SCHOOL of ENGINEERING & APPLIED SCIENCE
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Strain field and coherent domain wall effects on the thermal conductivity and Kapitza conductance in Bismuth Ferrite

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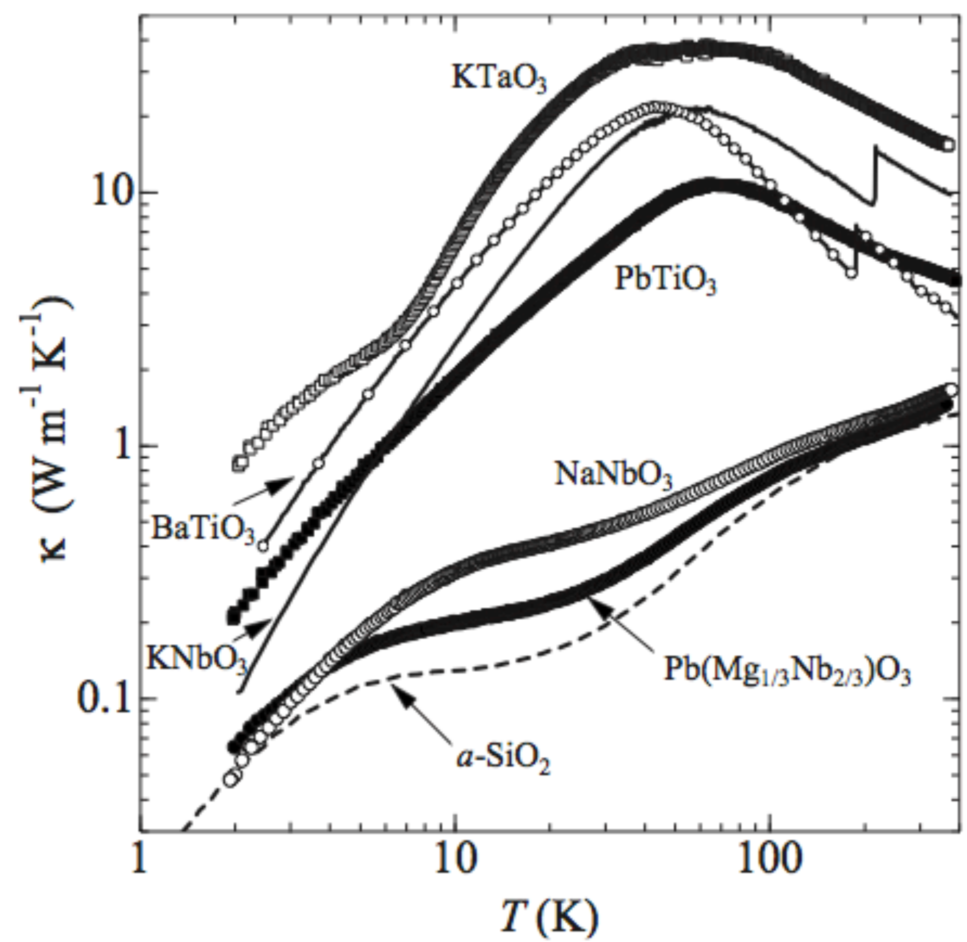
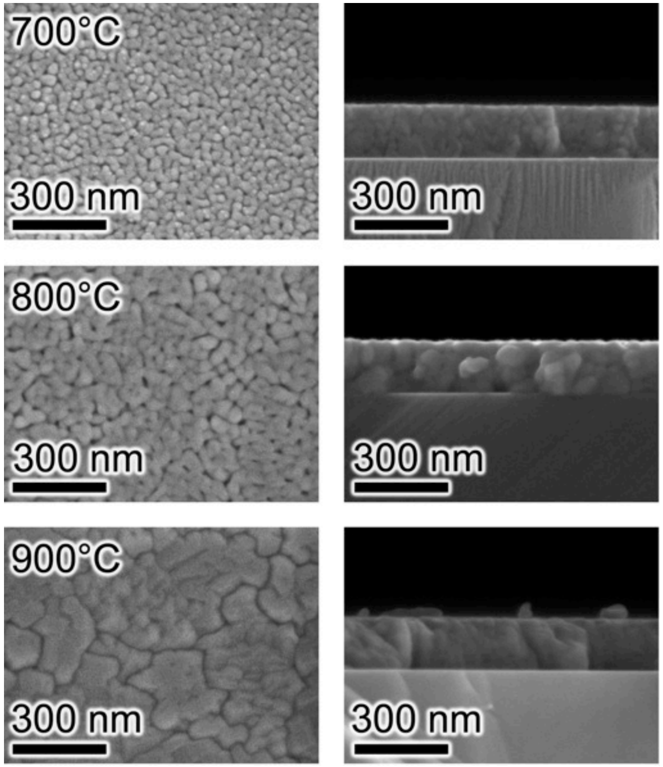
Thermal conductivity of Ferroelectrics

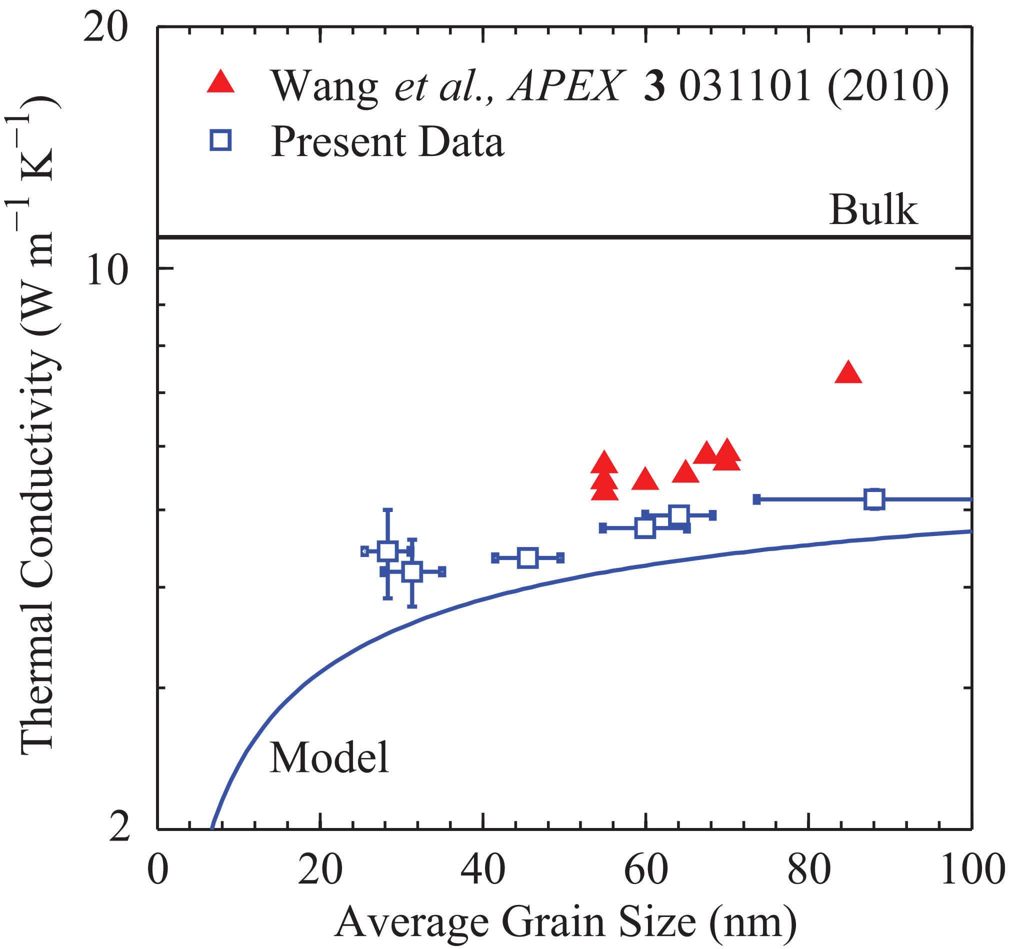
- Ferroelectrics and related materials can have low thermal conductivities
  - Complex phonon spectra
  - Soft modes
  - Anisotropy
- What role do internal boundaries/structures play??



Tachibani *et al*. *Appl. Phys. Lett.* **93**, 092902 (2008)

Grain boundaries: $SrTiO_3$





$$\tau_j = \left[\frac{1}{\tau_{\mathrm{a}}} + \frac{1}{\tau_{\mathrm{gb}}} + \frac{1}{\tau_{\mathrm{fb}}}\right]^{-1}$$

$$= \left[BT\omega_j^2 \exp\left(-\frac{C}{T}\right) + \frac{v_j}{d_{\mathrm{avg}}} + \frac{v_j}{170 \times 10^{-9}}\right]^{-1}$$

Foley *et al*. *Appl. Phys. Lett.* **101**, 231908 (2012)

What about domain boundaries/strain?

Grain boundaries = incoherent

Ferroelectric domain boundaries = coherent and strained

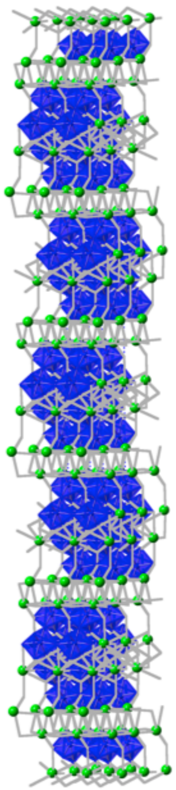
Outline

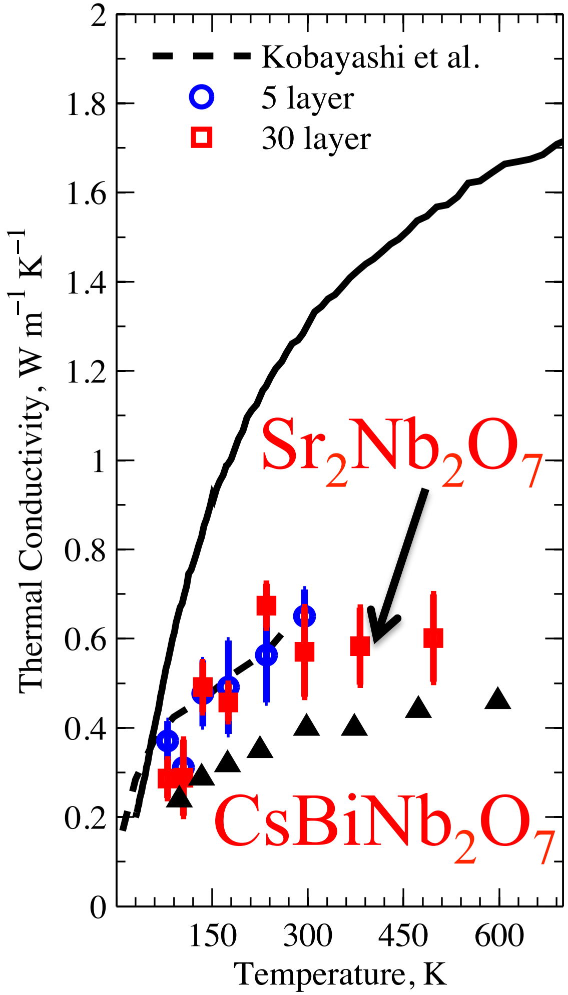
- Domains and domain walls in $BiFeO_3$
- Time domain thermoreflectance (TDTR)
- Domain effects on thermal transport in $BiFeO_3$
- “Domain wall” Kapitza conductance – phonon-strain field scattering

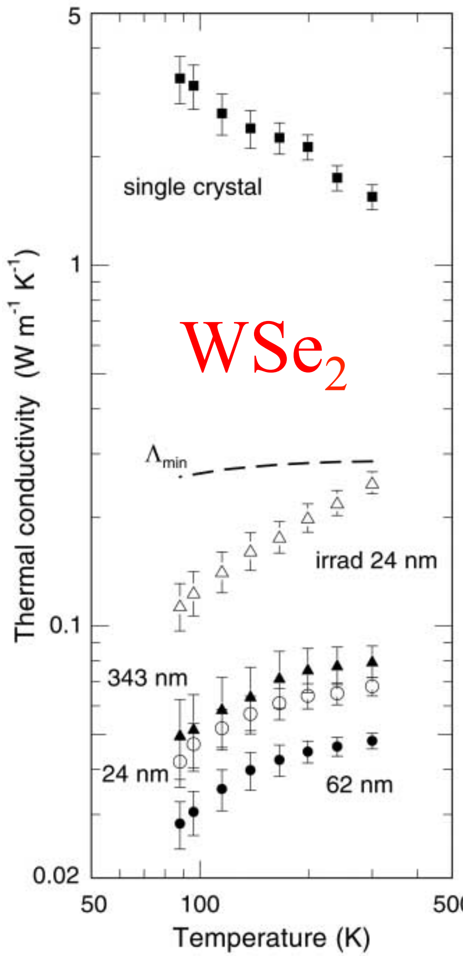
"Coherent interfaces" – think layers

- Layered structures can exhibit ultralow thermal conductivity

Ex. $Sr_2Nb_2O_7$





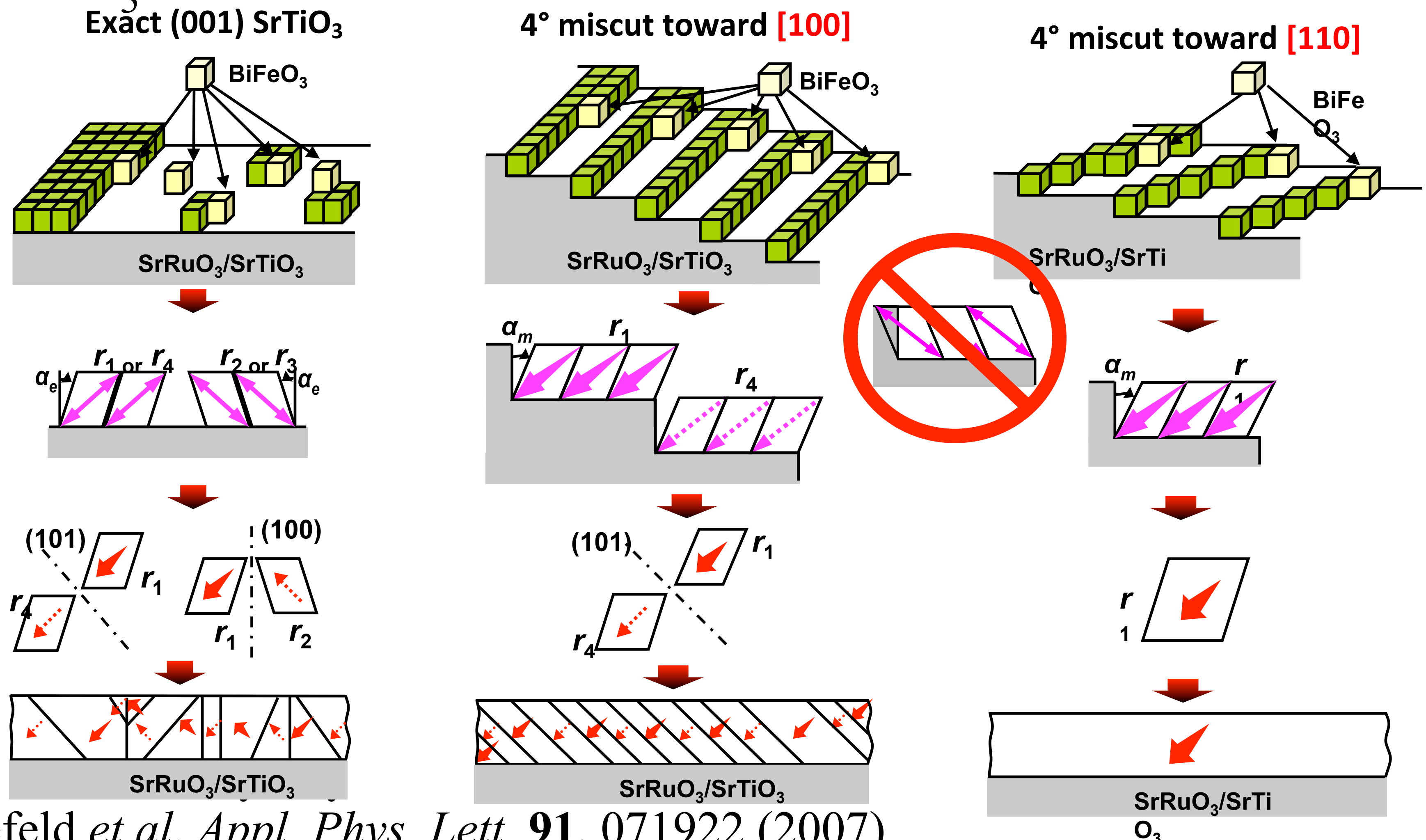


Cahill *et al*. *Appl. Phys. Lett*. **96**, 121903 (2010)
Chiritescu *et al*. *Science* **315**, 351 (2007)

"Coherent" interfaces – $BiFeO_3$ domains

Slide courtesy of Chang-Beom Eom and Jon Ihlefeld

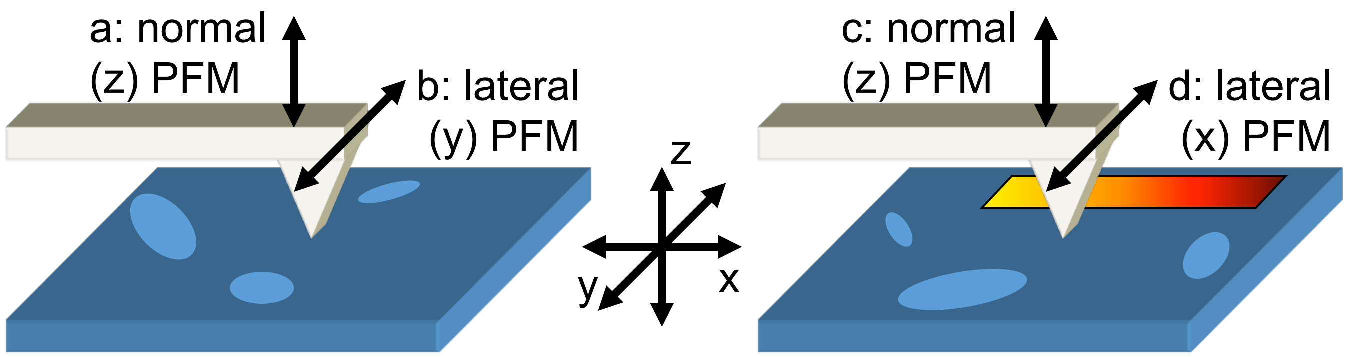
- Domain boundaries – other types of coherent interfaces
- Reactive molecular-beam epitaxy: 30 nm $BiFeO_3$ films on $SrTiO_3$ substrates



Ihlefeld *et al*. *Appl. Phys. Lett.* **91**, 071922 (2007)

Domain characterization - PFM

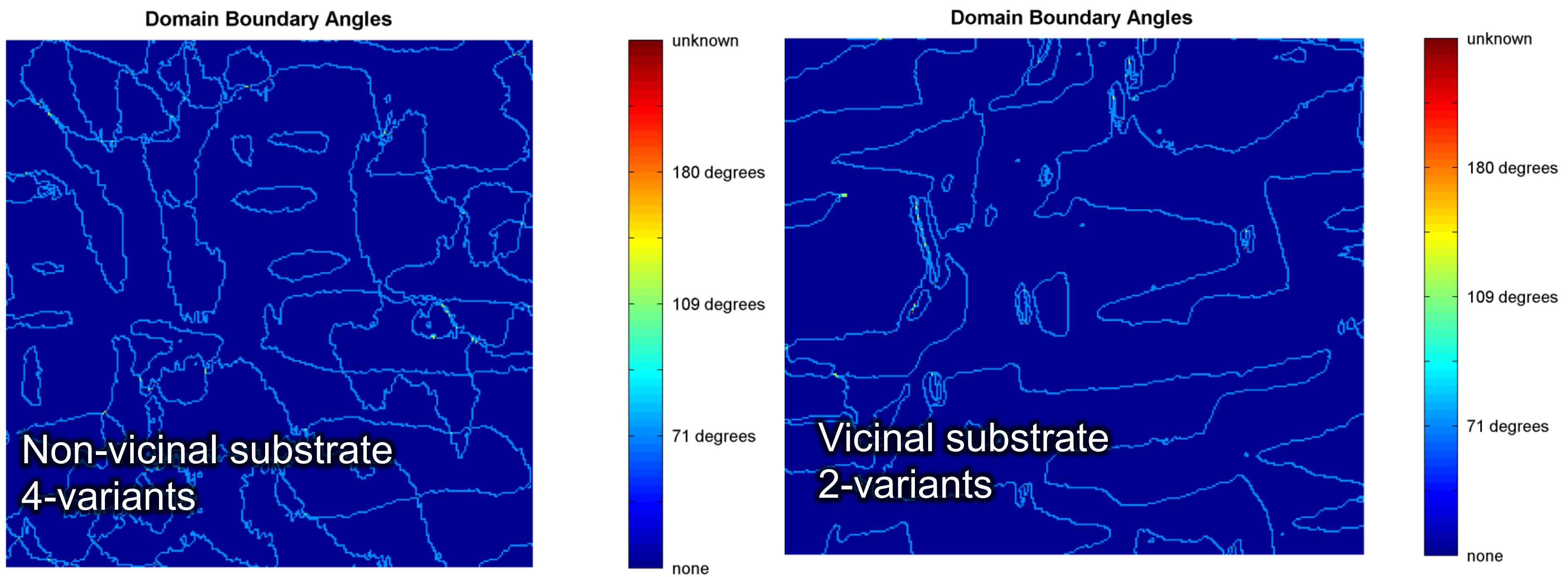
Prof. Bryan Huey
U. Conn.



- Standard domain imaging not sufficient
- Require quantification of domain boundaries
- Vector (angle-resolved) PFM: 2 steps
  - Out-of-plane (normal) z-direction
  - In-plane y-direction
  - Rotate specimen 90 degrees

Desmarais *et al*. *Appl. Phys. Lett.* **99**, 162908 (2011)

Domain boundary quantification

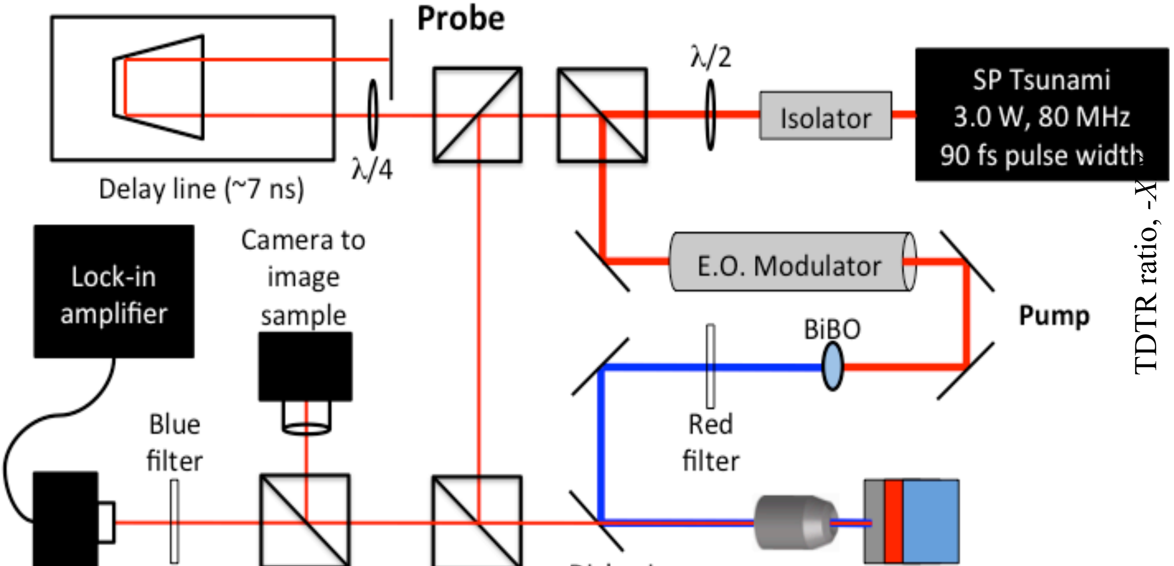


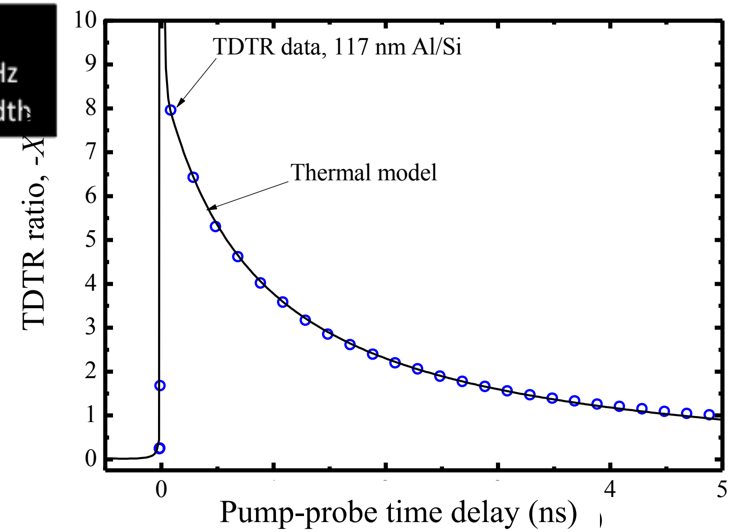
- Growth on vicinal substrate results in different domain structure
- Virtually all 71 deg. domain walls
- **4 variant: 16 μm domain wall/μm²**
- **2 variant: 11 μm domain wall/μm²**

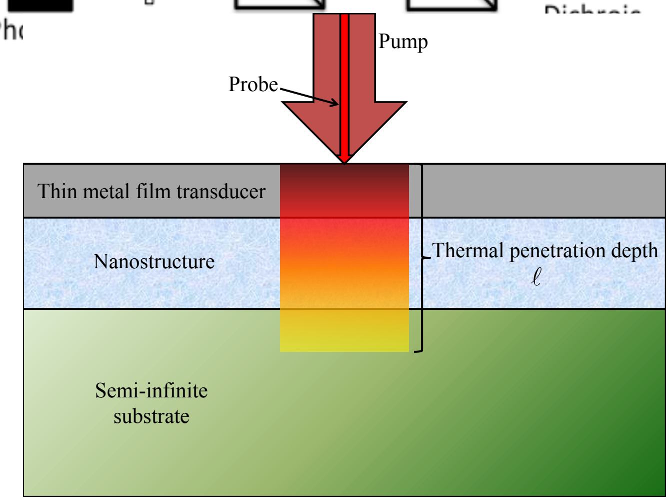
Hopkins *et al*. *Appl. Phys. Lett.* **102**, 121903 (2013)

Time domain thermoreflectance (TDTR)

- Thermal conductivity of series of $BiFeO_3$ films with different domain structures



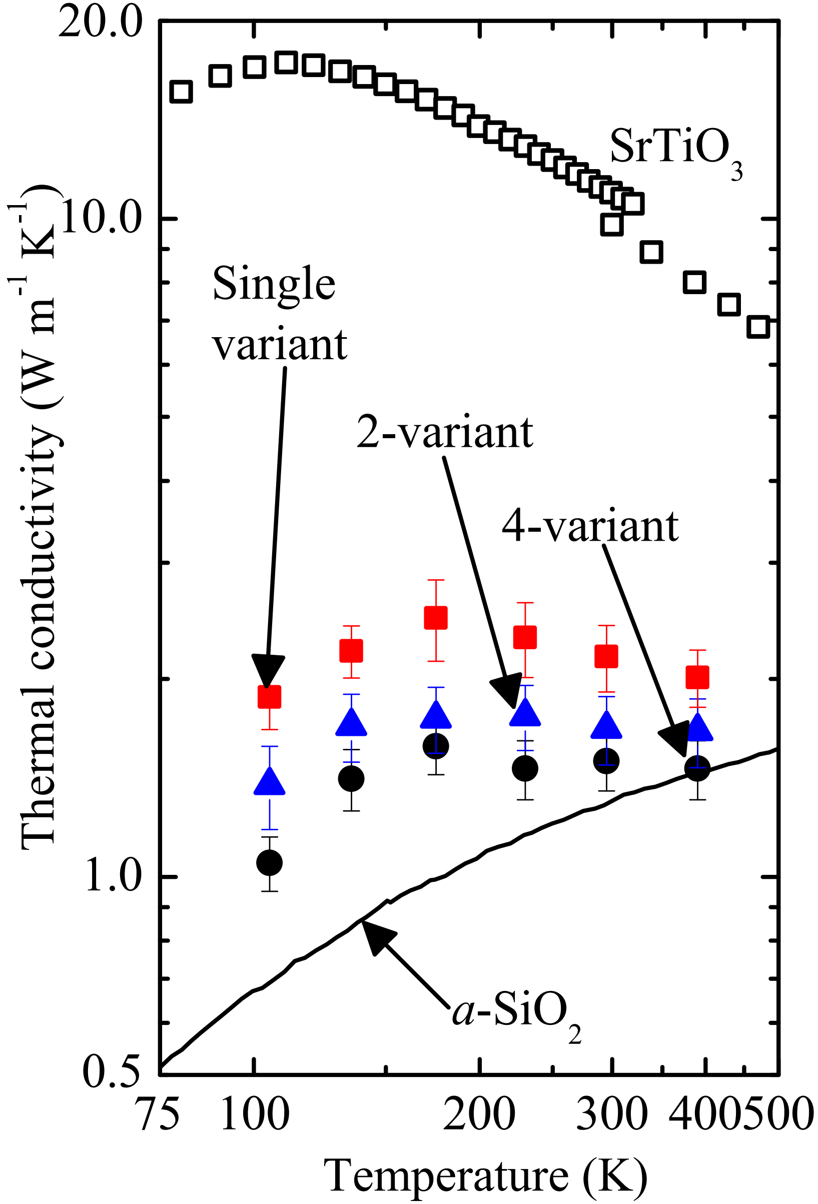




- Can measure thermal conductivity of thin films and substrates (κ) separately from thermal boundary conductance (h_K)
- Nanometer spatial resolution (~10's of nm)
- Femtosecond to nanosecond temporal resolution
- Noncontact

Domain effects on *effective* thermal conductivity

- Effective thermal conductivities of $BiFeO_3$ < 2.5 W m^{-1} K^{-1}
- Presence of domain walls reduces κ by ~30%
- ***Strain fields from domains are scattering phonons (previous speaker)***



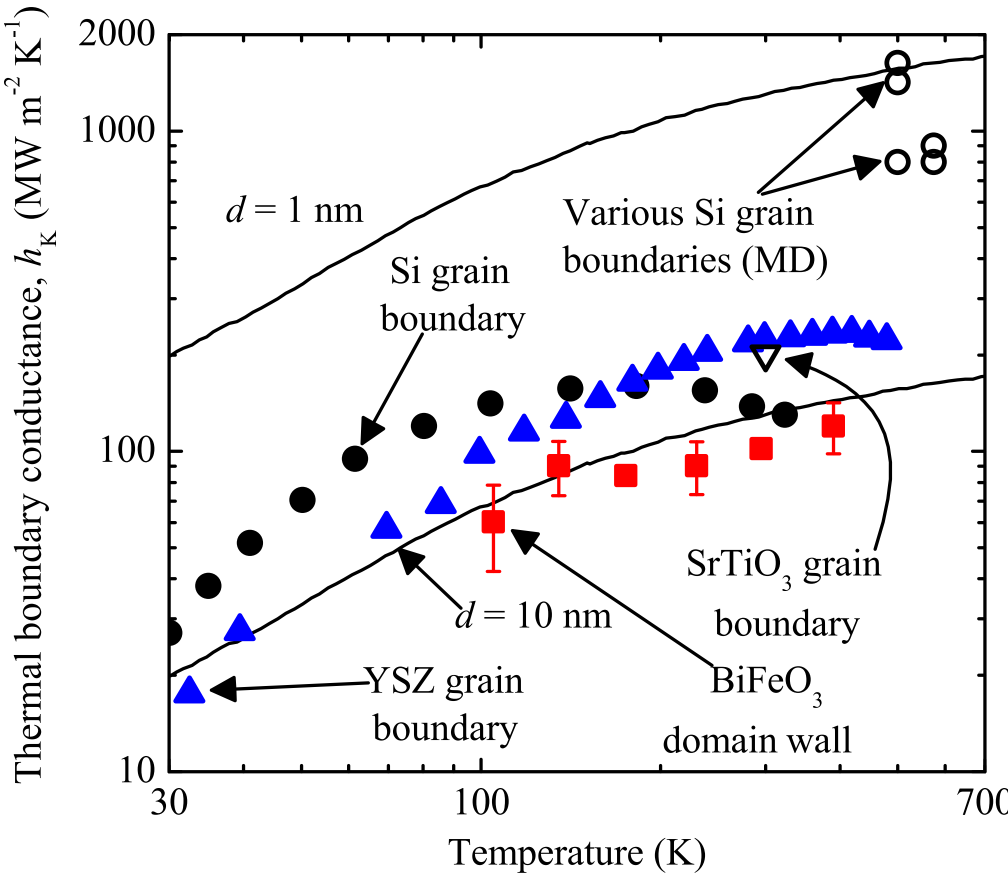
Hopkins *et al*. *Appl. Phys. Lett.* **102**, 121903 (2013)

Domain effects Kapitza conductance

- **4 variant: *D* = 16 μm domain wall/μm²**
- **2 variant: *D* = 11 μm domain wall/μm²**

$$h_K = \frac{\kappa_0}{D\left(\frac{\kappa_0}{\kappa} - 1\right)}$$

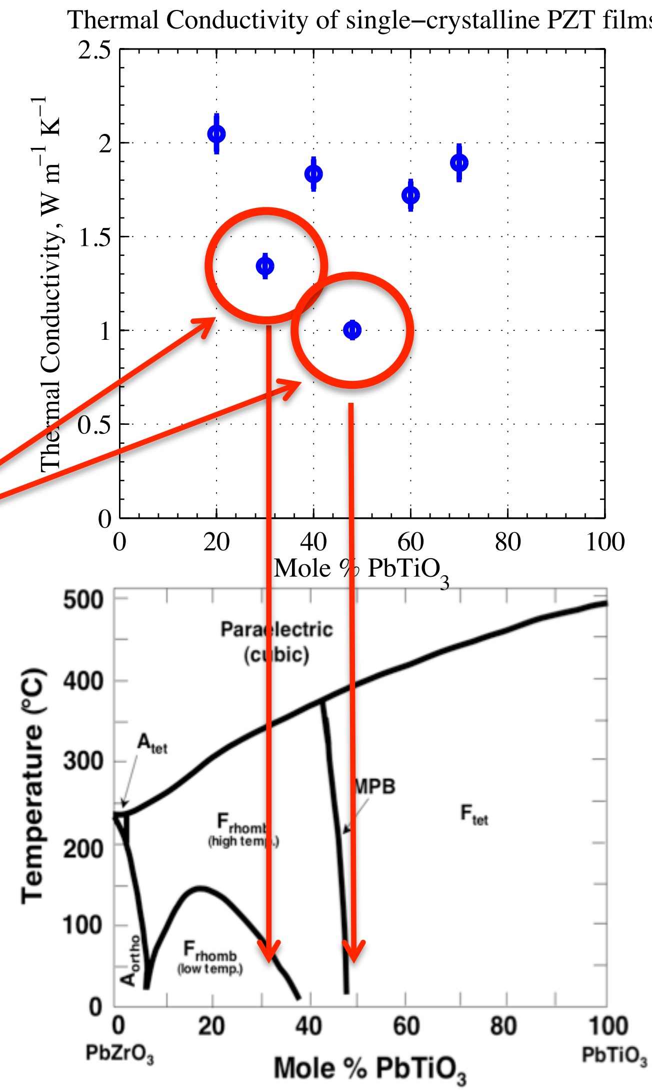
- Strain fields from coherent domain boundaries can scatter phonons like domain boundaries
- **Coherent domain walls offer as much resistance as 10 nm of SiO_2**



Hopkins *et al*. *Appl. Phys. Lett.* **102**, 121903 (2013)

Domain engineering of thermal properties

Single Crystalline $Pb[Zr_xTi_{1-x}]O_3$ (PZT) –
A LOT OF DOMAINS!



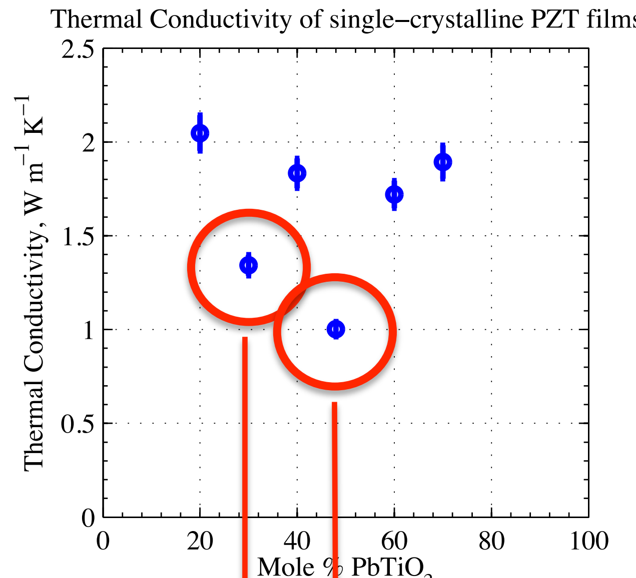
More domains and smaller domains at boundaries

Domain scattering stronger than alloy scattering

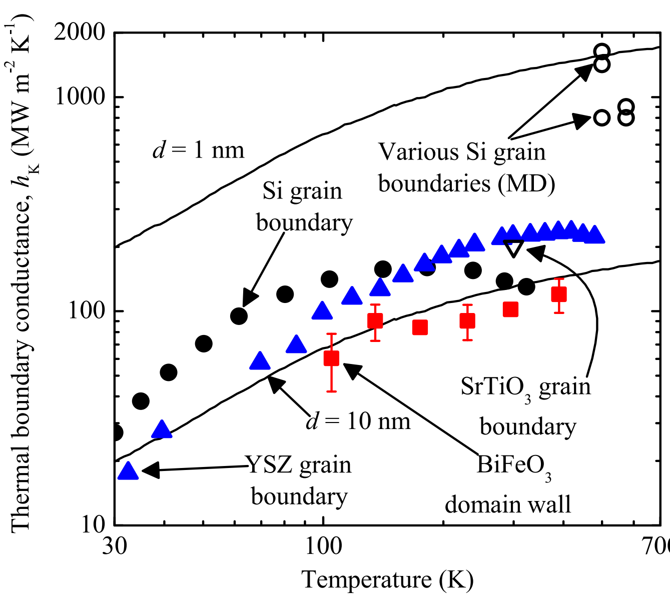
Schmitt *et al.* *JAP* **101**, 074107 (2007)

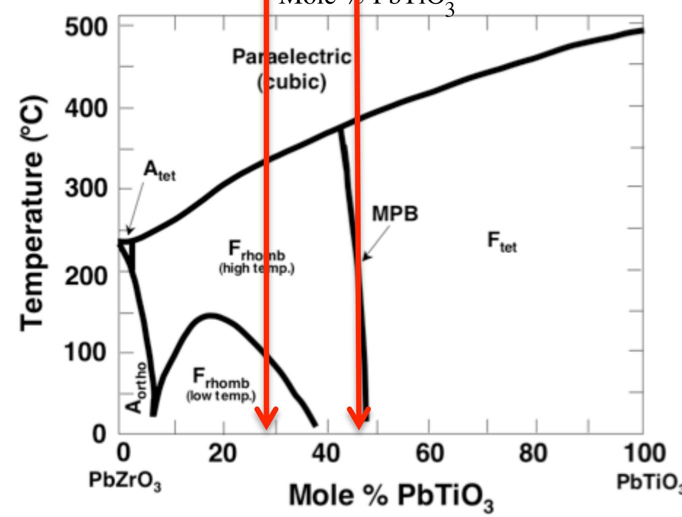
Conclusions - *Appl. Phys. Lett.* **102**, 121903 (2013)

- Domains boundaries scatter phonons
- Coherent strain fields have similar effects as incoherent grain boundaries



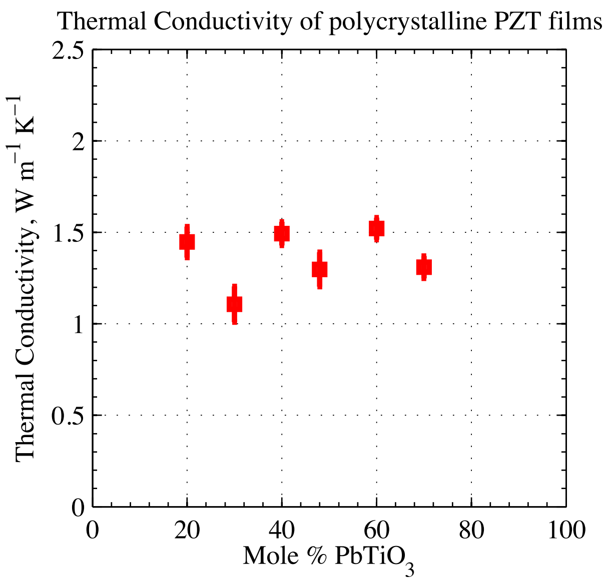
$$\frac{1}{\tau_{\text{domain wall}}} = \frac{v}{d_{\text{domain wall}}}$$

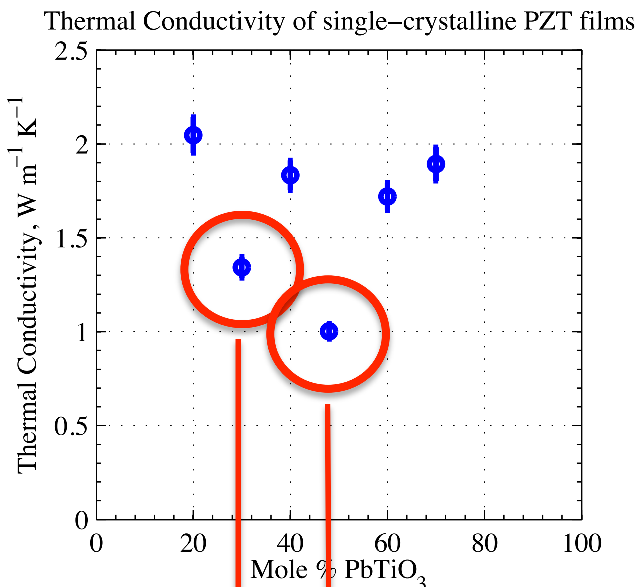


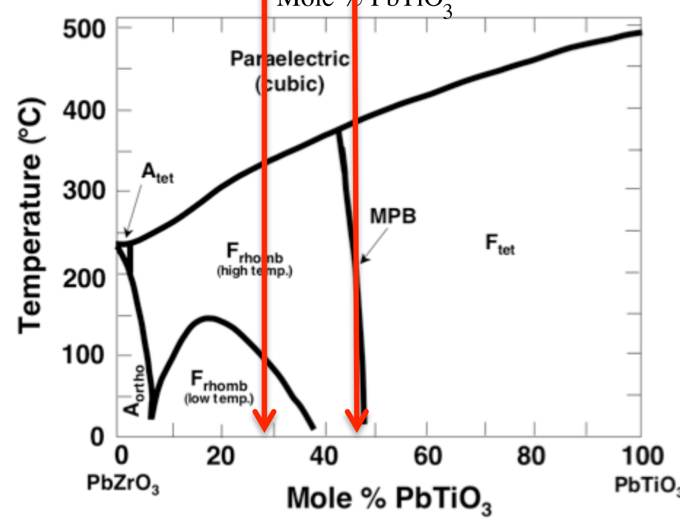


Young Investigator Program

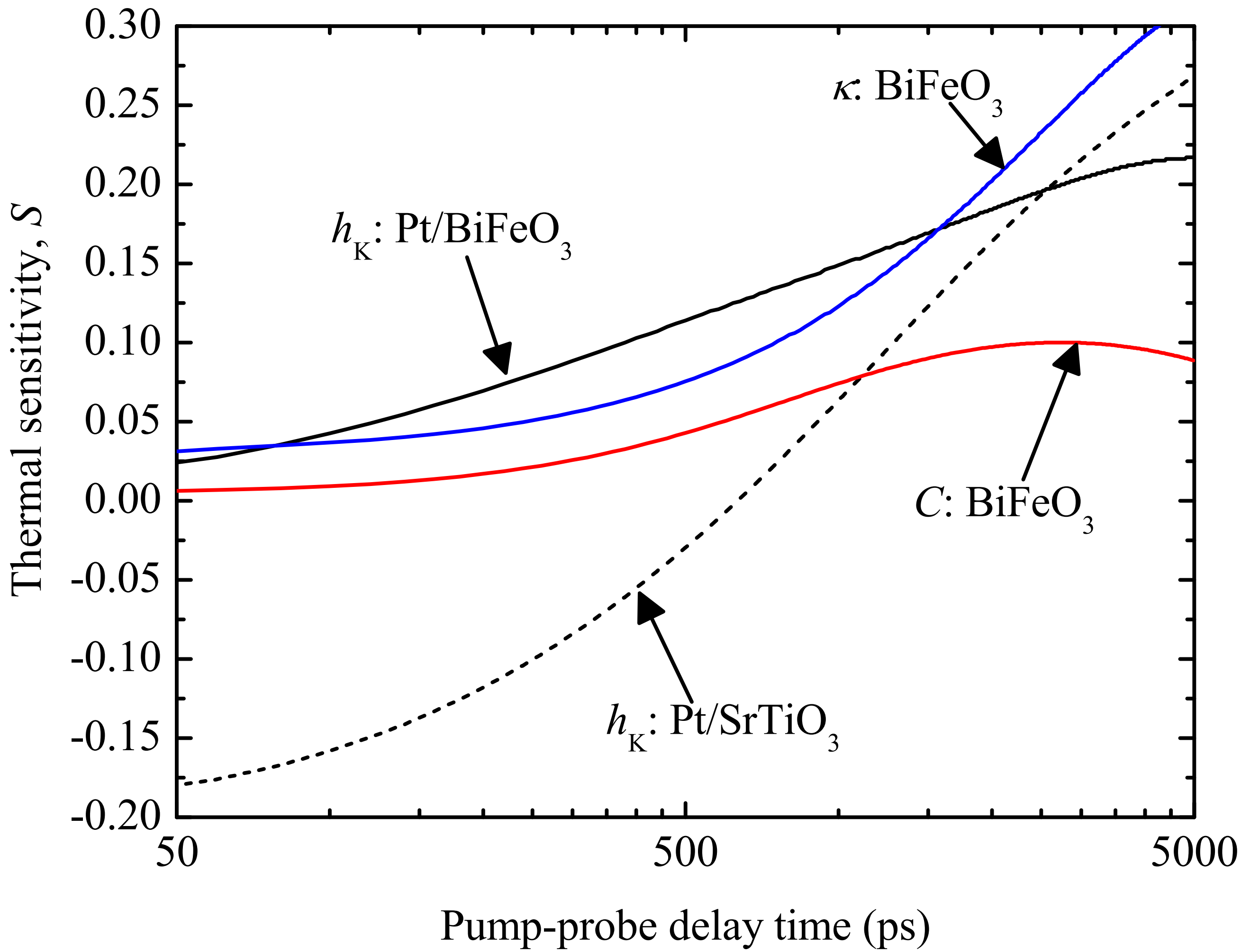
Single vs. poly PZT



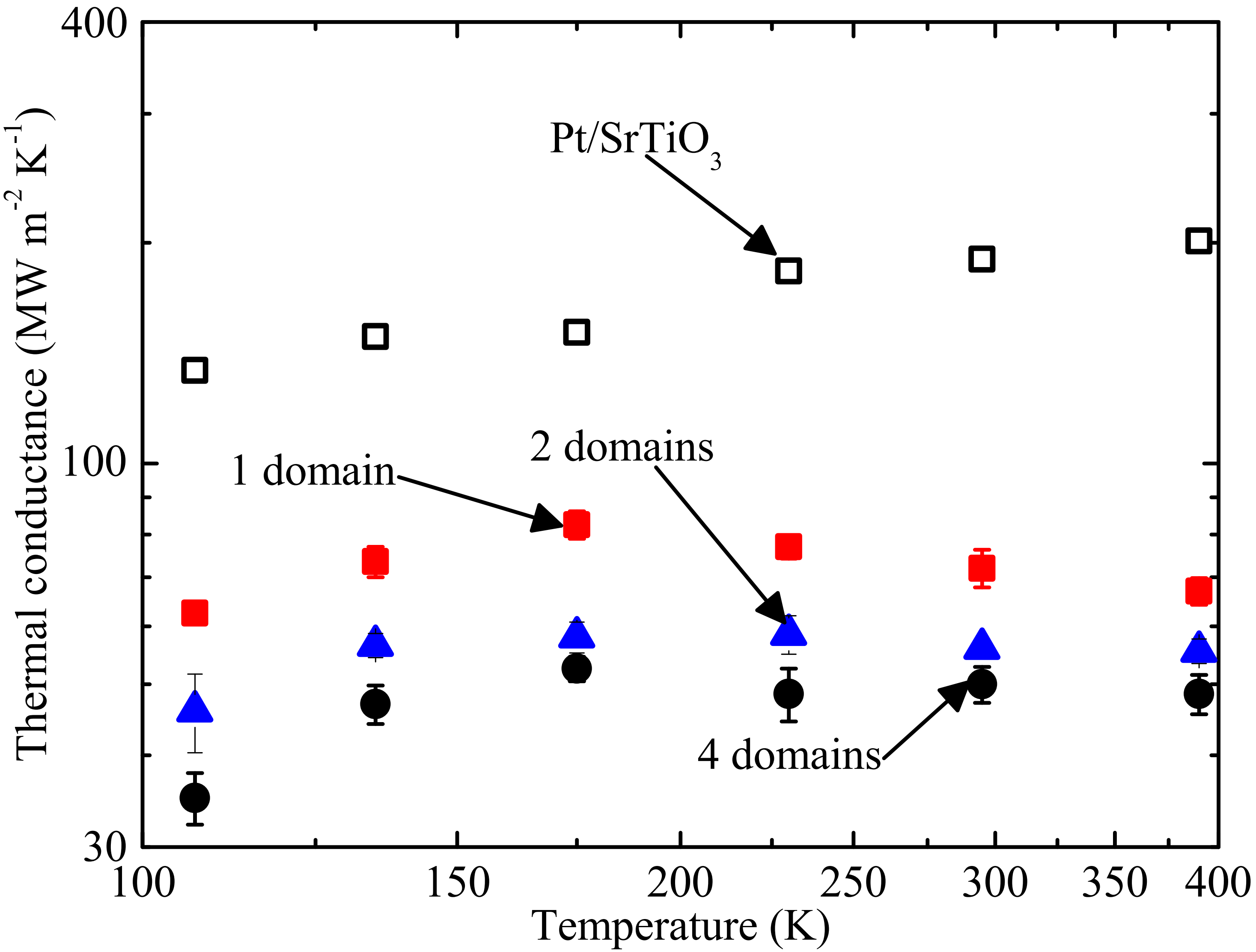




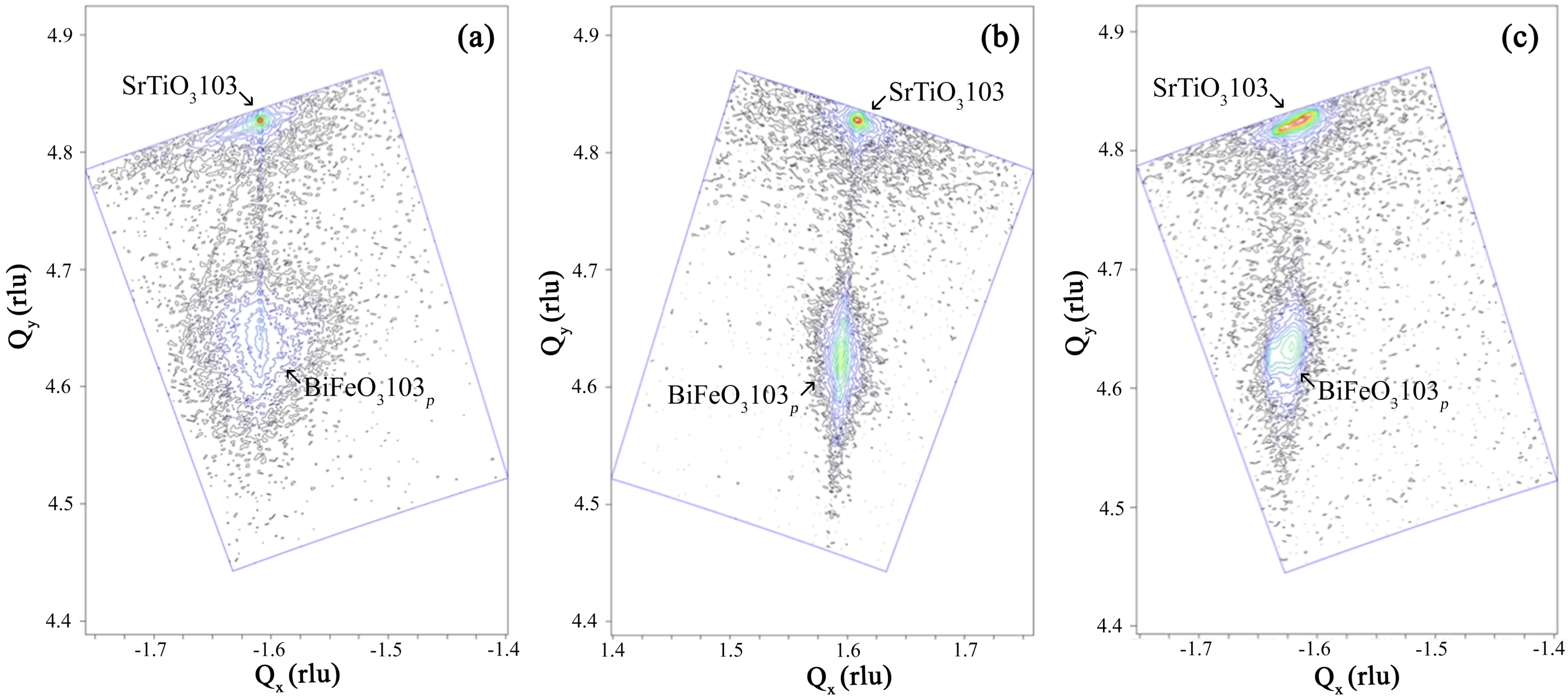
TDTR sensitivities – effective thermal conductivity



Conductance measurements



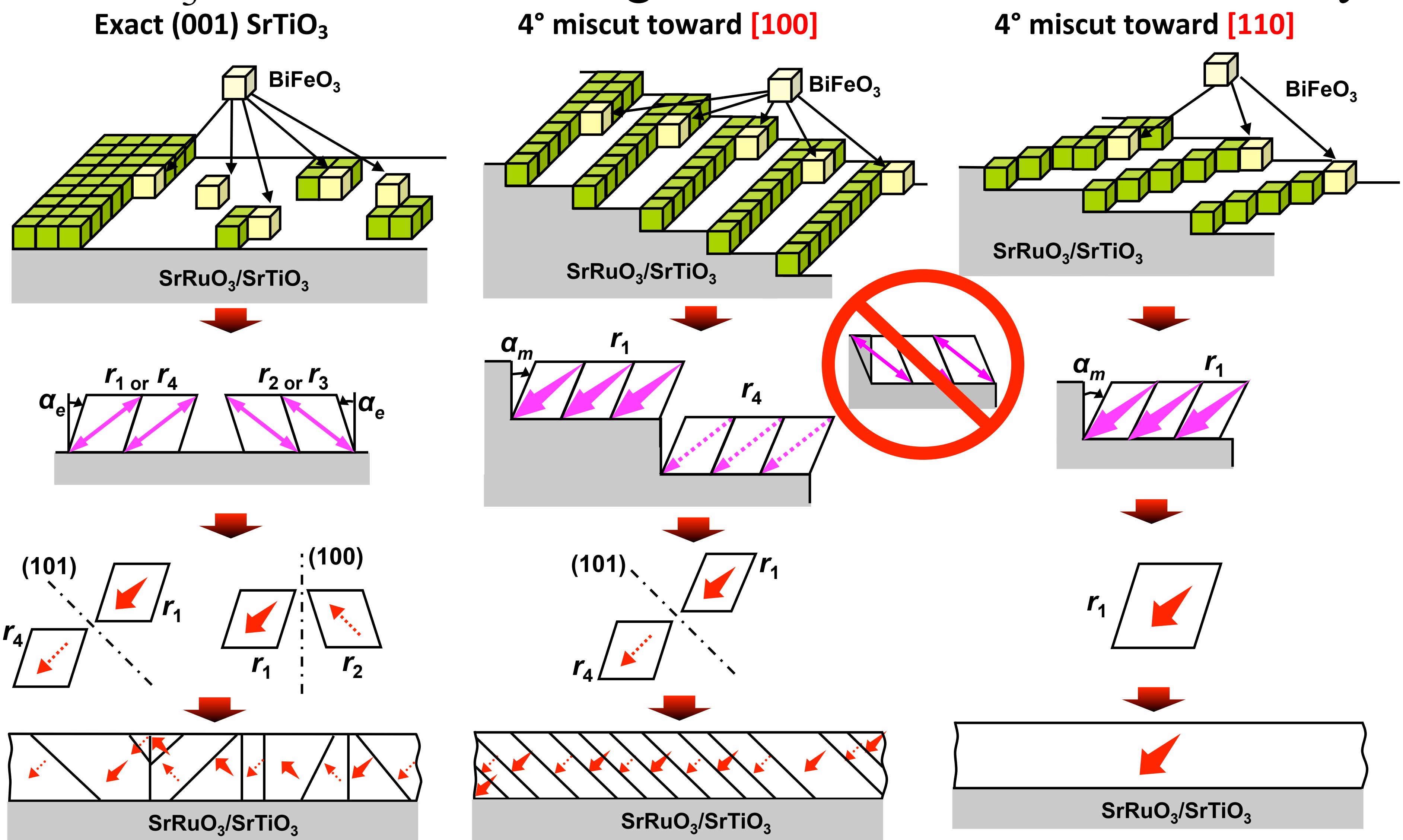
Reciprocal space mapping



“Coherent” interfaces – Domain boundaries

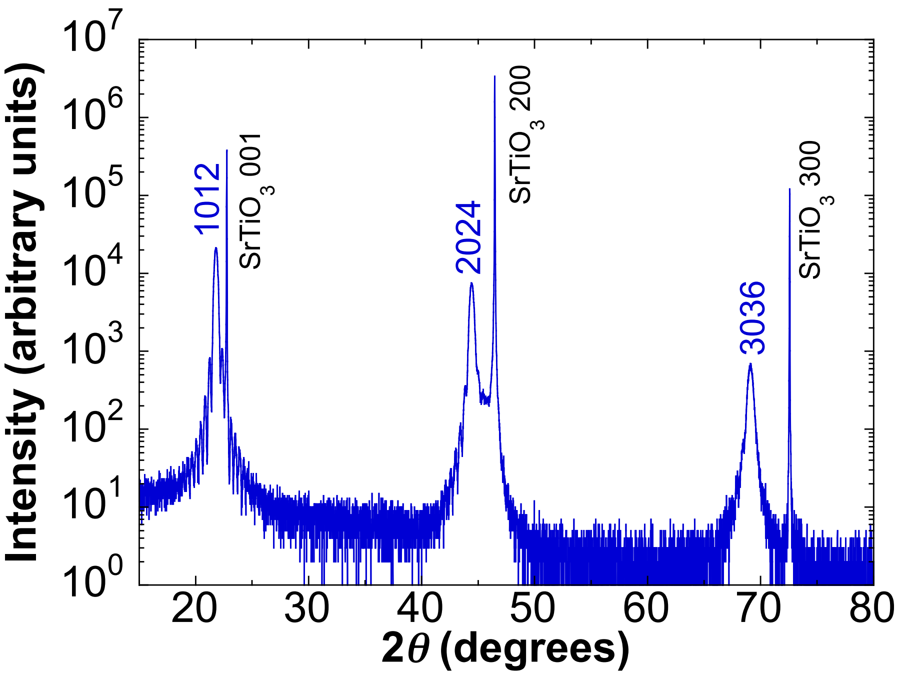
Slide courtesy of Chang-Beom Eom and Jon Ihlefeld

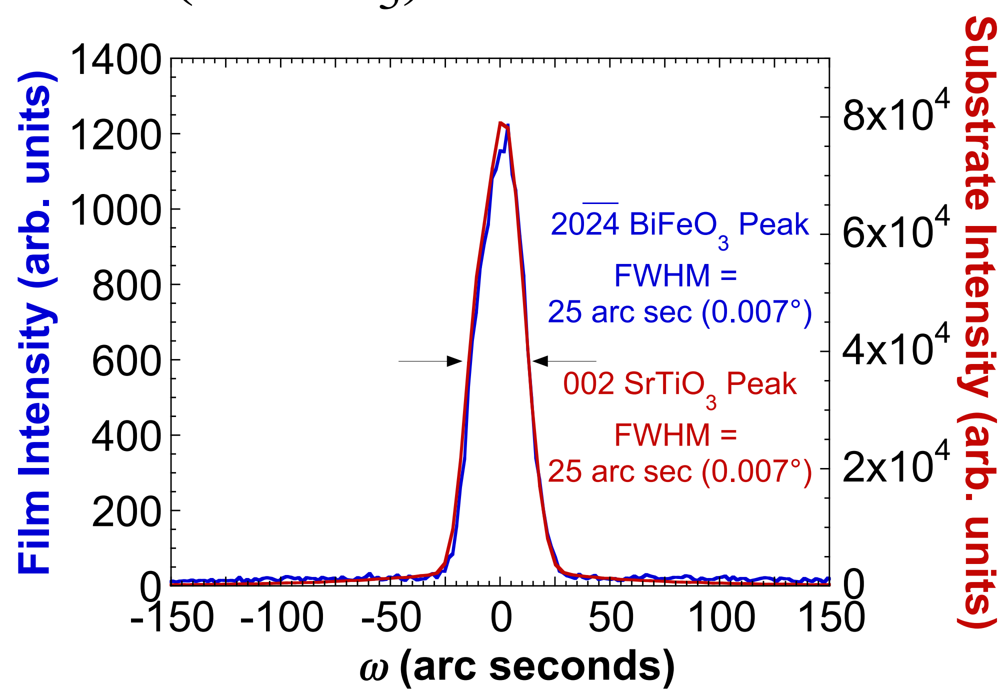
- Domain boundaries – other types of coherent interfaces
- $BiFeO_3$ domains can be engineered with substrate vicinality



BiFeO$_3$ film growth

- Reactive molecular-beam epitaxy: 30 nm BiFeO$_3$ films on SrTiO$_3$ substrates
- Phase-pure
- Smooth surface and interface
- Crystallinity limited by substrate (SrTiO$_3$)





Ihlefeld *et al*. *Appl. Phys. Lett.* **91**, 071922 (2007)

Does this make sense?

- Coherent domain wall scatters phonons like incoherent grain boundary?
- What's the mechanism???

Attenuation (Akhieser):

$$\frac{1}{\tau_{\mathrm{Akhieser}}} \propto \omega^2$$

Rayleigh:

$$\frac{1}{\tau_{\mathrm{impurity}}} \propto \omega^4$$

Incoherent (like a grain boundary):

$$\frac{1}{\tau_{\mathrm{grain}}} \propto \frac{v}{d_{\mathrm{grain}}}$$