Characterization of Strongly Correlated $Ca_3(Ru_{0.95}Ti_{0.5})_2O_7$ Domain Walls using Cryogenic High-Resolution STEM

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Correlated electronic perovskite oxides exhibits diverse phase diagrams, including ferroelectricity [1,2], magnetism [3], spin orbit coupling [4], charge density waves [5], metal to insulator transitions [3,6] and superconductivity [7,8]. An important unanswered question in this field is understanding the role domain walls play in the nucleation kinetics of these phases. In order to understand and exploit these extravagant phases, they must be observed in the vicinity of the phase transition, which mostly occur between room and liquid nitrogen temperatures. Because of advancements in drift correction in post processing and during acquisition, it is now possible to explored these regions of the correlated phase diagram [9,10] using aberration corrected scanning transmission electron microscopy (AC-TEM). This study will focus on combining cryogenic electron microscopy with emerging 4D-STEM techniques and electron energy loss spectroscopy (EELS) to understand the structure-property relationship of $Ca_3(Ru_{0.95}Ti_{0.5})_2O_7$ at a cryogenic temperature.

$Ca_3(Ru_{0.95}Ti_{0.5})_2O_7$ is of interest because it has a layered Ruddelsden-Popper structure and it exhibits a room-temperature metallic state and undergoes a sharp Mott Metal-Insulator Transition (MIT) at ~110 K [11]. Further, the previous room temperature measurements (Fig. 1) show that this material is isostructural to the improper ferroelectric $Ca_3Ti_2O_7$ at room temperature, suggesting that this is a “polar metal” at high temperatures, and ferroelectric below room temperatures [12]. Understanding the atomic structure, composition, electronic, and local symmetry in both the metallic and insulating phase will help to unlock the nature of this fascinating material.

Reference

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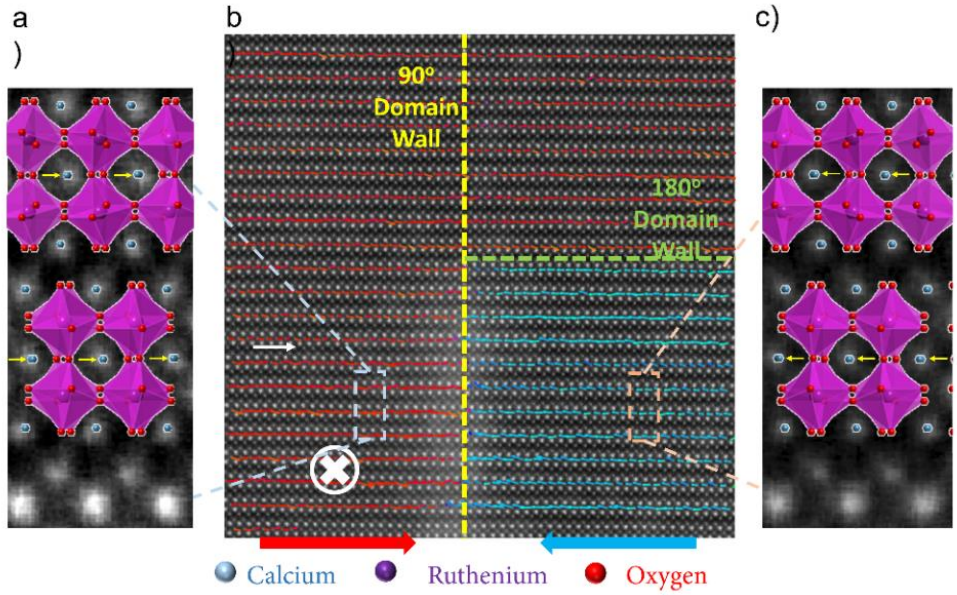

Figure 1. a) Zoomed in ADF–STEM image of $Ca_3Ru_{1.9}Ti_{0.1}O_7$ showing the ruthenate octahedra tilted left. Yellow arrows demonstrate the polar bending of the calcium columns. **b)** ADF-STEM image of $Ca_3Ru_{1.9}Ti_{0.1}O_7$ showing a domain junction with 90^0 and 180^0 domain walls. Calcium column displacement vectors are overlaid on top, with red pointing left and blue pointing right. **c)** Zoomed in section of ADF–STEM image showing ruthenate octahedra tilted right, with the yellow arrows demonstrating the corresponding polar displacement of calcium columns.