, Northwestern University; Advanced Photon Source, Argonne National Laboratory, JIAN LIU, B. GRAY, J. CHAKHALIAN, Department of Physics, University of Arkansas, J.M. RONDINELLI, E.A. KARAPETROVA, J.H. LEE, Advanced Photon Source, Argonne National Laboratory, M.J. BEDZYK, Department of Materials Science and Engineering, Northwestern University, J.W. FREELAND, Advanced Photon Source, Argonne National Laboratory — Understanding the structural and electronic behavior of ABO_3 thin films subjected to confinement, lattice misfit and broken symmetry at the interface in the ultra-thin limit is fundamentally important for the rational design of new materials [1]. However, the epitaxial strain will not only due to a change the in-plane lattice constants but also the octahedral rotations connected to bond angles and crystallographic symmetry. Here we present a study of the effect of the bulk lattice symmetry on octahedral rotations under epitaxial strain in thin films of $RNiO_3$ (R=La, Pr, Nd) grown on various substrates by pulsed laser deposition. A combination of high-resolution x-ray diffraction, polarization-dependent soft x-ray absorption spectroscopy, and first-principles density functional calculations has been applied to elucidate structural and electronic properties of the samples. Work at the Advanced Photon Source, Argonne is supported by the U.S. Department of Energy, Office of Science under Contract No. DE-AC02-06CH11357.

[1] J. Chakhalian et al., Phys. Rev. Lett., 107, 116805 (2011).

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