Visualizing Nanoscale Coexistence of Competing Phases In Ca_2RuO_4

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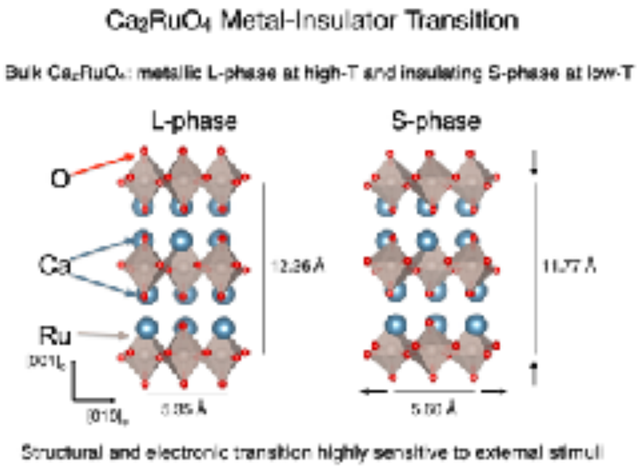
Introduction

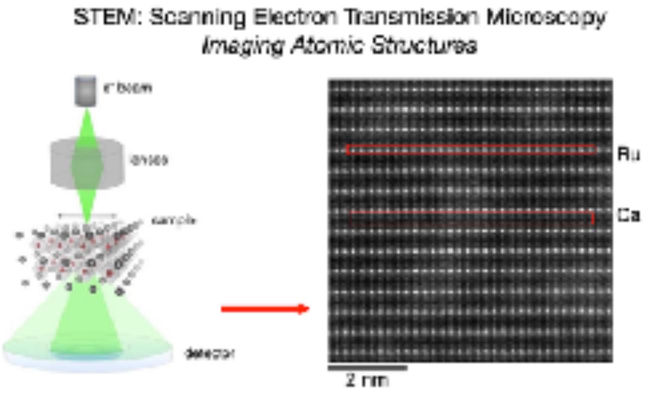
While most materials are either metallic or insulating, some materials exhibit a metal-insulator transition (MIT), a phase transition where a material switches from a metal to an insulator accompanied by a change in atomic scale structure. Metal-insulator transition materials have the potential to enable emerging technologies such as neuromorphic computing, but this will require a deep understanding of how these materials can be controlled by various external stimuli.

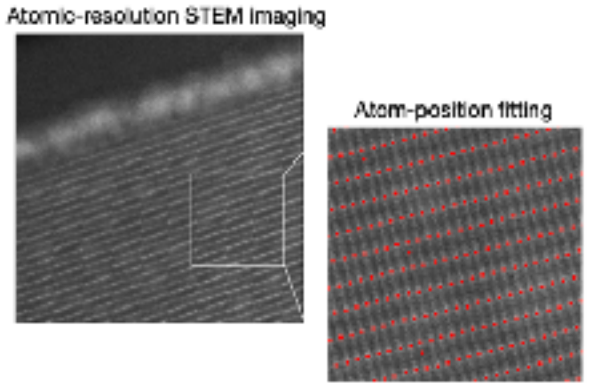


The 2D perovskite oxide Ca_2RuO_4 exhibits a metal-insulator transition, and the transition temperature can be tuned with epitaxial strain. Notably, compressively strained films grown on $LaAlO_3$ do not have a uniform transition in between phases, resulting in coexisting metallic and insulating areas of the film below the transition temperature. These phases can be differentiated by a change in lattice parameters — the metallic phase is stretched along the out of plane [001] direction. Here, this phase coexistence was measured with cryogenic scanning transmission electron microscopy (STEM), allowing the atomic scale features of the metal-insulator nanostructure to be characterized.

Methodology

Images of Ca_2RuO_4 were acquired with cryogenic high angle annular dark field STEM at ~100 K to directly visualize calcium ruthenate's atomic structure.

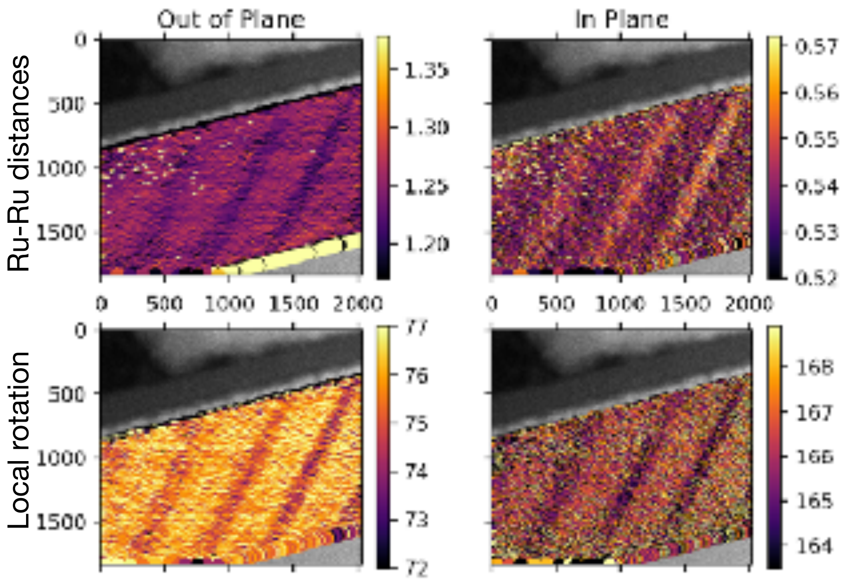




The STEM images went through a variety of processing steps to precisely identify the positions of the most prominent atom, Ruthenium, with the Python package STEMTool.

Several algorithms were then developed to identify locally variance in the film structure. In particular, distances and angles between ruthenium sites were calculated allowing local changes in the lattice parameters to be seen, visualizing the coexisting metallic and insulating domains present in the material.

Results



Visualizing the measured spacings of each Ruthenium site to its neighbors normal to the (001) plane ("out of plane") and in the (001) plane ("in plane"), striped domains with shorter out of plane and longer in plane lattice parameters can be seen revealing the phase coexistence.

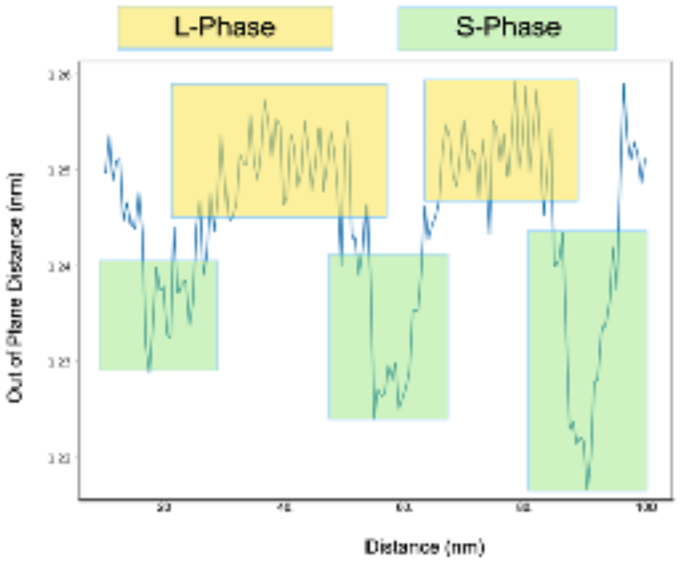
The change in lattice parameters is consistent with the narrow stripes belonging to the insulating S phase, while the surrounding film is the metallic L phase.

Mapping the local rotation of the lattice, a corresponding mis-orientation is measured along each of the stripes.

To investigate the nature of the interface between the coexisting phases, the out of plane Ru-Ru distance was profiled along the stripes, visualizing the change in the lattice parameter inside and outside of the stripes.

Consistent with the maps of the lattice parameter above, the stripes are clearly visible as significant reduction in the out of plane lattice parameter from ~1.25(5) nm in the L phase matrix to ~1.23(0) nm in the S phase stripes.

Intriguingly, the interfaces between the phases are not sharp — instead, the lattice parameter gradually changes over 2-5 unit cells.



Conclusions and future work

Characterizing the coexisting metallic and insulating phases and quantifying the nanoscale structure of Ca_2RuO_4 helps us to understand the material's metal insulator transition. Looking forward, this work will be expanded upon to characterize the structure and in particular the interfacial reconstructions at higher precision. In addition, for this study other areas of the film were not able to be analyzed because of severe defects in the atomic structure, however the phase coexistence in these areas must also be characterized to understand how the transition is modulated by defects in the lattice.