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Electronic Structure of New Line Defect in Strained $NdTiO_3$ on $SrTiO_3$

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$NdTiO_3$ is a Mott insulator with an orthorhombic perovskite structure [1] and $NdTiO_3/SrTiO_3$ heterostructure is of interest for a new platform material to study two-dimensional electron gases which can be produced by charge rearrangement and/or atomic reconstruction at the interface [2,3]. Our recent study has shown that high-quality stoichiometry-controlled $NdTiO_3$ film can be grown on $SrTiO_3$ by a hybrid molecular beam epitaxy approach and can generate high carrier density in room temperature [4]. Bulk orthorhombic $NdTiO_3$ (*Pbnm*) has lattice parameters a=5.525 Å, b=5.659 Å, and c=7.791 Å. It is useful to consider tetragonal lattice parameters $a_t=b_t=d_{110}$=3.953 Å and $c_t=d_{002}$=3.896 Å—where the subscript "t" represents tetragonal lattice—since the tetragonal unit in the $NdTiO_3$ lattice is analogous to the $SrTiO_3$ cubic lattice (a=3.905 Å). When it is grown on a $SrTiO_3$, it yields strain to accommodate the lattice mismatch with the substrate. According to our scanning transmission electron microscopy (STEM) analysis, the $NdTiO_3$ film grows on the $SrTiO_3$ (001) with a specific crystallographic orientation—a_tc_t plane as in-plane of the heterostructure and b_t as out-of-plane direction. Interestingly it is found that the strain in the $NdTiO_3$ film interplayed with stoichiometry supplies driving force to form a new type of line defect to adapt the strain (Figure 1). Here, we present the analysis of the atomic and electronic structure of the line defect using analytical STEM with the assistant of density functional theory (DFT) calculation.

High-angle annular dark-field (HAADF) STEM imaging, energy dispersive X-ray spectroscopy (EDX), and electron energy-loss spectroscopy (EELS) were performed using an aberration-corrected monochromatic FEI Titan G2 60-300 STEM equipped with a CEOS DOCR probe corrector, Super-X EDX spectrometer, and Gatan Enfinium ER spectrometer. First-principles calculations were performed in the framework of DFT as implemented in Vienna *ab initio* Simulation Package (VASP) code [5].

The defect has been detected in HAADF-STEM images viewed only along the c_t-axis, indicating that the line defect is parallel to the c_t-axis (Figure 1), which is in agreement with energy calculation results. The determined structure of the defect is described in Figure 1b and is known to have a relatively relaxed Ti-deficient structure (from EDX, not shown here). This defect structure is energetically more favorable than a strained structure without the defect. The calculated oxygen partial-density of states (DOS) and experimental O *K* core-loss EELS spectra show good agreement (Figure 2) and further confirm the validity of the determined defect structure. EELS and DFT calculation results indicate that Ti atoms in the core of the line defect have Ti^{4+} character in contrast to Ti^{3+} in the bulk structure, meaning alterations of the DOS and narrowing of $NdTIO_3$ band gap occurred with defect formation. We also expect that other perovskite materials can possibly have this type of defect when they have proper amount of strain and certain crystallographic growth direction on substrates [6].

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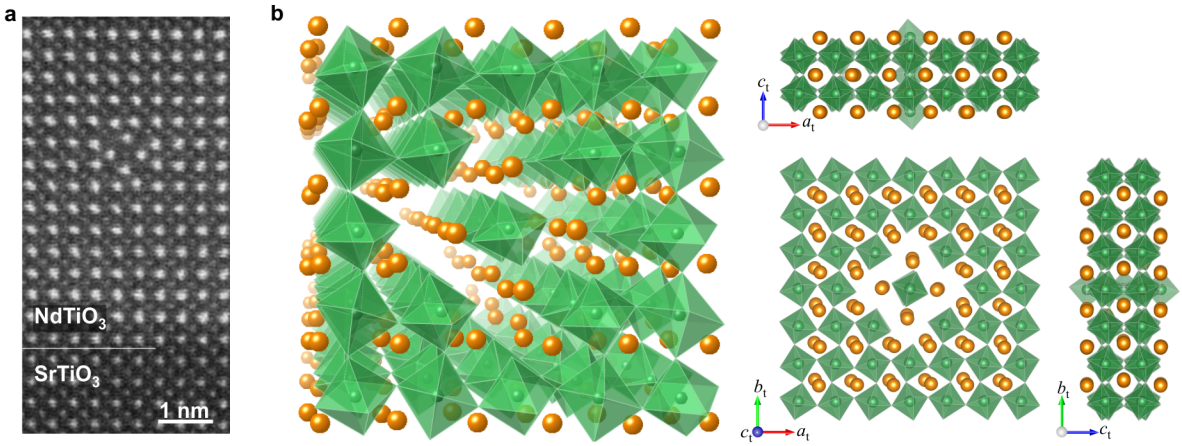

Figure 1. (a) HAADF-STEM image of a line defect in a NTO film on a STO substrate, where the NTO film is viewed along the c_t axis. (b) Perspective atomic model for the defect and its a_t, b_t, and c_t axis projections. Yellow spheres are Nd and green octahedrons represent Ti coordinated by six O.

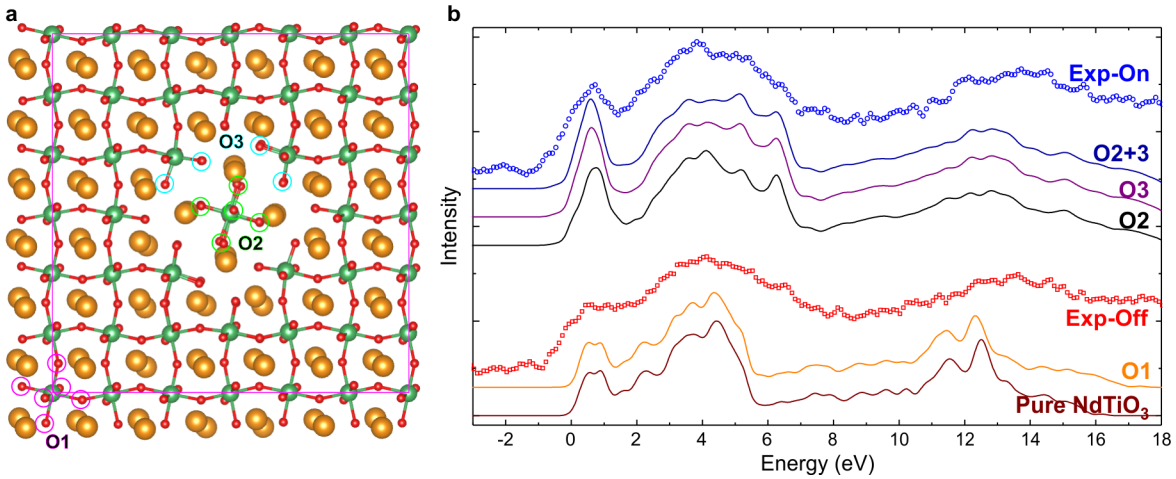

Figure 2. (a) c_t axis-projected defect supercell (supercell boundary is presented by the pink box) for DFT calculation, where each position of O of interest are indicated. (b) Experimental O *K* core-loss EELS fine structures and calculated O partial-DOS; "Exp-On" and "Exp-Off" represent experimental EELS on and off the defect and the calculated partial-DOS for the O positions in (a) are accordingly labeled. The calculated O partial-DOS for pure $NdTiO_3$ is also presented.