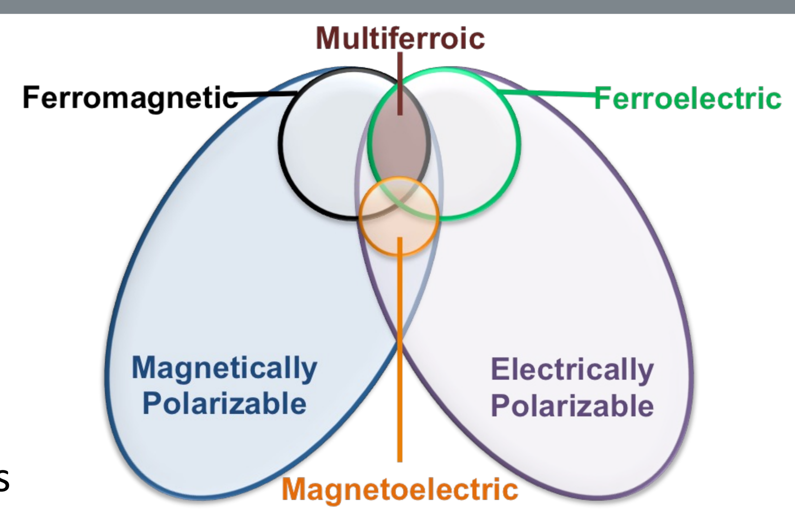
Epitaxial stabilization of the hexagonal polymorph of $ScFeO_3$

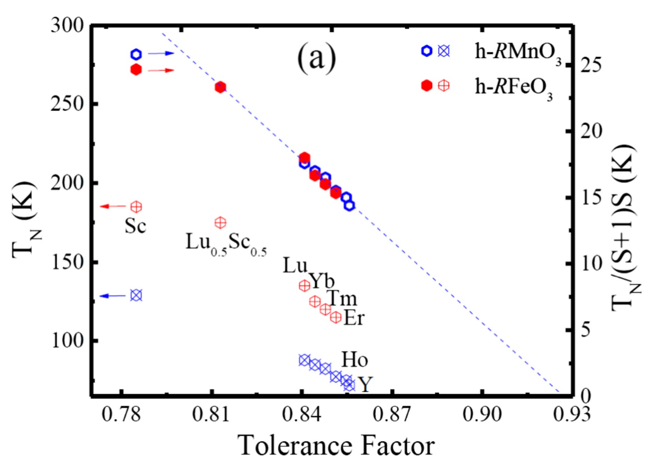
N. D. Redwing[1], N. A. Parker[2], J. R. Wright[3], M. R. Barone[2], and D. G. Schlom[2]
[1]Department of Materials Science and Engineering, Pennsylvania State University
[2]Department of Materials Science and Engineering, Cornell University

Introduction

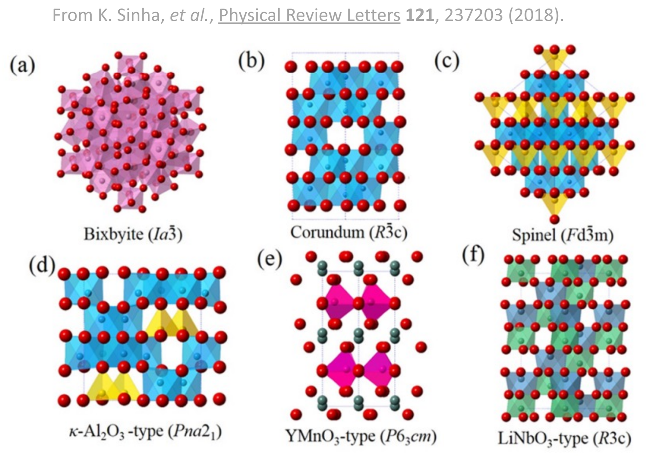
- **Ferroelectric** materials exhibit spontaneous and switchable polarization through an external electric field
- **Ferromagnetic** materials instead have spontaneous and **switchable** magnetism with a magnetic field
- **Coupled multiferroic** materials (in this case ferromagnetoelectric), allow for the control of both polarization and magnetization by both fields **simultaneously**. This leads to potential use in devices that already use either property



From Complex Oxide Superstructures & Emergent Phenomena Research Group, Tsinghua University



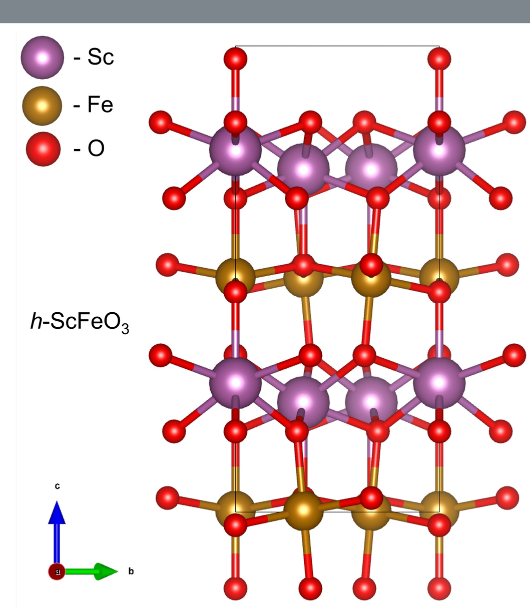
From K. Sinha, et al., Physical Review Letters 121, 237203 (2018).



From Y. Hamasaki, et al., Crystal Growth & Design 16(9), 6214-5222 (2016).

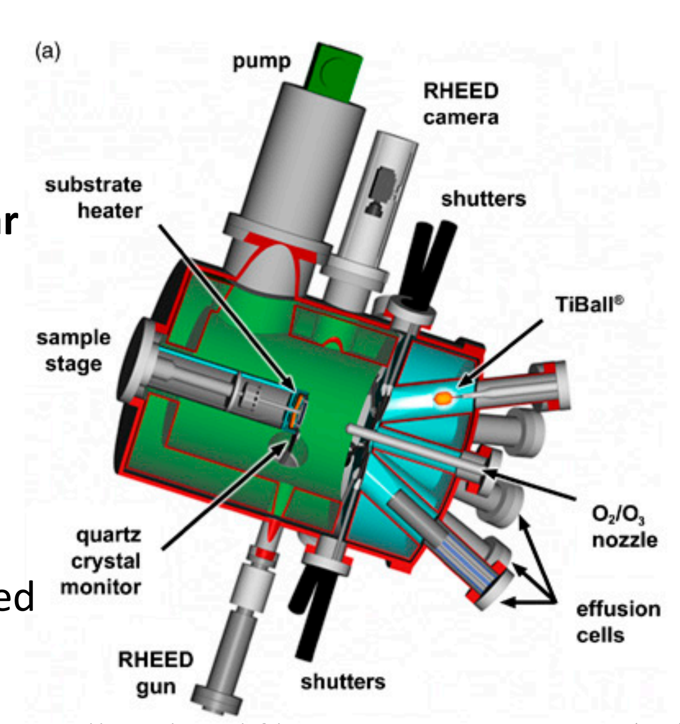
- **Hexagonal rare earth ferrites** are a group of materials that exhibit coupled multiferroic behavior under a certain transition temperature, the **Néel temperature** (T_N)
- The Néel temperature of the rare earth ferrites have been previously reported to increase linearly relating to a decrease in A-site rare earth ionic radius
- **Hexagonal scandium ferrite (*h*-$ScFeO_3$)** has high interest due to scandium's small ionic radius compared to other rare earth elements, allowing for a transition temperature potentially near room temperature
- Previous attempts to synthesize $ScFeO_3$ produced transition temperatures much lower than expected, indicating potential improvement through phase pure, properly ordered *h*-$ScFeO_3$

Molecular Beam Epitaxy



- One potential Multiferroic, $ScFeO_3$, in it's hexagonal polymorph is characterized by its **alternating stacking layers** of scandium oxide and iron oxide
- Precise **stoichiometry** and ordered layering required to stabilize hexagonal polymorph, else the ground state bixbyite polymorph begins to form

- To control stoichiometry and create layered growth, **molecular beam epitaxy (MBE)** is used as deposition method
- MBE uses elemental sources heated at high temperatures to create a molecular beam whose flow is controllable through shuttering
- Through alternating shuttered deposition, layered hexagonal structure is **epitaxially stabilized** on substrate
- To allow for *h*-ScFeO3 nucleation, $ScFeO_3$ is epitaxially stabilized on substrate of significant lattice mismatch
- **C-plane Al_2O_3 (0001)** was used to due small mismatch (5.3%) compared to in-plane lattice parameter of *h*-$ScFeO_3$

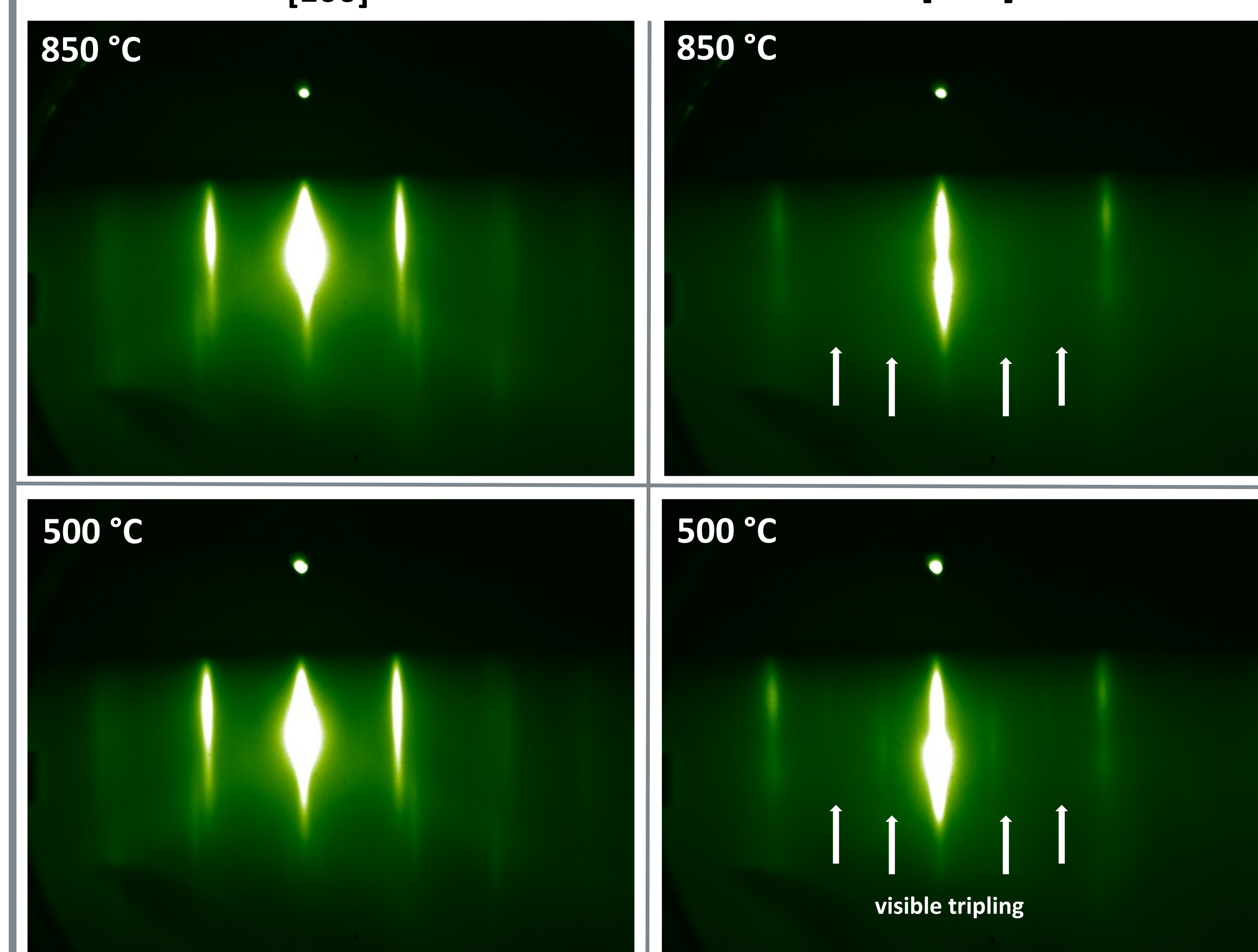


From D. Schlom, et al., Journal of the American Ceramic Society, 91, 2429-2454 (2008).

Characterization and Results

RHEED Analysis

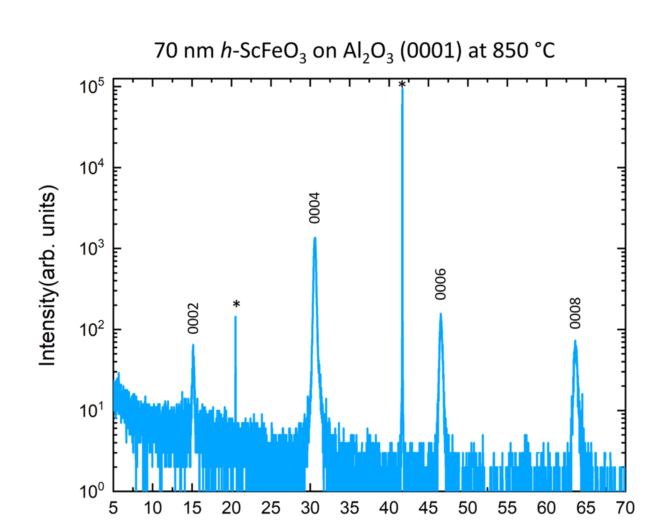
70 nm *h*-$ScFeO_3$ on Al_2O_3 (0001)

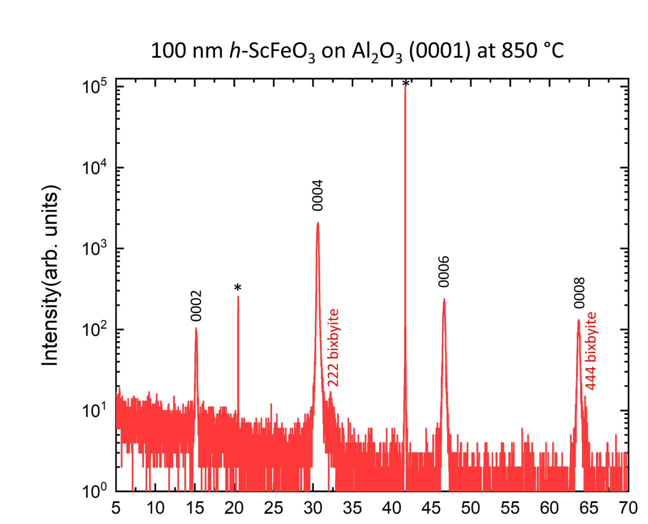


- In-situ characterization of material depending on diffraction pattern
- Presence of *h*-$ScFeO_3$ deposition observed using diffraction line spacing during growth
- Tripling appearing during cool down indicates asymmetric hexagonal polymorph on sample surface

X-ray Diffraction

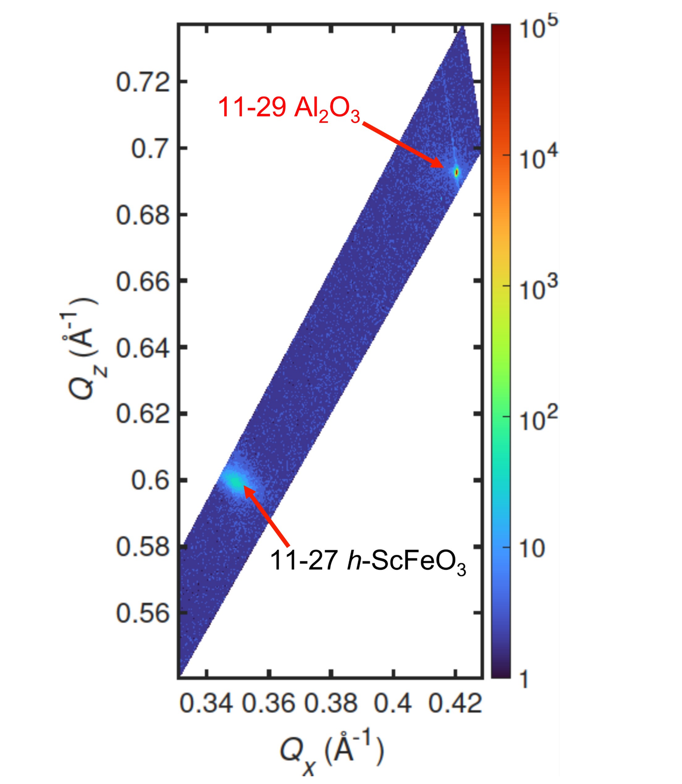
- XRD diffraction patterns indicate that *h*-$ScFeO_3$ was successfully deposited with no apparent impurities at thicknesses **up to 70 nm**
- At thickness greater than 70 nm, $Fe3O_4$ or bixbyite impurities begin to dominate the spectra

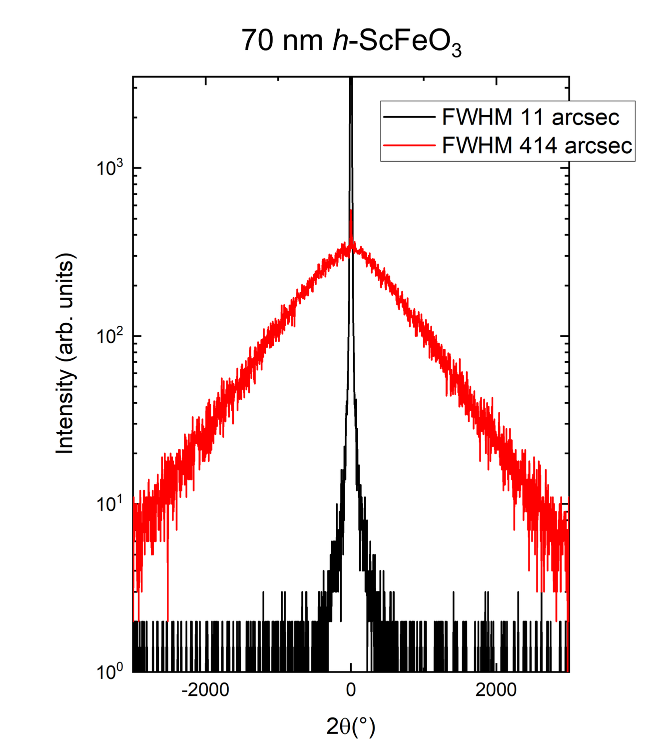




Reciprocal Space and Crystallinity

- Reciprocal space mapping of 70 nm sample showed difference in in-plane lattice parameter, indicating epitaxial stabilization
- Compactness of *h*-$ScFeO_3$ points show overall crystallinity of film

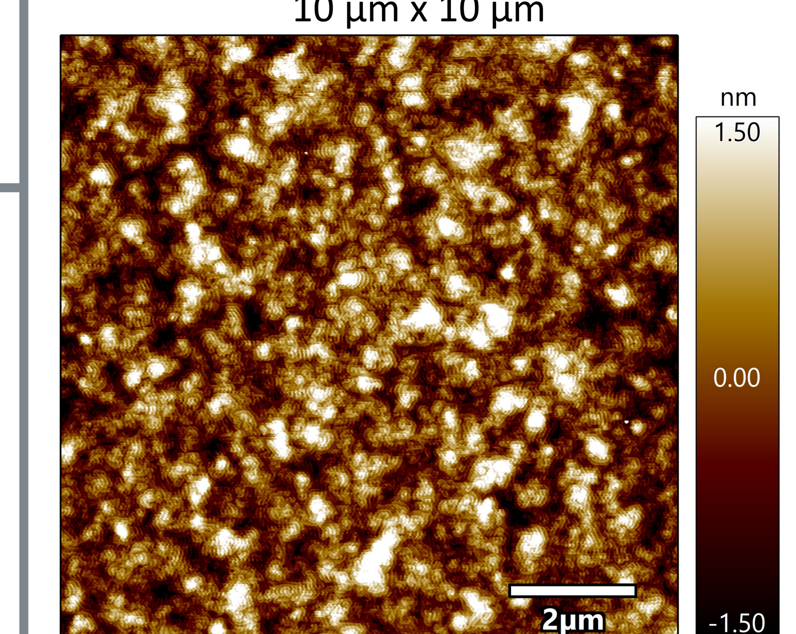




- Rocking curve of 0004 *h*-$ScFeO_3$ x-ray peak displayed wide outer peak, indicative of complete relaxation
- Central thin inner peak points to crystallinity of grown film

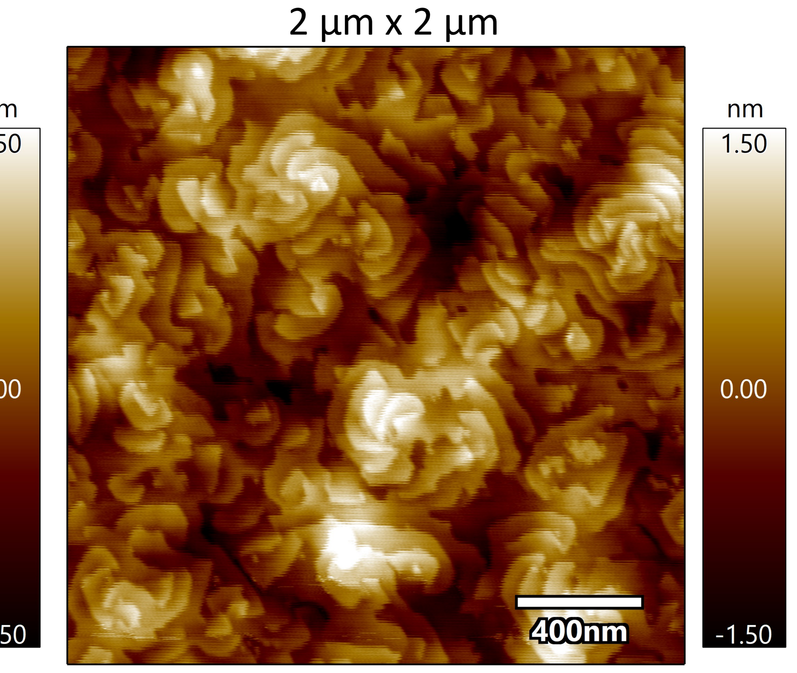
Atomic Force Microscopy

10 μm x 10 μm



RMS: 579 pm

2 μm x 2 μm



RMS: 449 pm

- No impurities visible during AFM imaging of 70 nm sample
- Overall RMS indicates smooth surface of film

Summary

- Through Molecular Beam Epitaxy, *h*-$ScFeO_3$ was epitaxially stabilized on Al_2O_3 (0001)
- In-situ and ex-situ characterization confirmed purity and crystallinity
- Atomic Force Microscopy further indicated lack of impurities and smoothness
- Up to 70 nm of pure-phase *h*-$ScFeO_3$ was deposited onto substrates
- Future magnetic analysis will determine transition temperature of deposited material

NSF Grant DMR-2104918