The role of oxygen octahedra connectivity in orthorhombic perovskite heterostructures

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Controlling the atomic structure in epitaxial transition metal perovskite thin films is an effective way to tune their properties or to achieve new functionalities. This is linked to the intimate coupling of the electronic and structural degrees of freedom in this family of materials. For instance, the rotation angle of the oxygen octahedra is directly linked to the electronic bandwidth in nickelates or to the orbital ordering temperature in vanadates. Another example is a predicted novel ferroelectric state due to a tailored coupling of rotations in epitaxial heterostructures of different symmetries [1]. Achieving such a control requires an understanding of the mechanisms that determine the atomic structure - and may compete - in an epitaxially strained structure. In this work, we investigate orthorhombic perovskite films grown by pulsed laser deposition on orthorhombic substrates [2]. We show that there is a competition between oxygen octahedra connectivity and macroscopic strain leading to an ”intermediate layer” and a ”switching plane” that allow a re-orientation of the orthorhombic unit cell [3]. The detailed atomic structure of these oxide material combinations is probed using X-ray diffraction and scanning transmission electron microscopy.

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