Interfaces in Complex Functional Oxides

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Background

Epitaxial heterostructures as model systems
Role of defects
Reliability and Yield

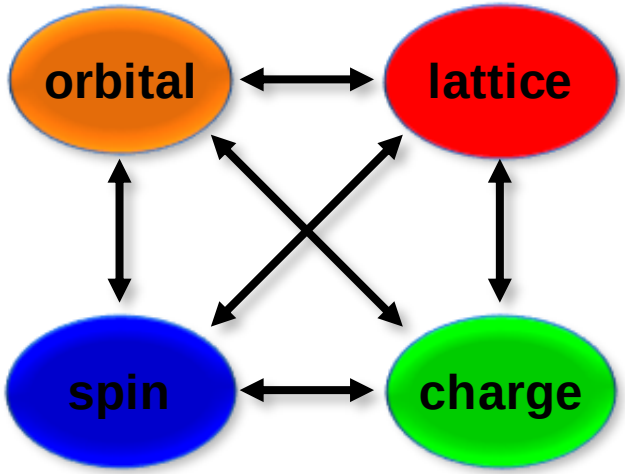
Complex Oxides : Many Possibilities

A-site (La) Oxygen

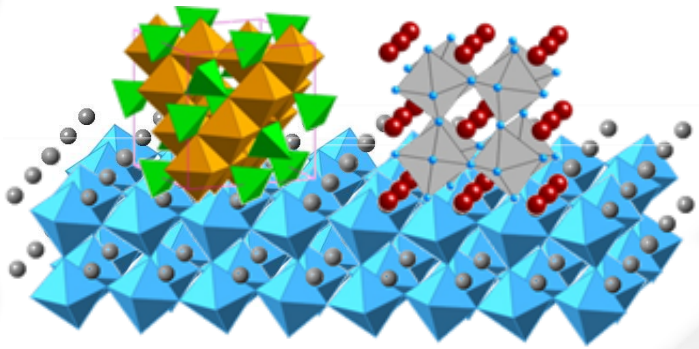
- Superconductors (YBCO)
- Ferroelectrics ($BaTiO_3$)
- Colossal Magnetoresistance ($(La,Sr)MnO_3$)
- Multiferroics ($BiFeO_3$)
- Topological Insulators ($Y_2Ir_2O_7$)
- Thermoelectrics (doped $SrTiO_3$)
- Ferromagnets ($SrRuO_3$)
- Photovoltaics (copper oxides)

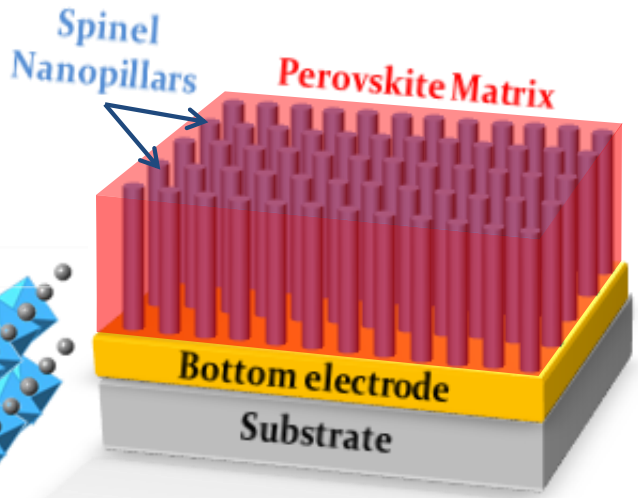
A huge range of oxide crystals : pyrochlores, layered structures, spinels, rock salt, …

Creating Coupled Systems



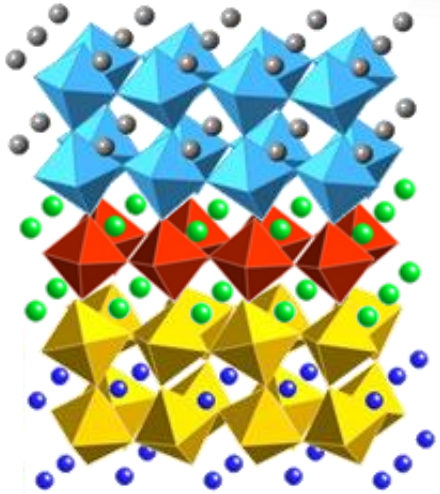
I. Interface-mediated functionality

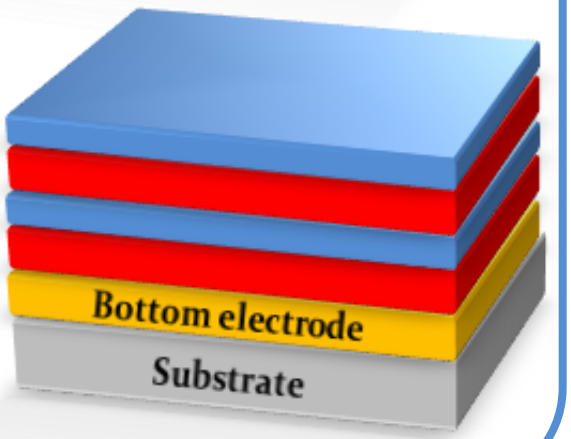




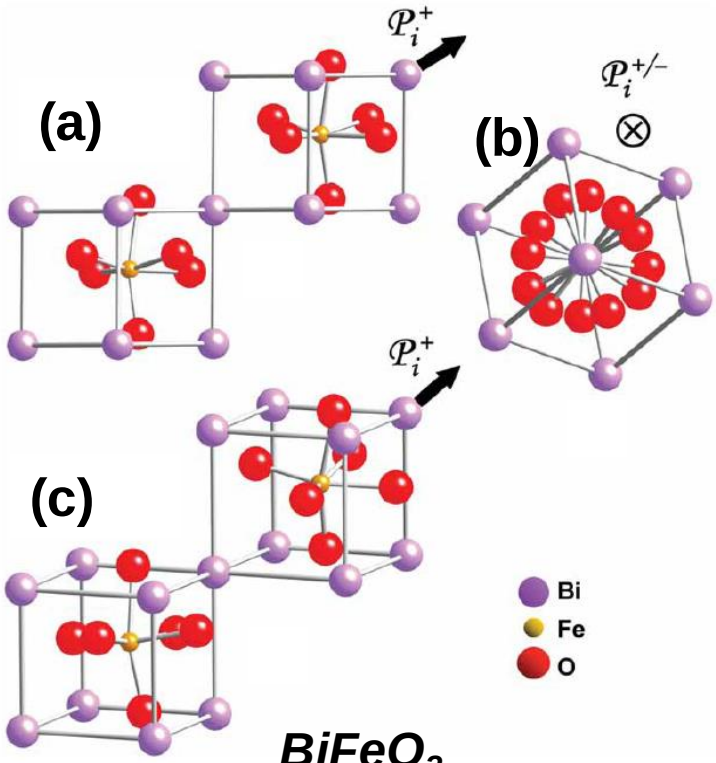
Energy Conversion/ Transduction
Field Tunable Photonic Bandgap Structures
Information Storage
Radiation Sensing
Energy Storage

II. Functional interfaces





Bismuth Ferrite, $BiFeO_3$: Model Multiferroic

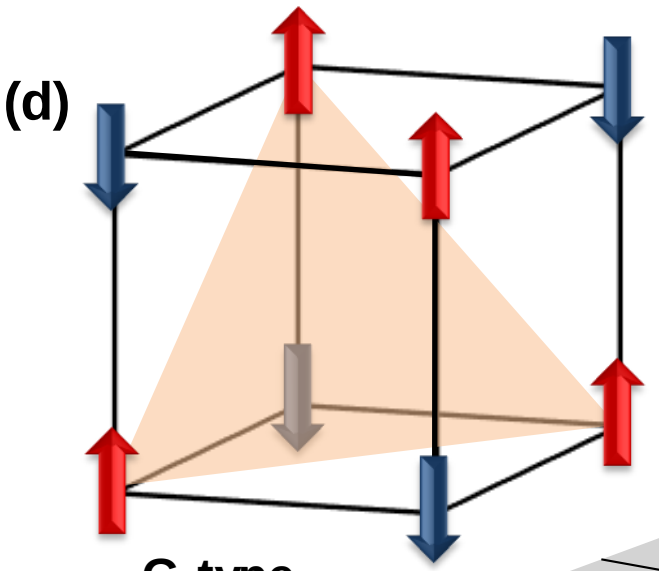


$BiFeO_3$

Rhombohedral, *R*3*c*

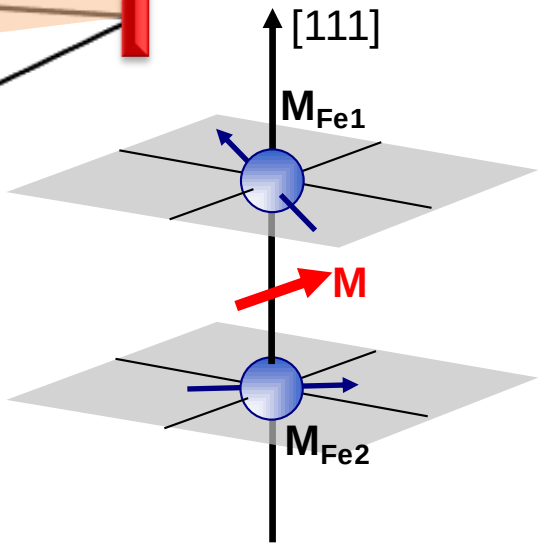
a_{hex} = 5.58 Å; c_{hex} = 13.86 Å

a = 3.96Å, a_r = 0.6°

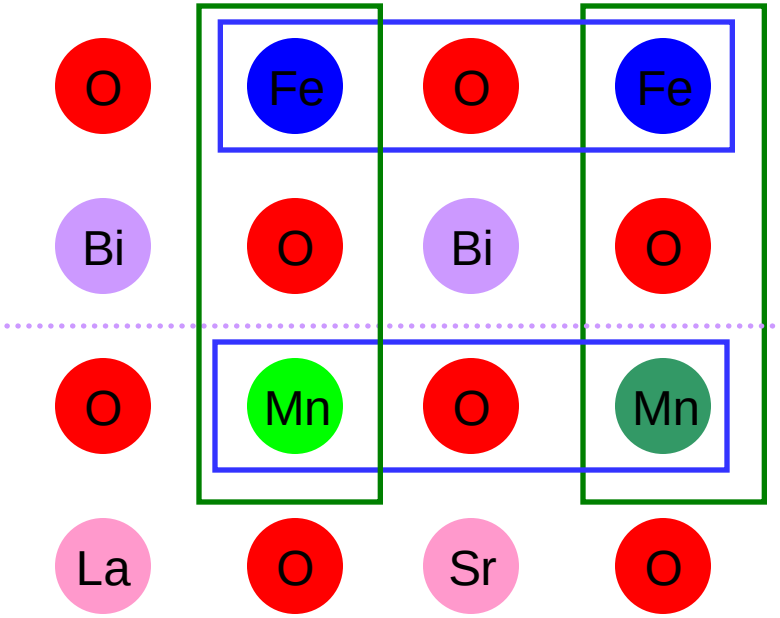


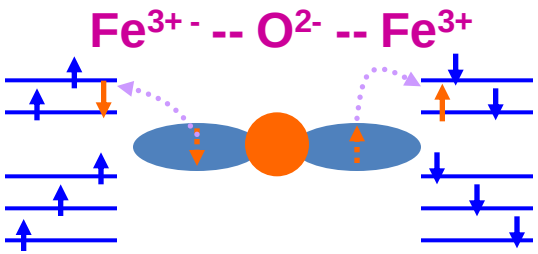
Weak Ferromagnetic Moment

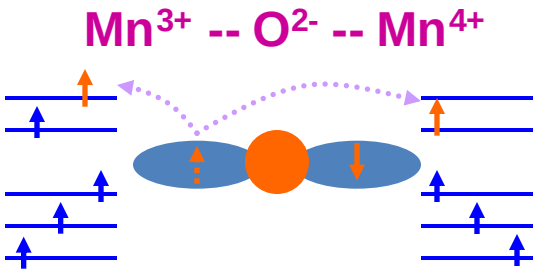
G-type Antiferromagnetic Order

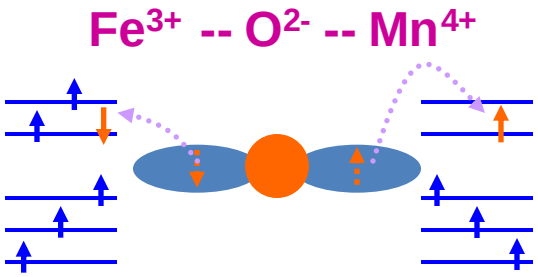


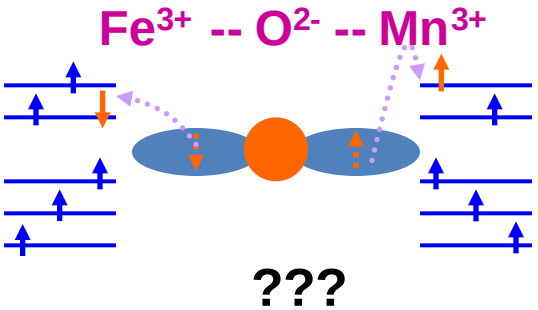
Interfaces III: Artificial Interfaces





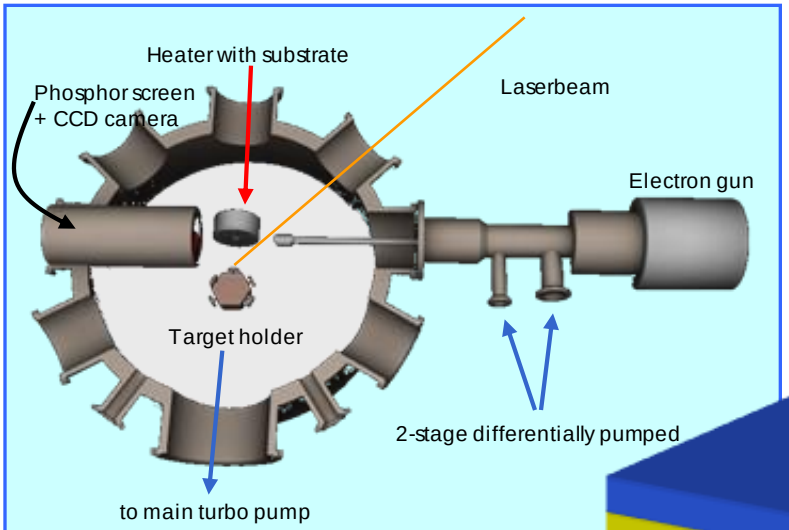






--- what's the coupling mechanism at the interface ?
--- Role of Orbital physics ?
--- can we use an electric field to control this coupling ?

Creating and Understanding Interfaces



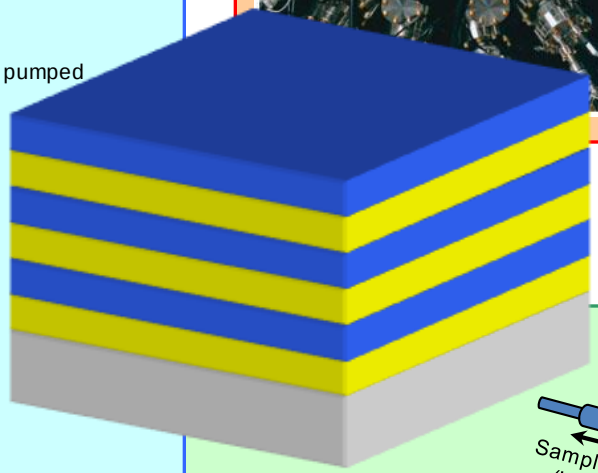
Laser-MBE

- Highly controlled growth
- Controlled interfaces

MBE

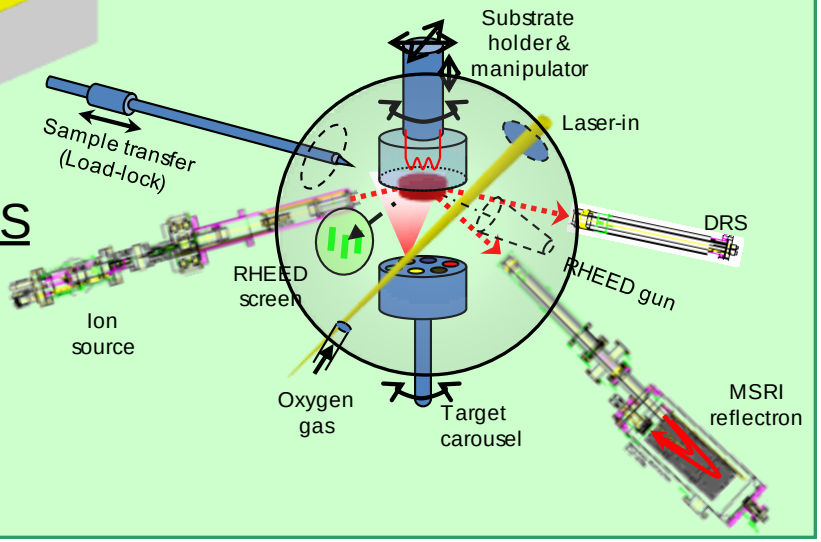
e.g., Schlom Group

- Highly controlled growth
- Extremely high structural quality

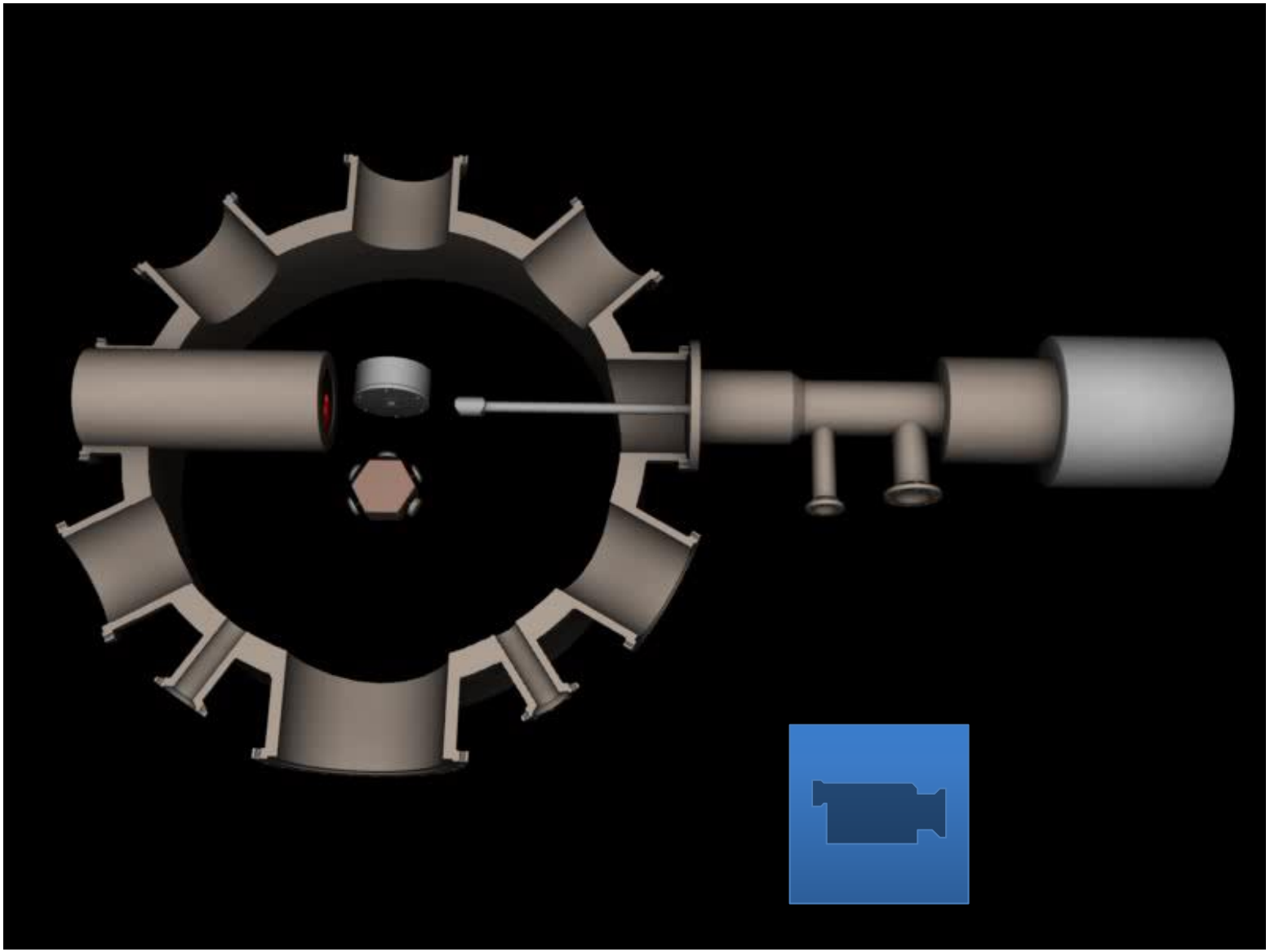


RHEED, TOF-ISARS

- Highly controlled growth
- Interface chemistry

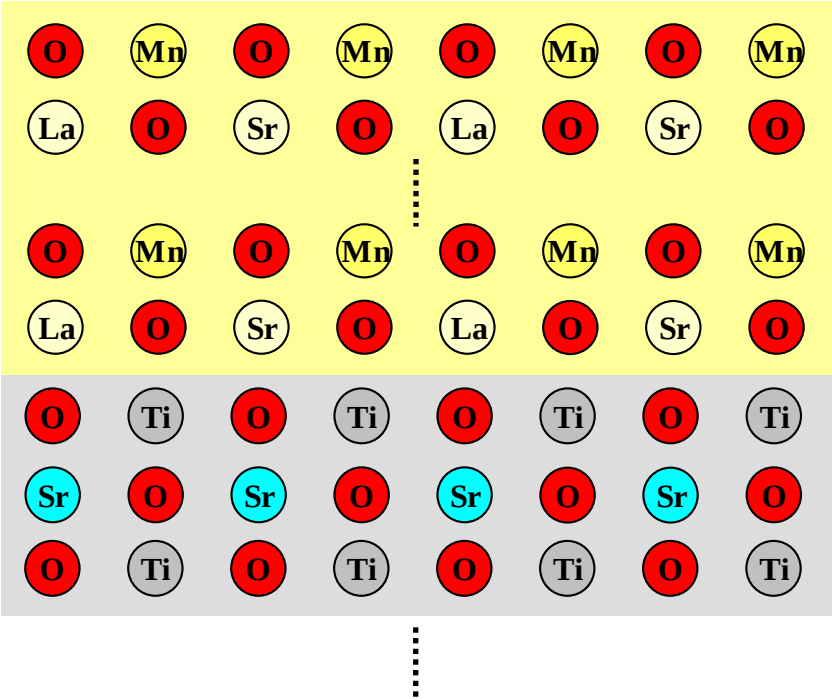


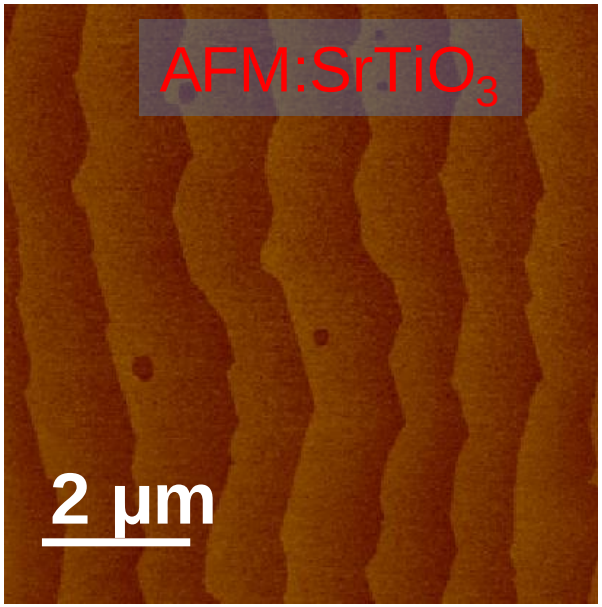
Atomic Control of Oxide Heterostructures

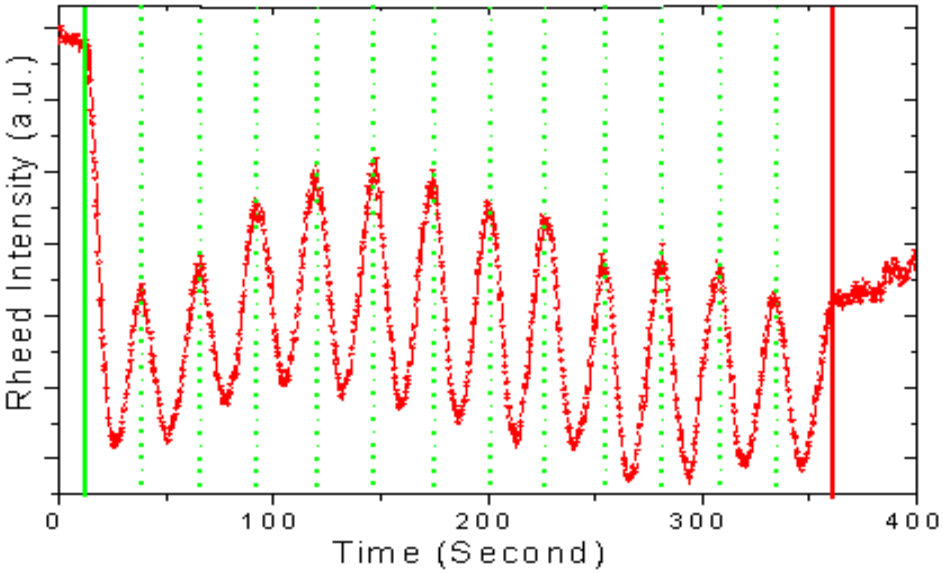


J. Huijben,…, D. Blank, Univ. of Twente

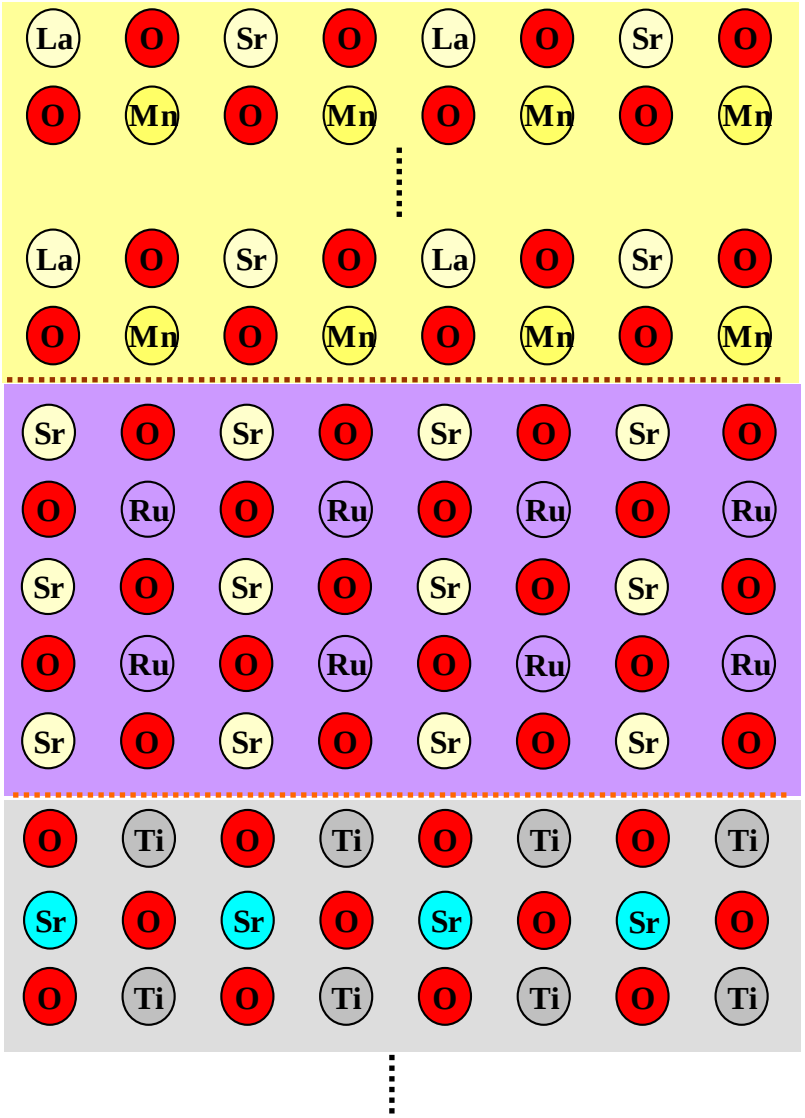
All Oxide Interfaces : BFO/LSMO



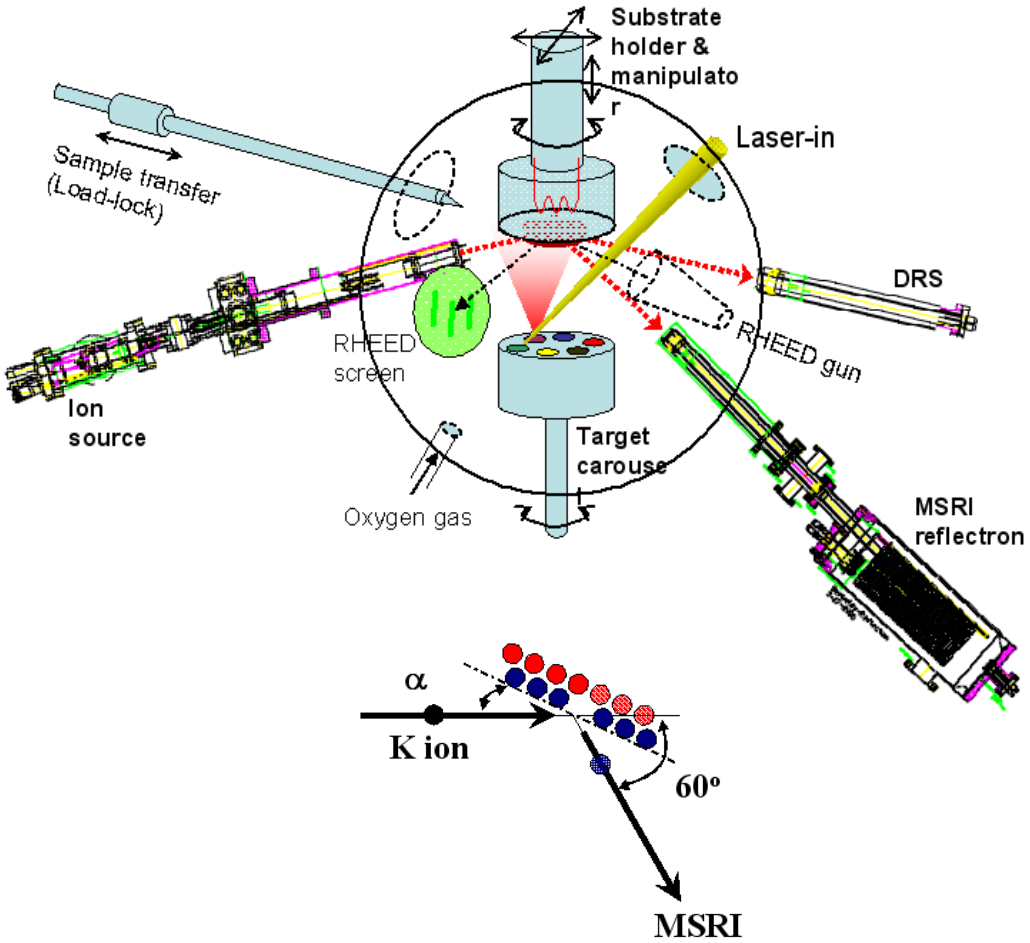




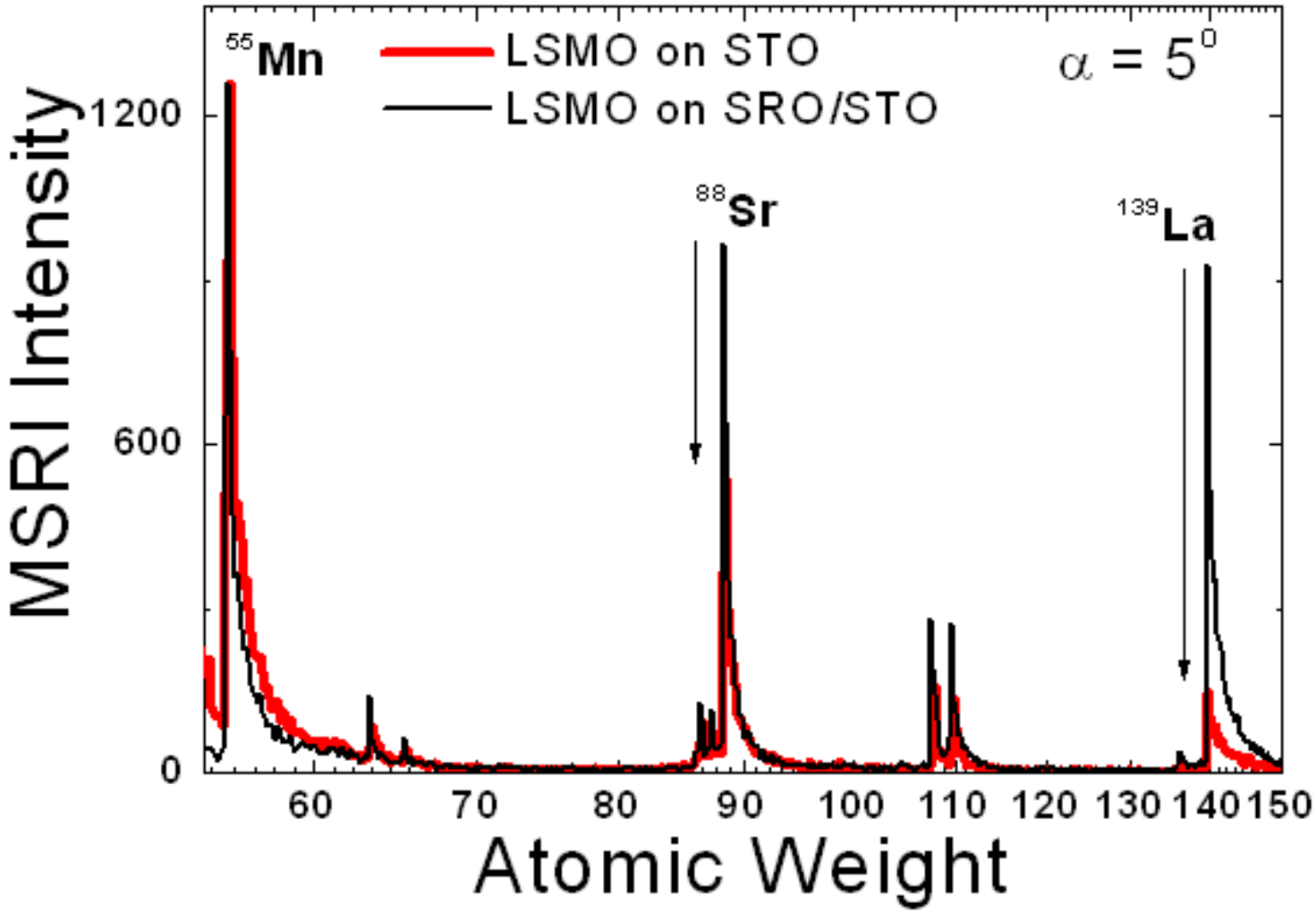
Controlling Surface Termination



Time Of Flight-Mass Spectroscopy of Recoil Ion (TOF-MSRI)

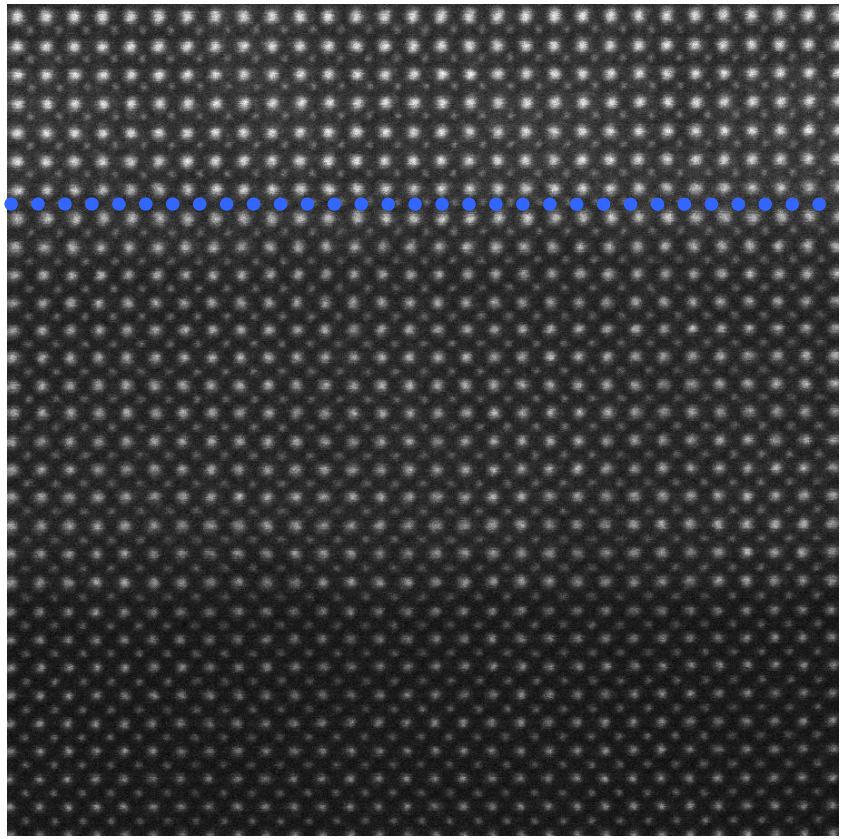


Probing Surface Termination

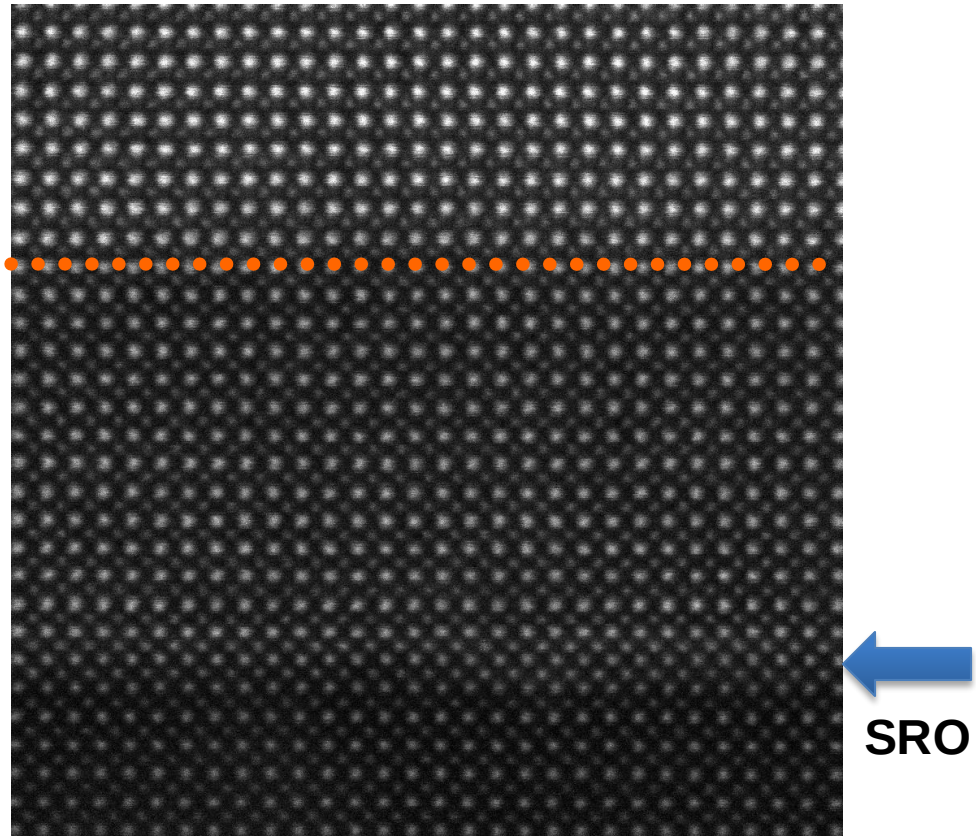


Atomic Structure of interfaces

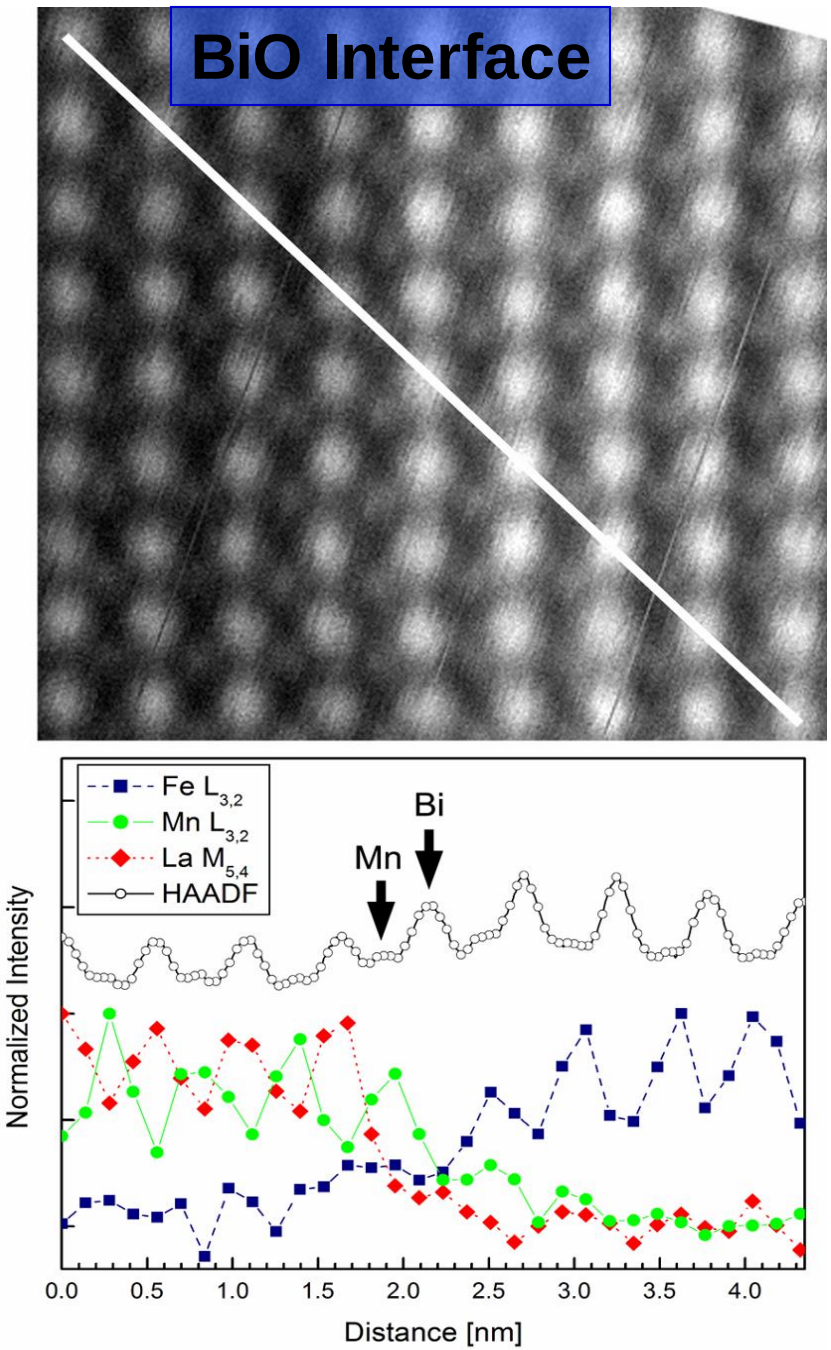
BiO Interface

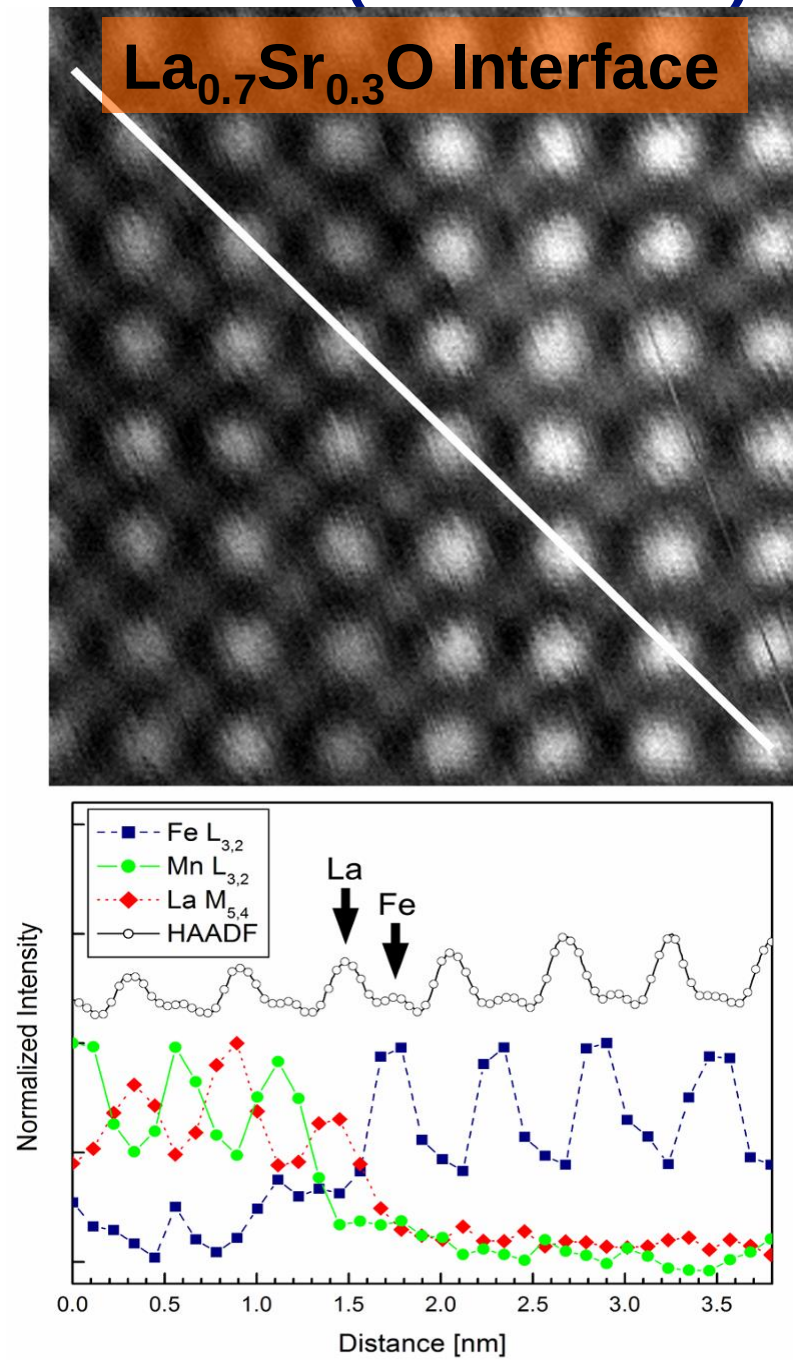


$La_{0.7}Sr_{0.3}O$ Interface



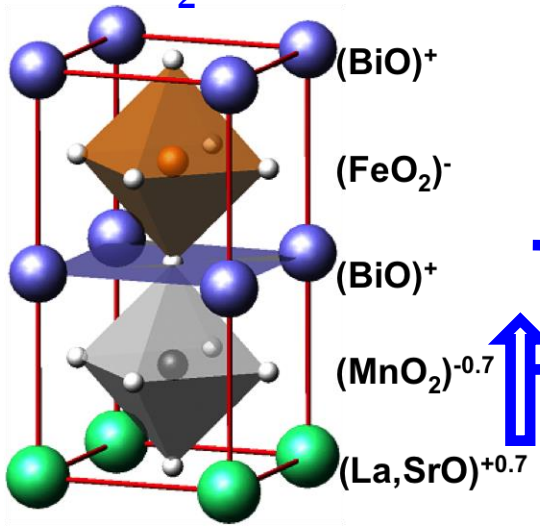
Structure and Composition of Interfaces (STEM-EELS)





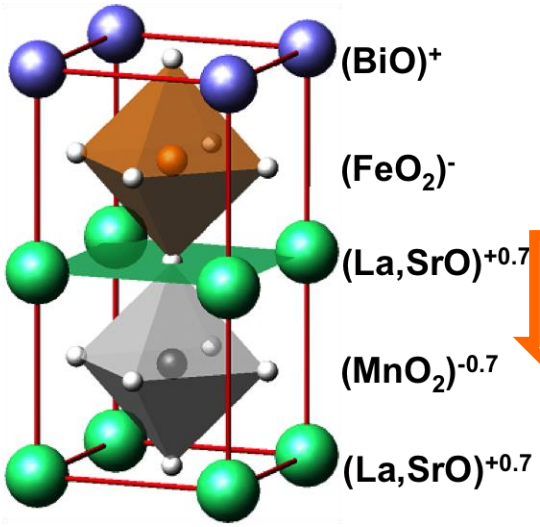
Interface Termination Controls Bulk properties

MnO_2 interface



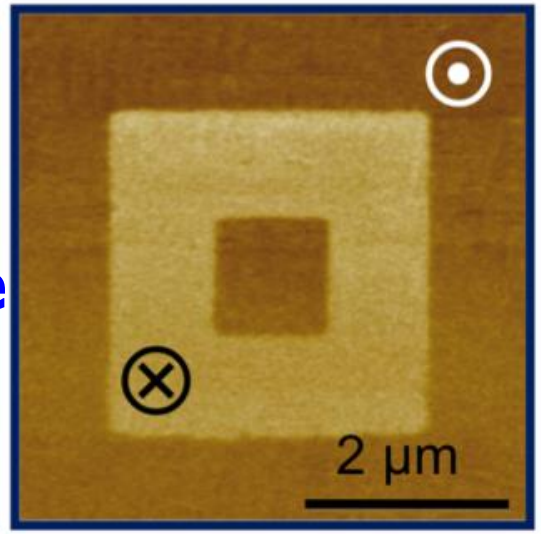
+0.15 e

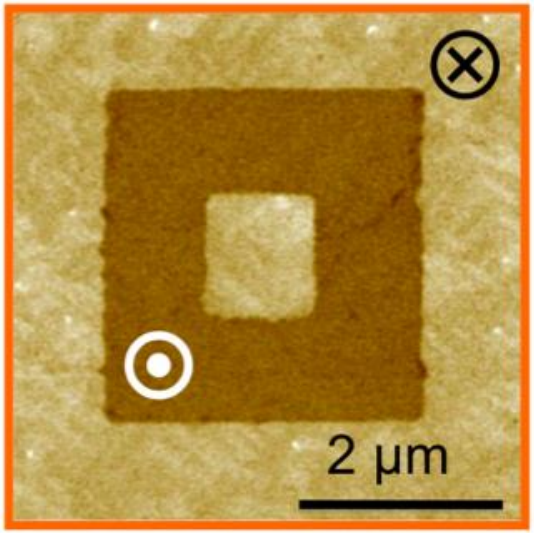
$La_{0.7}Sr_{0.3}O$ interface



-0.15 e

Out of plane PFM image

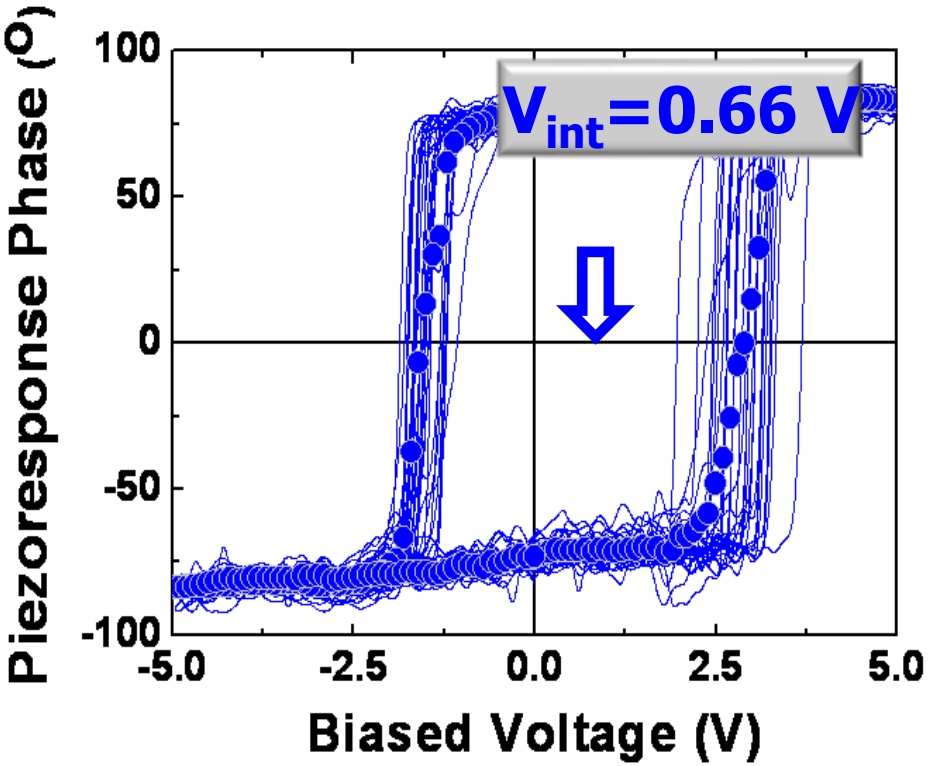




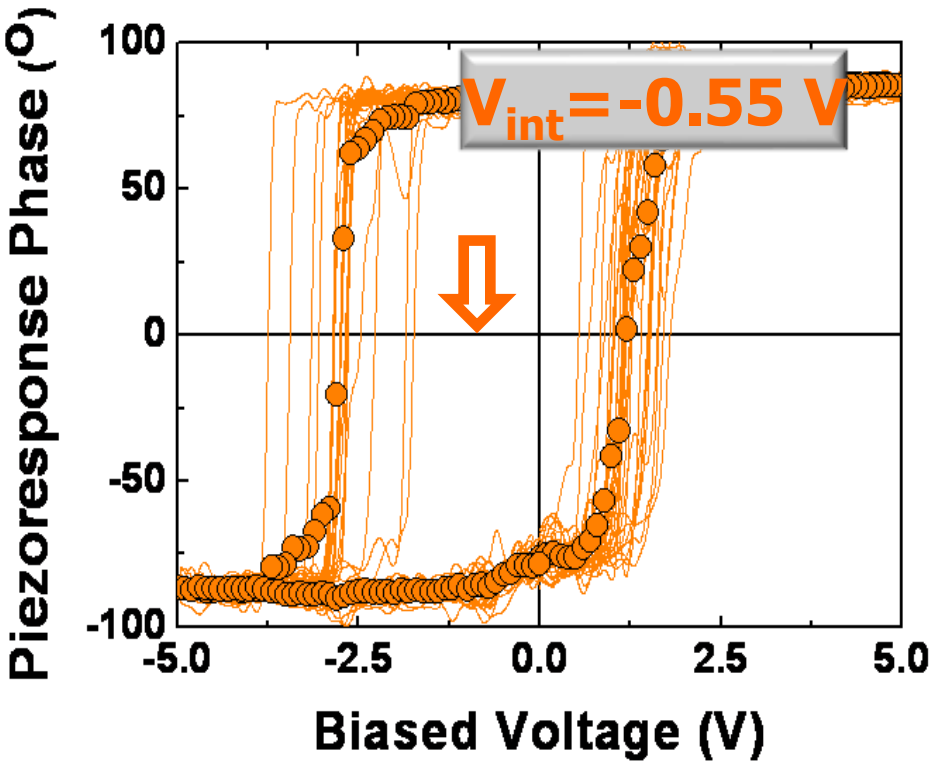
P. Yu *et al.*, under review(2011)

Interface Termination Controls Bulk properties

***BiO* interface**

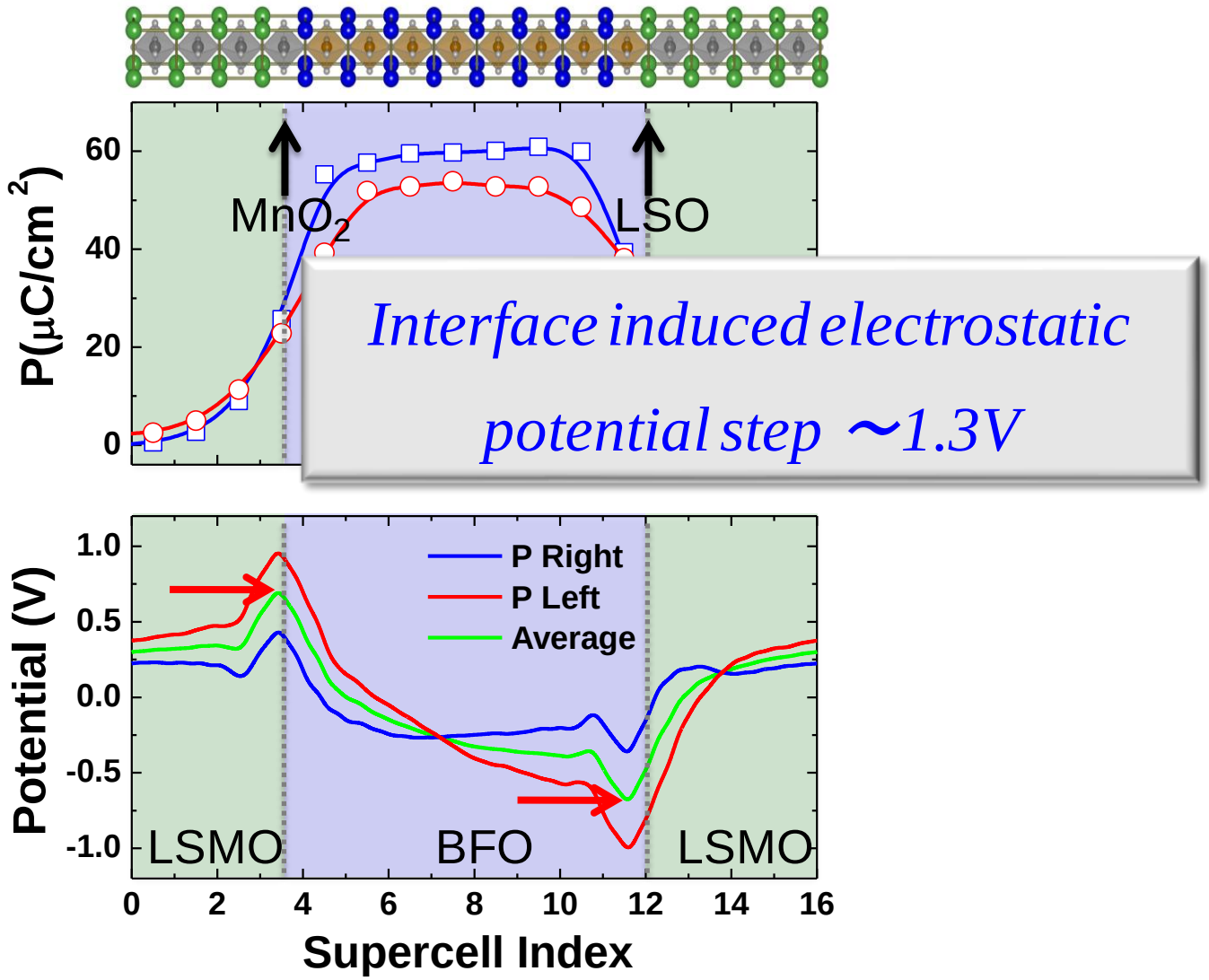


***$La_{0.7}Sr_{0.3}O$* interface**



- Internal field: shift of piezoresponse hysteresis loop;
- Interface induced electrostatic potential step ~ difference between internal fields ~ 1.2 Volts.

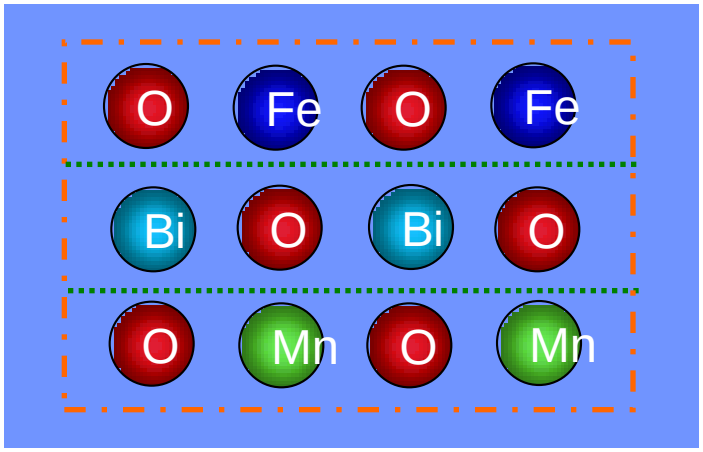
Interface Termination Controls Bulk properties

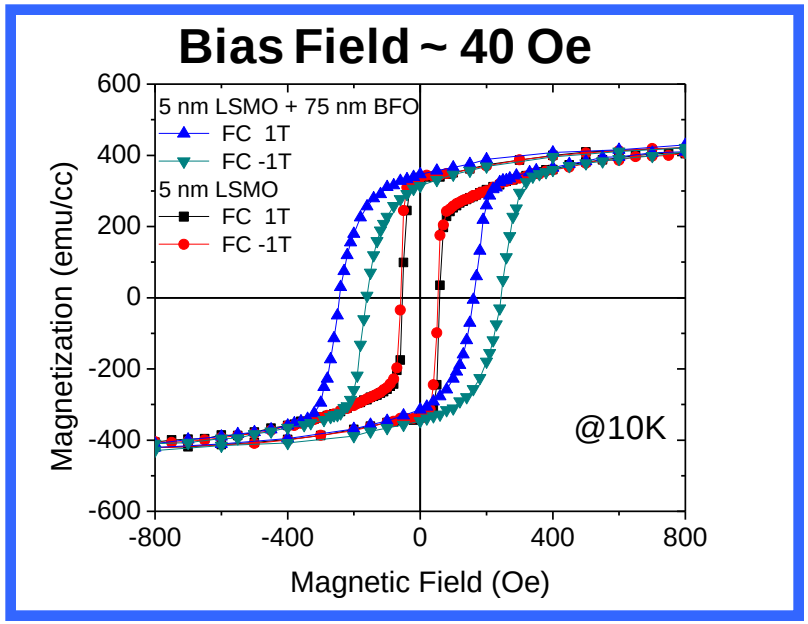


Collaboration with Dr. Luo, W. D., Prof. Pennycook, S. J. and Prof. Pantelides, S.T. at ORNL.

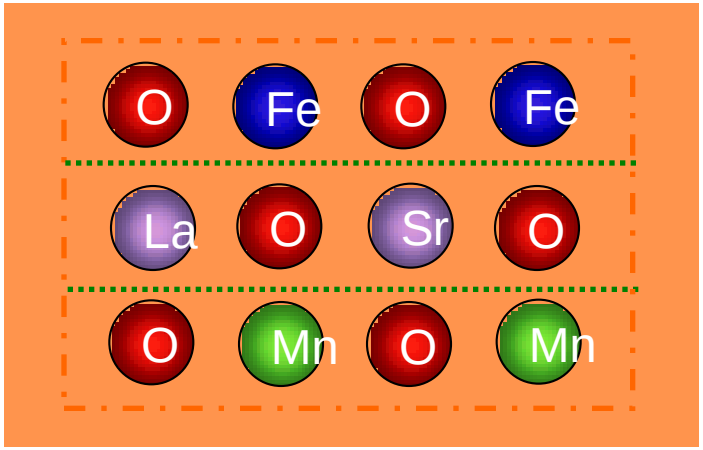
Exchange coupling changes with Interface termination!!

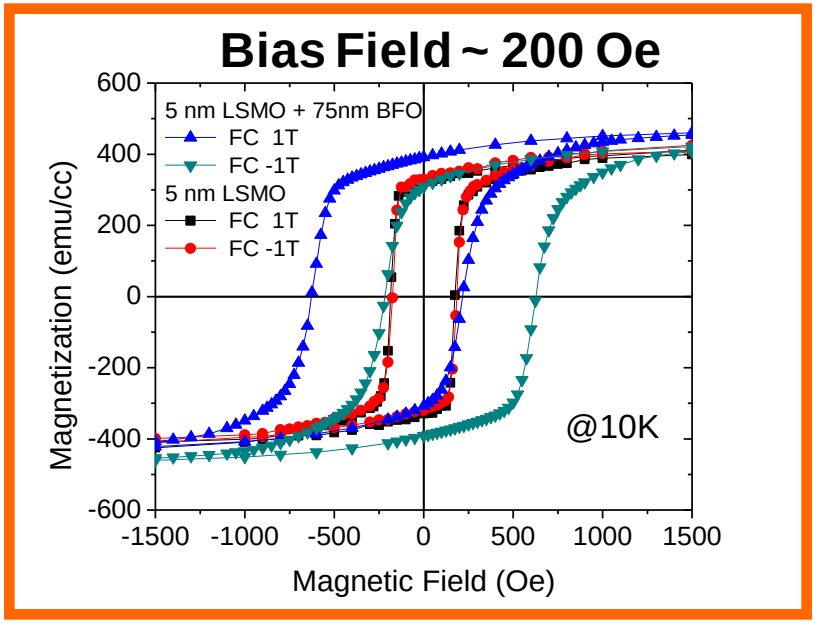
BiO Interface



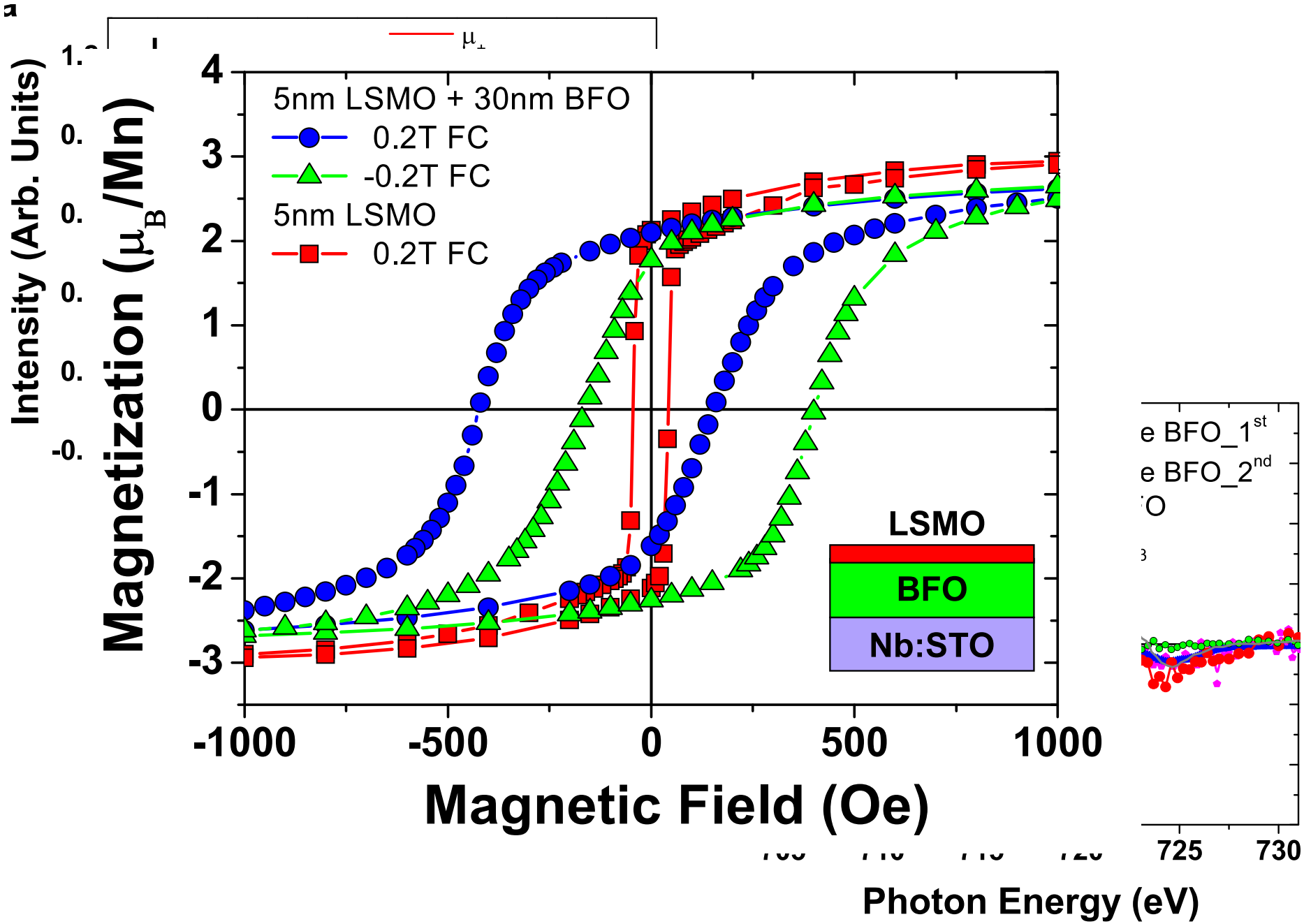


$La_{0.7}Sr_{0.3}O$ Interface





Probing Exchange Coupling with XMCD



FeRAMs: Solving Technology Challenges through Science

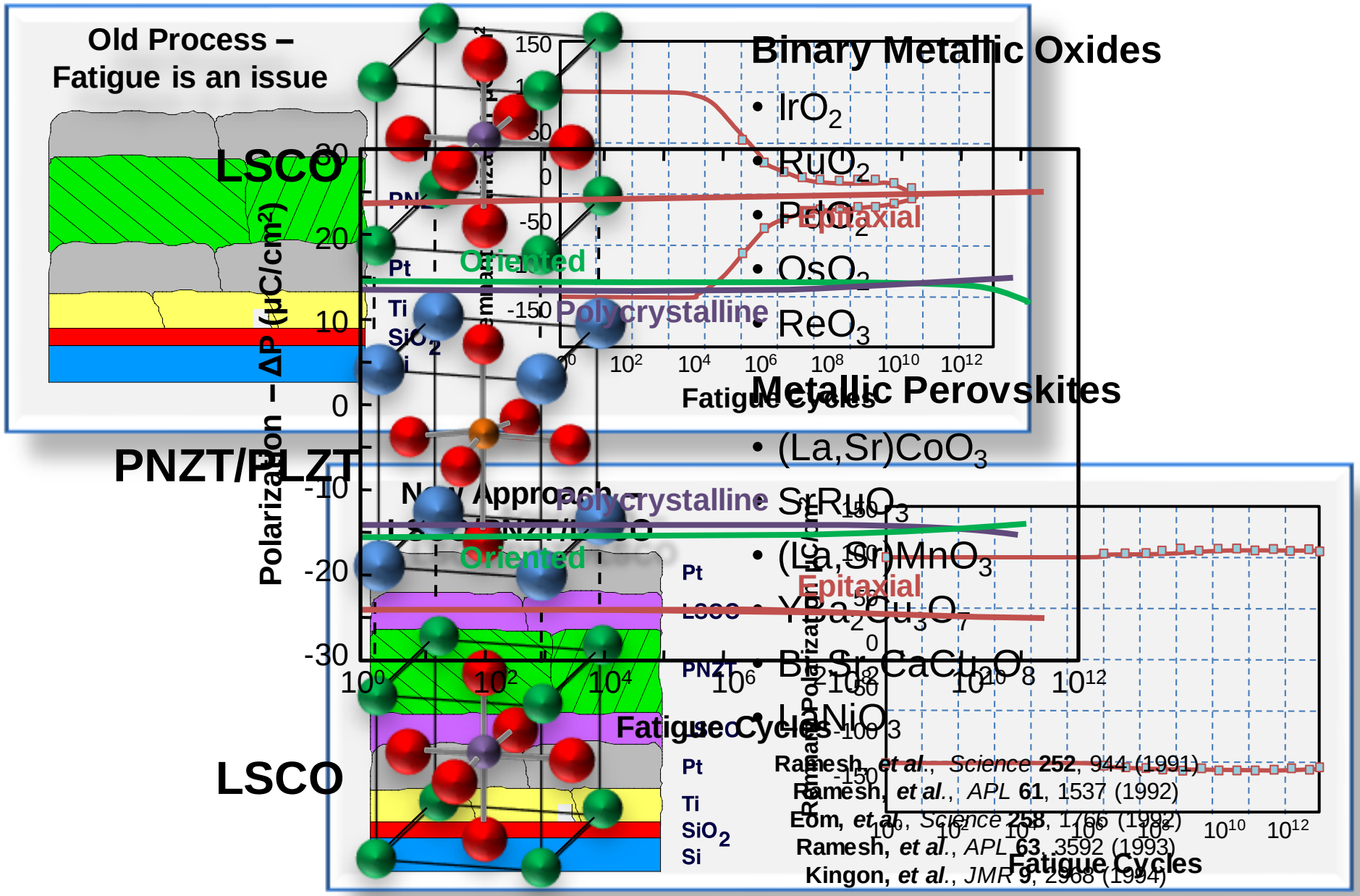
Memory Parameter	DRAM		FeRAM	
	Min	Max	Min	Max
Supply Voltage	3.15 V	3.45 V	3.15 V	3.45 V
Low Power Standby	-	-	-	10 µW
Operating Active Current	-	25 mA	-	25 mA
Operating Temperature	0°C	70°C	0°C	70°C
Storage Temperature	-55°C	125°C	-55°C	125°C
Non-Volatile Data Storage	-	-	0°C	70°C
Read Cycle Time	50 ns	-	50 ns	-
Address Access Time	-	26 ns	-	26 ns
Read Cycles Per Byte	$>10^{15}$	-	$>10^{13}$	
Write Cycle Time	50 ns	-	50 ns	-
Non-Volatile Data Retention	-	-	-	10 yrs.
Write Cycles Per Byte	$>10^{15}$	-	$>10^{13}$	

Imprint

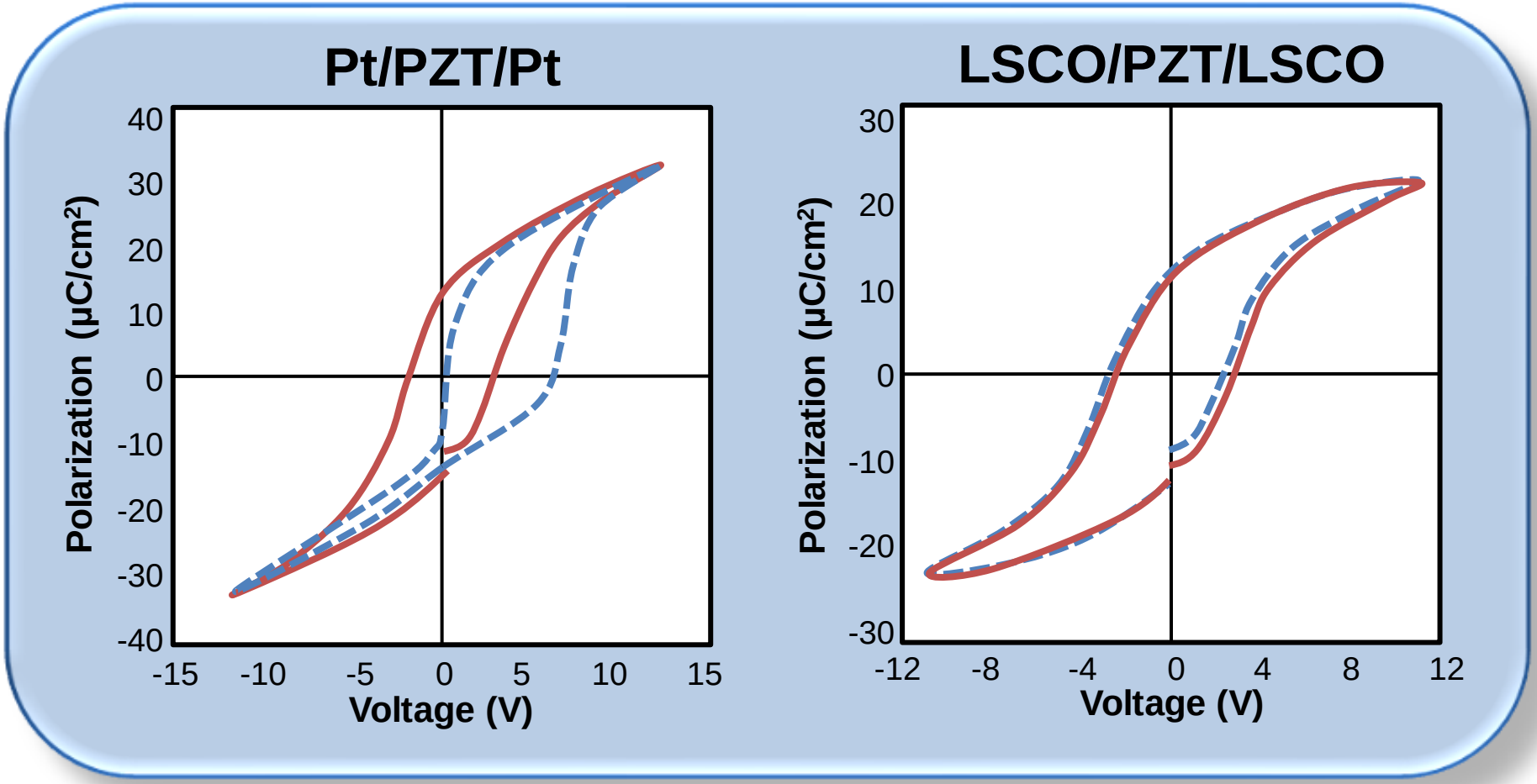
Fatigue

Scott & Araujo, *Science* **246**, 1400 (1989)

Basic Science Solves Applied Problems



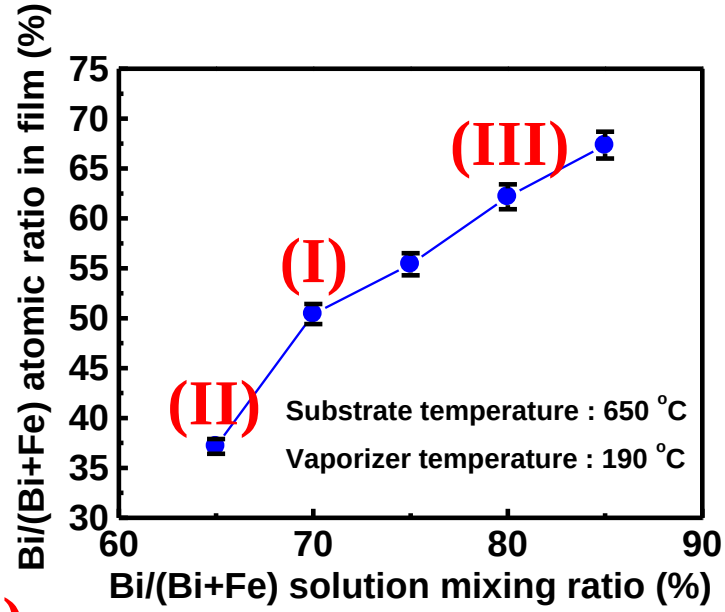
Oxide Electrodes: Eliminate Imprint

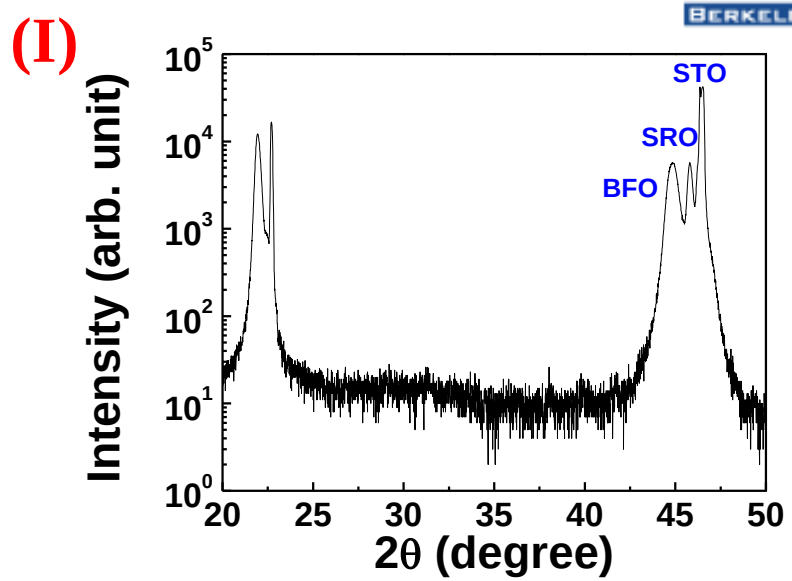


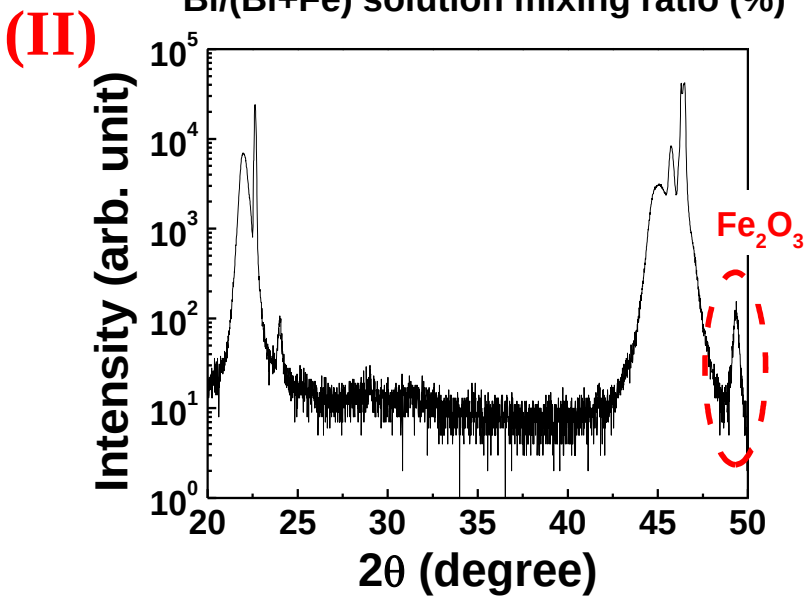
Oxide Electrodes Solve the Imprint (Internal Field) Problem

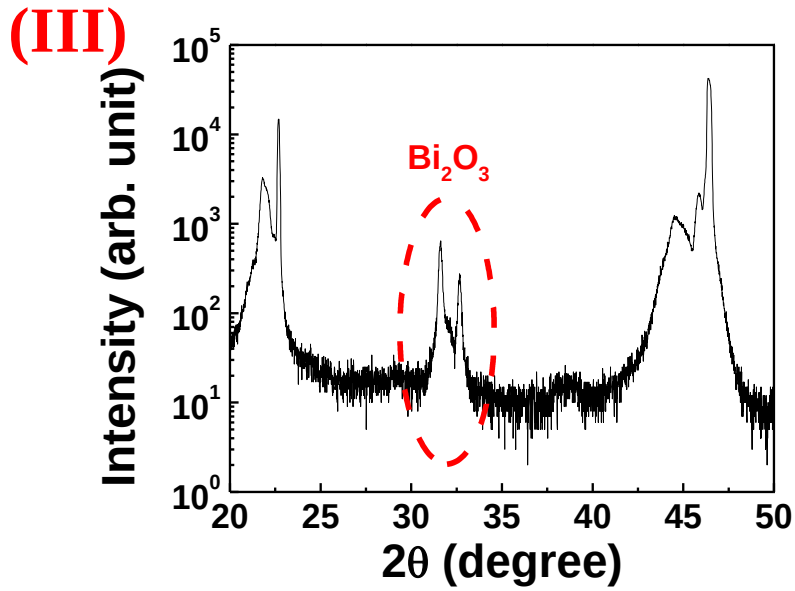
Pike, *et al.*, *APL* **66**, 484 (1995) & **Warren, *et al.*,** *APL* **67**, 866 (1995)

Processing Issues in CVD: Role of Composition

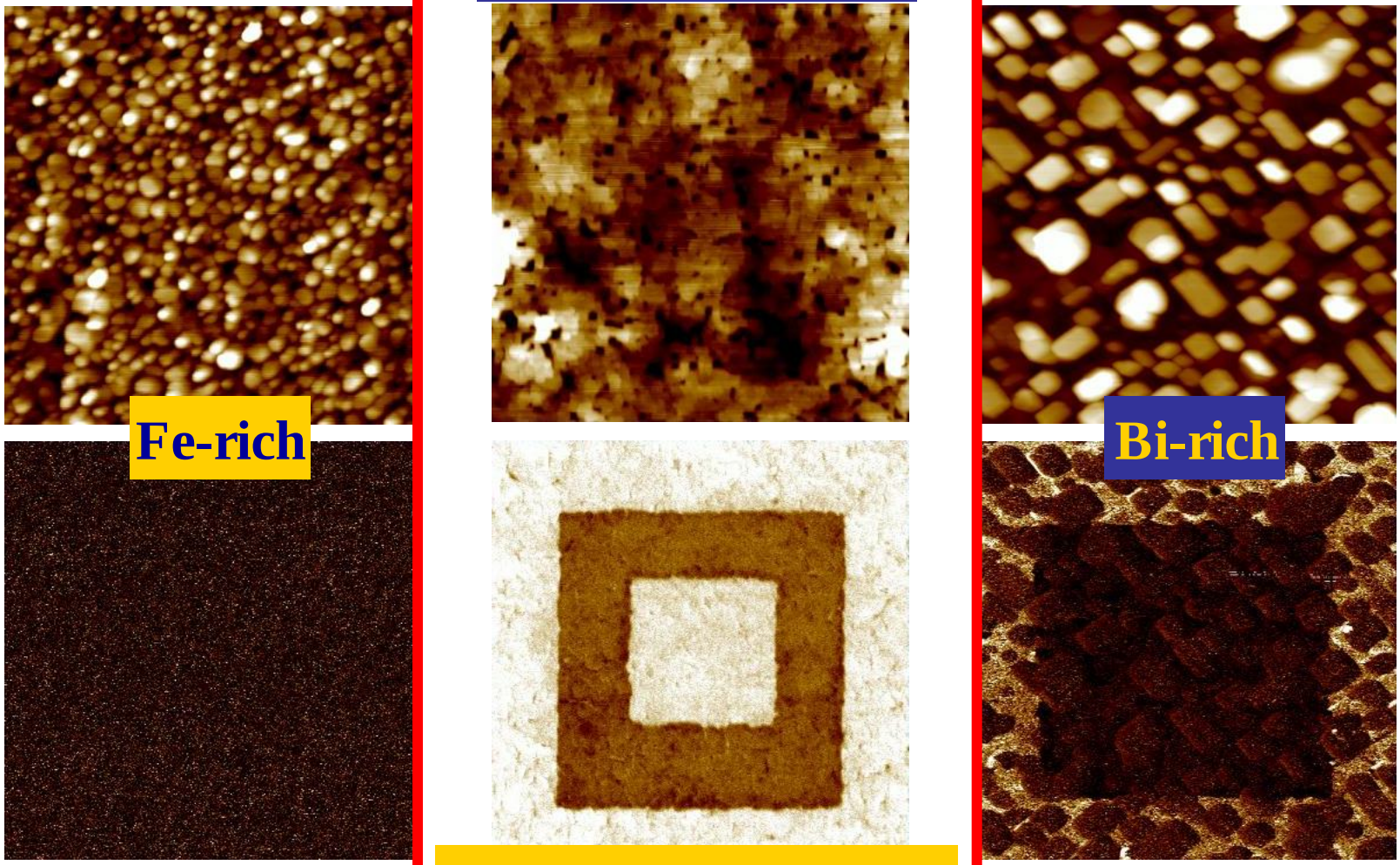






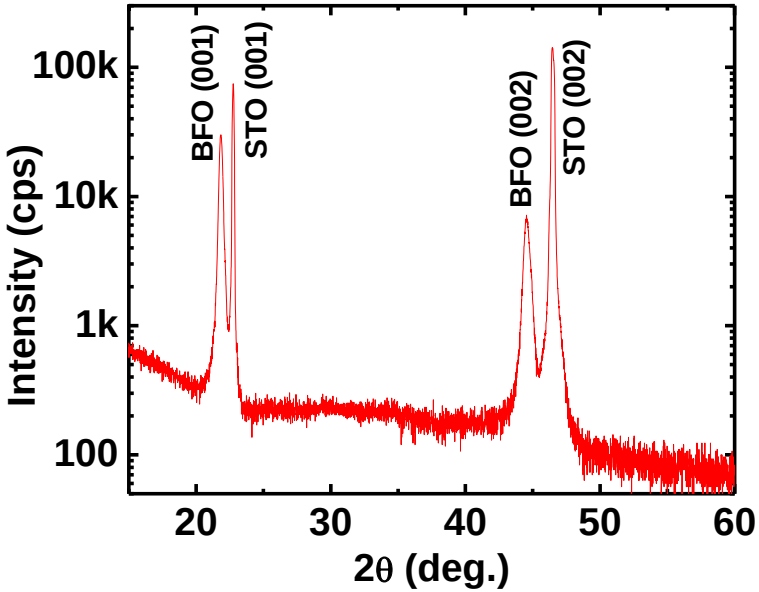


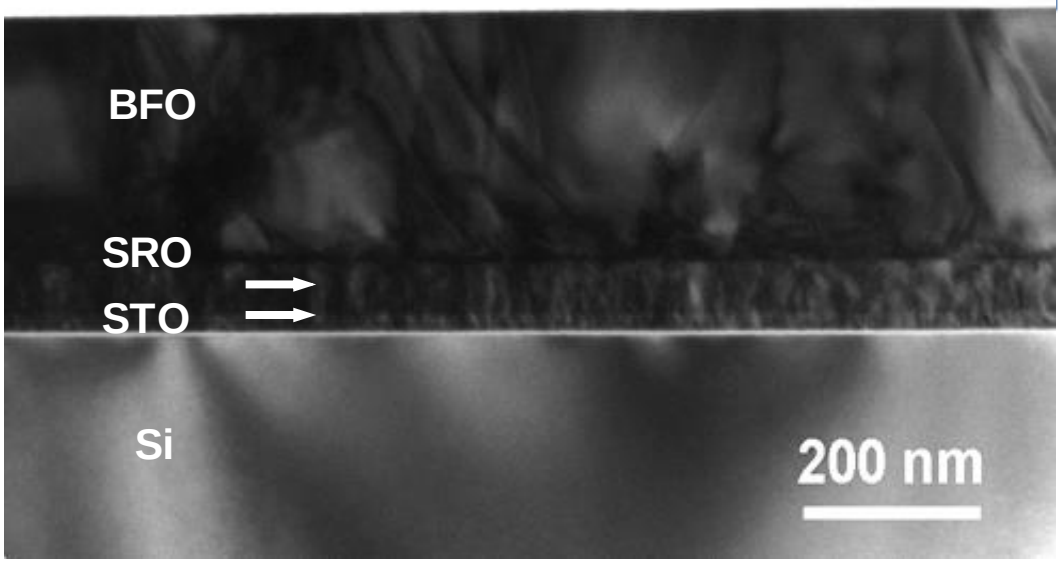
Composition effect

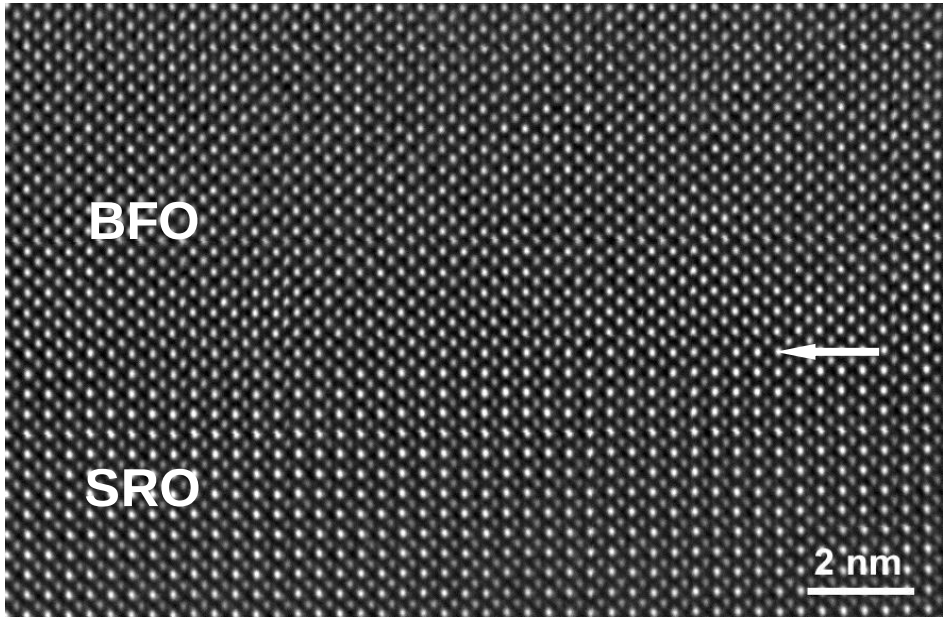


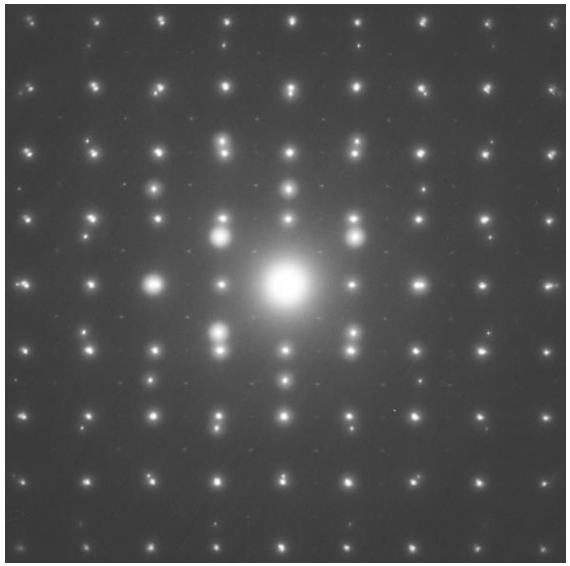
Need for careful composition control!!

High quality epitaxial BFO films









Possible conduction mechanisms

$$J_S = RT^2 \exp - \left[\frac{\Phi}{k_B T} - \frac{1}{k_B T} \left(\frac{q^3 E}{4\pi\varepsilon_o K d} \right)^{1/2} \right]$$

Schottky emission

$$J_{\mathrm{SCLC}} = \frac{9\mu\varepsilon_o K}{8} \frac{V^2}{d^3}$$

Space charge limited conduction

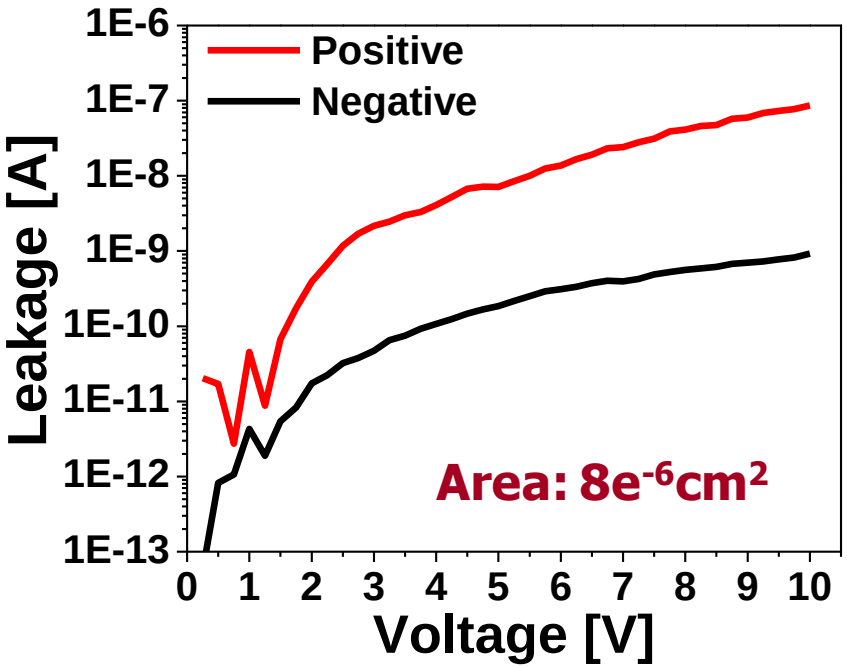
$$\sigma_{\mathrm{PF}} = c \exp - \left[\frac{E_I}{k_B T} - \frac{1}{k_B T} \left(\frac{q^3 E}{\pi\varepsilon_o K d} \right)^{1/2} \right]$$

Poole-Frenkel emission

$$I = A_{\mathrm{eff}} \frac{e^3 m_{\mathrm{Pt}}}{8\pi\, h m_{BFO}\, \phi_{\mathrm{B}}} \times E^2 \exp\left(-\frac{8\pi\sqrt{2m_{BFO}}}{3he} \frac{\phi_{\mathrm{B}}^{3/2}}{E} \right)$$

Fowler-Nordheim tunneling

Leakage

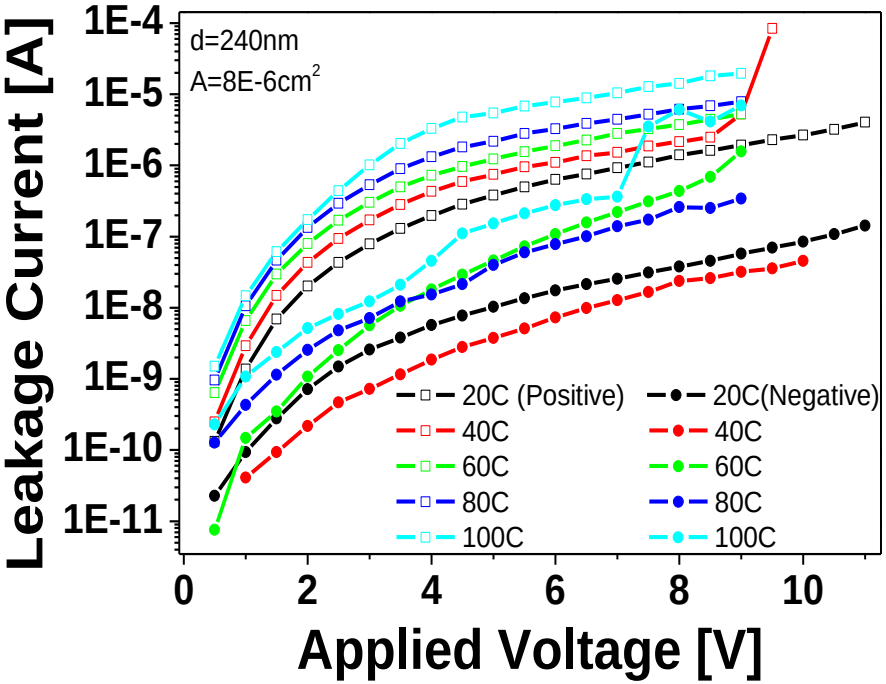


Poole-Frenkel Emission : $Fe^{3+} \rightarrow Fe^{2+} + h^{+}$

Schottky Emission

Electron Hopping : From Fe^{2+} to Fe^{3+}

Space-Charge-Limited Conduction



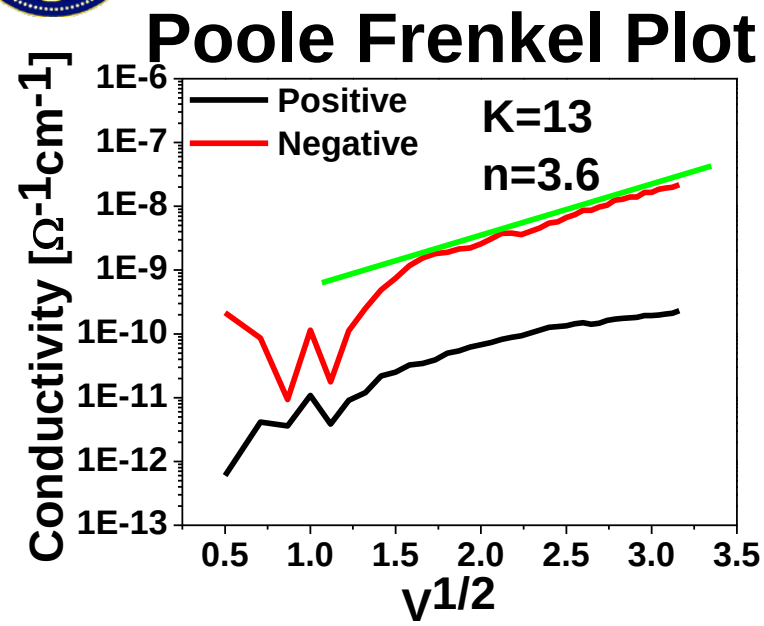
Critical Issue #2

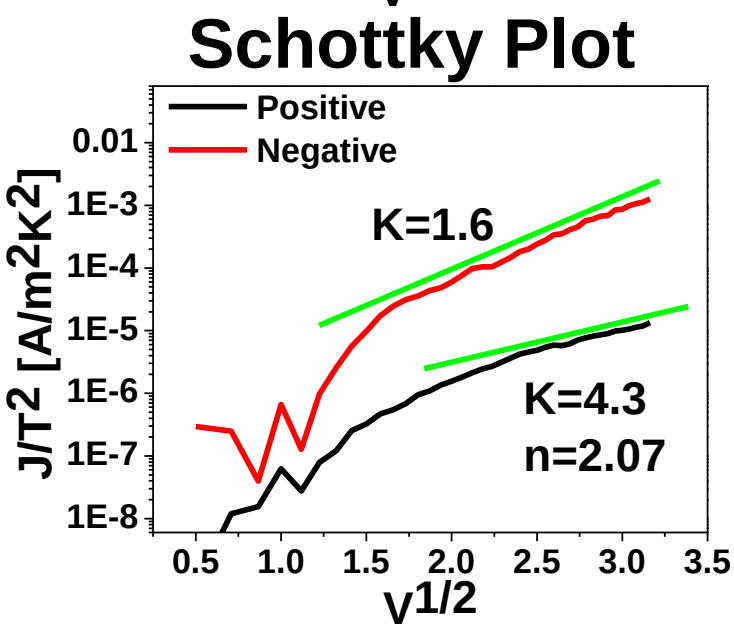
How to reduce leakage ?

Understand leakage mechanisms

Chemical doping

Identifying the leakage mechanism





Poole-Frenkel

The extracted dielectric constant is too high, about twice that of the expected 6.25-6.5

Schottky

The extracted dielectric constant is too low for the negative direction, but not far off for higher fields

Space Charge Limited

Log-log plots (not shown) do not follow the expected trend

Need more thickness, T and E dependent measurements