Department of Materials Science and Engineering,

PhD Defense

June 16, 10:00 AM

Zoom Meeting
https://drexel.zoom.us/j/99107996915?pwd=VVVHemN1bTI5MnBHSkxxNWFGb0U1UT09
Meeting ID: 991 0799 6915
Password: 261325

Processing of Epitaxial Oxyfluoride Films and Characterization of Their Physical Properties

Jiayi Wang
Advisor: Steven J. May, Ph.D.

Abstract

Controlling the carrier concentration in electronic materials via doping is of fundamental importance in engineering physical properties for applications in electronic devices. In ABO_3 perovskites, altering the electron count on the *B*-site cation is typically achieved through *A*-site cation substitution. In contrast, there has been less exploration of anion substitution. For example, F^- substitution for O^{2-} provides an alternative

means to tailor the nominal *B*-site valence, the ionicity of the *B*-O bond, and the lattice volume. In the study of anion substitution, while bulk oxyfluorides have received interest over the last two decades, epitaxial perovskite oxyfluorides have only been reported in recent years. The goal of this project is to develop a mechanistic understanding of topotactic fluorination reactions in epitaxial perovskite films and the resultant effects on physical properties of the incorporated F content.

In this work, I demonstrate a highly controllable fluorination process using as-grown $SrMnO_{2.5}$ epitaxial thin films as a model system with polytetrafluoroethylene (PTFE) as F source. The F content is systemically controlled by the fluorination time. The F is found to incorporate by substituting for the in-site O, which provides a means of electron doping the transition metal perovskites. Upon fluorination, a *c*-axis expansion, resistivity increase, and blue-shift of the optical absorption features are observed. In addition, the F/O site occupancy in the $SrMnO_{2.5-\delta}F_{\gamma}$ epitaxial thin film is successfully engineered using substrate-induced biaxial strain. The F is found to have an apical site preference under compressive strain while it has an equatorial site preference under tensile strain. This is the first report of the strain-induced anion arrangement in oxyfluoride thin films. The *B*-cation alloyed $SrFe_xMn_{1-x}(O,F)_{3-\delta}$ system with different Fe substitution level is also investigated to reveal the *B*-cation and anion composition influence on structural, electronic, and optical properties.