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Quantification of Epitaxial Strain and Crystal Structure in Nanoscale Oxide Films Using Position Averaged Convergent Beam Electron Diffraction

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Strongly correlated ABO_3 "Mott" perovskite thin films show unique properties, such as superconductivity and metal-insulator transitions. The film properties depend on its internal structure, which is closely related to the epitaxial strain and the BO_6 octahedral tilt [1-4]. In-plane epitaxial strain can change lattice parameters and affect octahedral tilts (Fig. 1) [3], but measuring such small changes in a spatially confined system is often difficult with conventional imaging or diffraction techniques. We use position averaged convergent beam electron diffraction (PACBED) [5] to measure the strain and crystal structure of the perovskite films. PACBED measures spatially averaged STEM CBED patterns from one or a few unit cells. It combines the resolution of STEM probe and the precision of electron diffraction. PACBED is sensitive to lighter elements and to the displacement of atoms as small as a few picometers.

Using PACBED, we examined the structure of $[LaNiO_3/SrTiO_3]_3$ superlattice films on $(LaAlO_3)_{0.3}(SrAl_{0.5}Ta_{0.5}O_3)_{0.7}$ (LSAT) substrates [4]. We found that the structure of $LaNiO_3$ layers is determined by both the epitaxial strain and the oxygen connectivity at the interfaces. Figure 2(b) shows a PACBED pattern acquired from the $LaNiO_3$ layer in Fig. 2(a). The pattern is laterally elongated (inset), indicating the pseudocubic $LaNiO_3$ unit cell is elongated in the growth direction, despite the tensile strain from the LSAT substrate. By mapping the χ^2 image match [Fig. 2(d)] between the experimental and simulated patterns, we found that this 'negative Poisson's ratio' is due to a decrease in the out-of-plane tilts, which is caused by the oxygen connectivity at the interfaces. The decrease in the out-of-plane tilt expands the unit cell, but the in-plane lattice parameter is constrained by the substrate, causing an increase in the in-plane tilt angles to accommodate the strain. Such changes in the lattice parameters and the tilts result in a monoclinic $LaNiO_3$ film, as opposed to the rhombohedral bulk $LaNiO_3$, and cause a metal to insulator transition [2, 4].

In $NdNiO_3$ films, we found that the symmetry of the substrate also influences the film structure. A $NdNiO_3$ film grown on $LaAlO_3$ showed a rhombohedral PACBED pattern, same as the substrate, as opposed to the orthorhombic bulk $NdNiO_3$ (Fig. 3). This shows that the structure of the film can follow the symmetry of the substrate, defying the original bulk structure [6].

References
[1] J. Son et al., *Appl. Phys. Lett*. **96**, 062114 (2010).
[2] J. Son, J. M. LeBeau, S. J. Allen, and S. Stemmer, *Appl. Phys. Lett*. **97**, 202109 (2010).
[3] J. Hwang, J. Y. Zhang, J. Son, and S. Stemmer, *Appl. Phys. Lett*. **96**, 062114 (2012).
[4] J. Hwang et al., *Phys. Rev*. B **87**, 060101(R) (2013).
[5] J. M. Lebeau, S. D. Findlay, L. J. Allen, and S. Stemmer, *Ultramicroscopy* **110**, 118 (2010).
[6] This work is supported by DOE (DEFG02-02ER45994) and Army Research Office (W911-NF-09-1-0398).

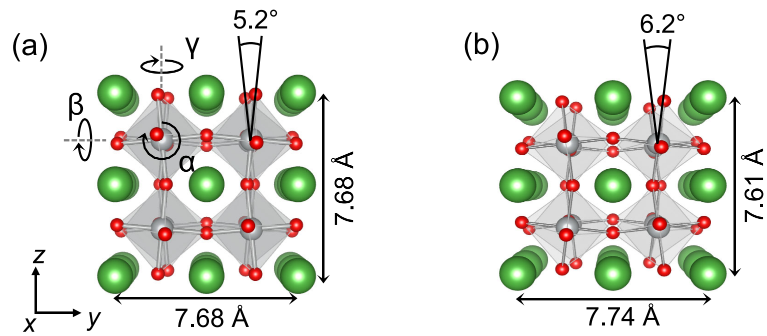

Fig. 1. (a) Schematic drawing of bulk $LaNiO_3$. α, β are out-of-plane tilts, γ is in-plane tilt, and $\alpha = \beta = \gamma = 5.2°$. (b) $LaNiO_3$ film on LSAT substrate showing strained lattice and $\alpha = \beta = 6.2°$, $\gamma = 0.9°$ [3].

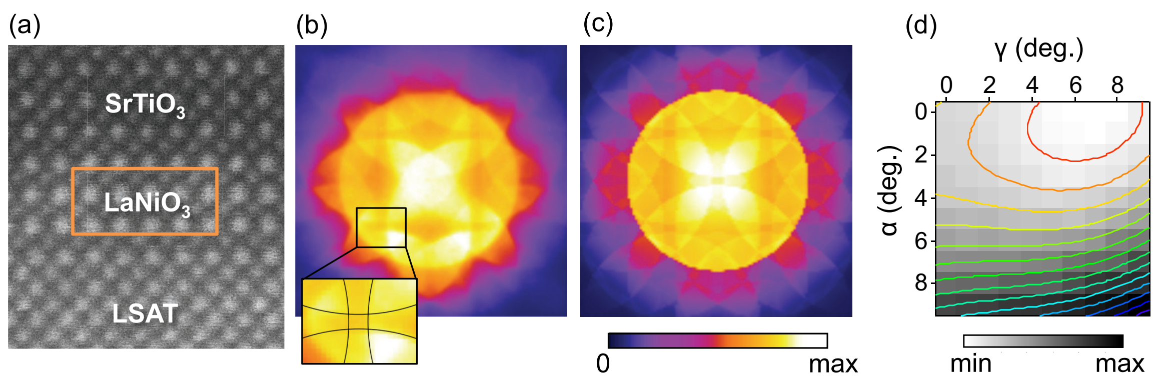

Fig. 2. (a) HAADF image of a $[LaNiO_3/SrTiO_3]_3$ superlattice. Orange block indicates the area where the PACBED was acquired. (b) Experimental PACBED patterns from the $LaNiO_3$ layer in the superlattice. Inset shows magnified portion of the PACBED showing the unit cell elongation in the growth direction. (c) A best matching simulated pattern to the experiment according to the (d) χ^2 map, which show the minimum (best match) at $\alpha = \beta = 0.5°$, $\gamma = 6.5°$ [4].

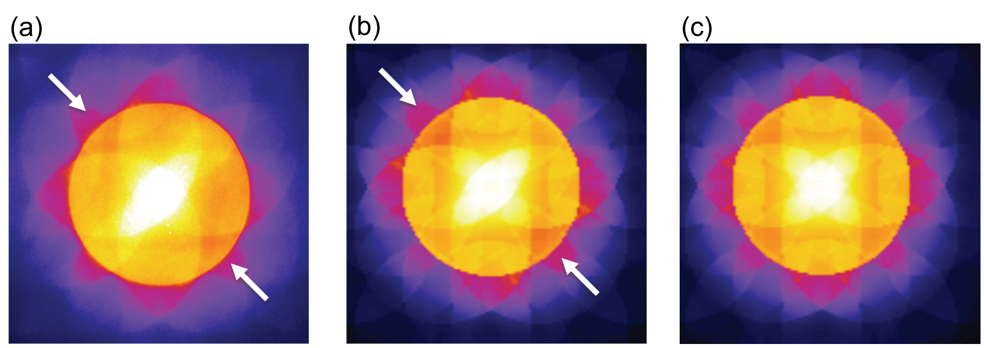

Fig. 3. (a) Experimental PACBED from $NdNiO_3$ films on $LaAlO_3$. Simulated PACBED patterns of (b) rhombohedral and (c) orthorhombic $NdNiO_3$. Arrows indicate the diagonal asymmetry that appears in rhombohedral patterns.

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