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Characterization and Growth of Quad Unit Cell Linear Defects in Potassium Tantalate

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Perovskite oxides are functional materials with current and potential industrial applications. These materials have demonstrated many useful and novel properties, including two-dimensional (2D) superconductivity at heterogeneous interfaces [1], high piezoelectric responses [2], and tunable ferroelectricity [3]. The properties can be tuned by modifying the structures, for example, controlling the level of oxygen vacancies can tune the charge carrier concentration [4], local strain can modify the polarization patterns, and varying the composition changes the curie temperatures. Defects and structural fluctuations also play important roles in determining the electronic structures, such as the new polarization states. To design new functional oxides, not only correlating the structure with the properties is important, understanding the formation of the defect states is also critical. However, discovery and characterization of the defects remain challenging. Here we show the visualization of the formation of linear defects in potassium tantalate ($KTaO_3$) using atomic resolution scanning transmission electron microscopy (STEM) and studies of the strain and polarization states using four-dimensional (4D) STEM.

$KTaO_3$ is a paraelectric perovskite oxide, with K at the A sites and Ta at the B sites. Recently it was discovered that 2D superconductivity exists along its interfaces with EuO and $LaAlO_3$. Engineering novel strain and electronic states inside this wide bandgap material may also prove key to unlocking future possibilities. The STEM samples of $KTaO_3$ were prepared by thinning a single crystal with the [001] in the plane of the wafer, followed by wedge polishing before ion milling in a Gatan PIPS II. The final thickness of the sample is about 5-20 nm with suitable flatness. Atomic resolution STEM and 4D-STEM Data sets were acquired using an aberration corrected FEI-Titan STEM operated at 200 kV outfitted with a 128 x 128 pixel EMPAD detector as the diffraction camera.

In this work, unlike prior defects under study in perovskite materials which are the result of strain, stoichiometry, or other conditions during growth [5], the defects, found in $KTaO_3$, are formed in-situ using the driving force of the electron probe in STEM. Using medium-angle annular dark field (MAADF) and integrated differential phase contrast (iDPC) we are able to present images of the formation of these defects, which can be grown in-situ in targeted locations. As shown in Fig.1, the novel one-dimensional (1D) line defect in $KTaO_3$ emerges by the removal of K atoms, resulting in a 45 degree shift in the Ta column positions around a center. EDS and EELS mapping were used to provide information on the elemental composition and mechanism for these structures. Combining the elemental data with intensity analysis of MAADF data acquired during growth of a defect, by tracking the image intensity of individual atomic columns in Fig.2, it can be demonstrated that the Ta columns shift in a layer by layer transformation that propagates along the beam direction. Strain mapping and polarization measurement of the region close to the defects reveals new polarization states. In situ results showing the control of defect formation with larger sizes will also be discussed in the presentation [6].

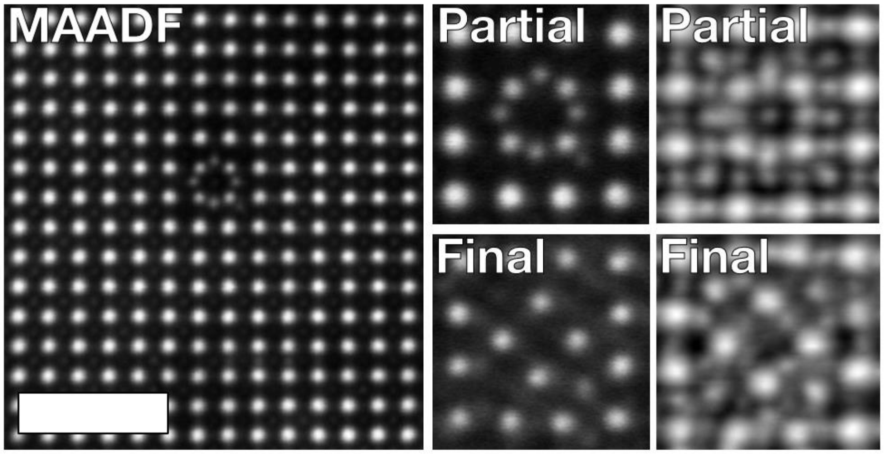

Figure 1. (left) MAADF image of an isolated linear defect (2 nm scale bar). (right) MAADF and iDPC images showing the oxygen and potassium position shifts during the formation of the defect.

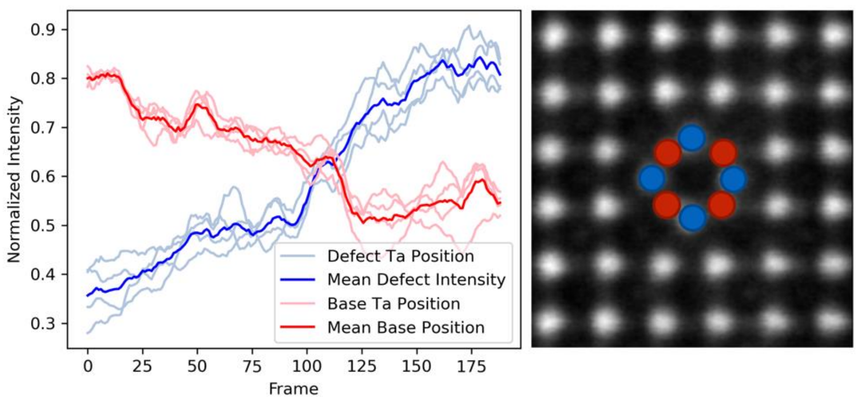

Figure 2. (left) Intensity analysis of the base Ta positions and defect positions from a MAADF data series of 200 frames. (right) Column assignments for the base and defect sites.

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[6] The electron microscopy was carried out at the Analytical Instrumentation Facility (AIF) at North Carolina State University, which is supported by the State of North Carolina and the National Science Foundation (award number ECCS-2025064). The AIF is a member of the North Carolina Research Triangle Nanotechnology Network (RTNN), a site in the National Nanotechnology Coordinated Infrastructure (NNCI).

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