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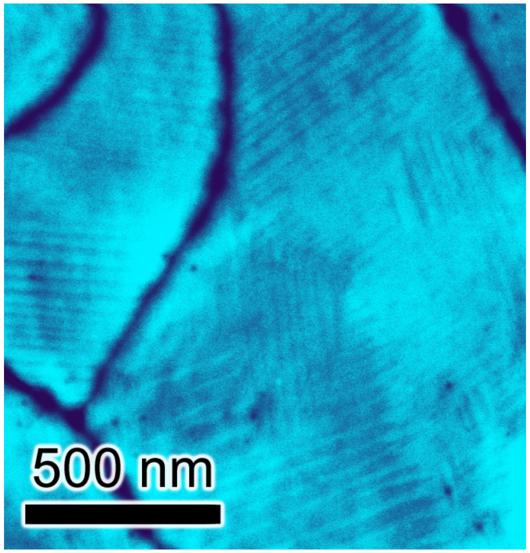

Thermal Conductivity and Phonon Scattering Mechanisms in Ferroelectric Thin Films

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NNSA National Nuclear Security Administration

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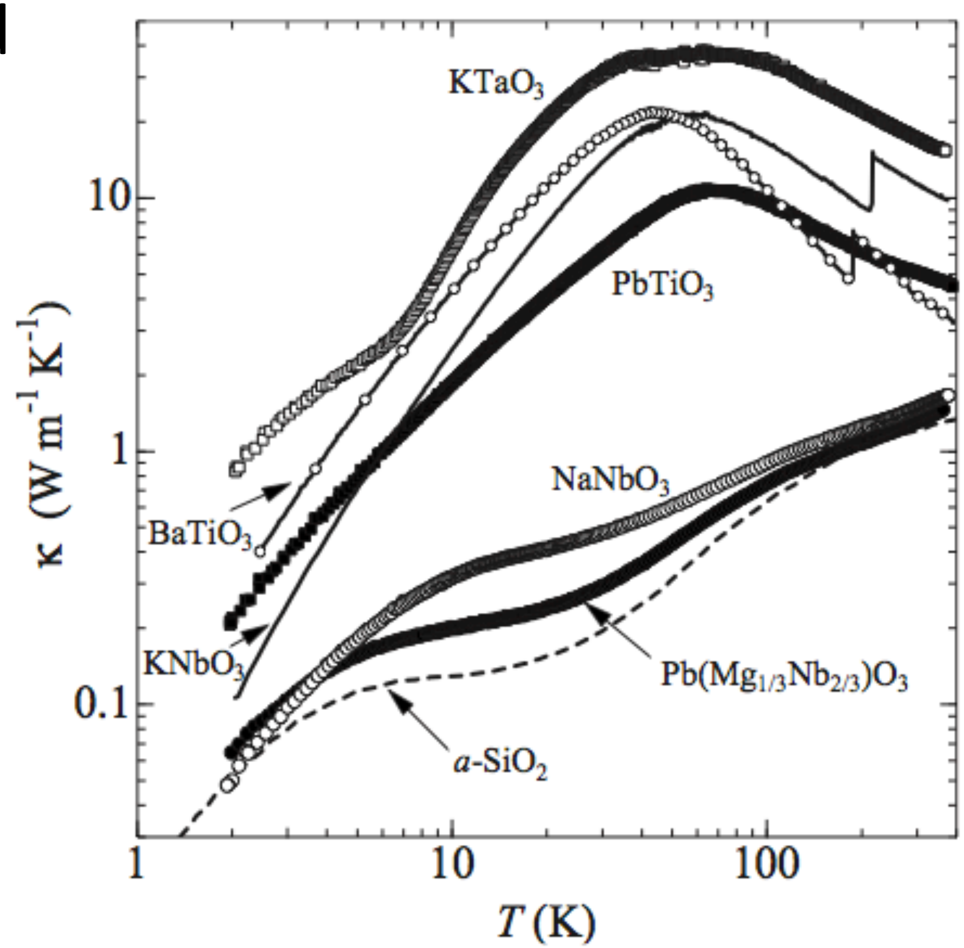
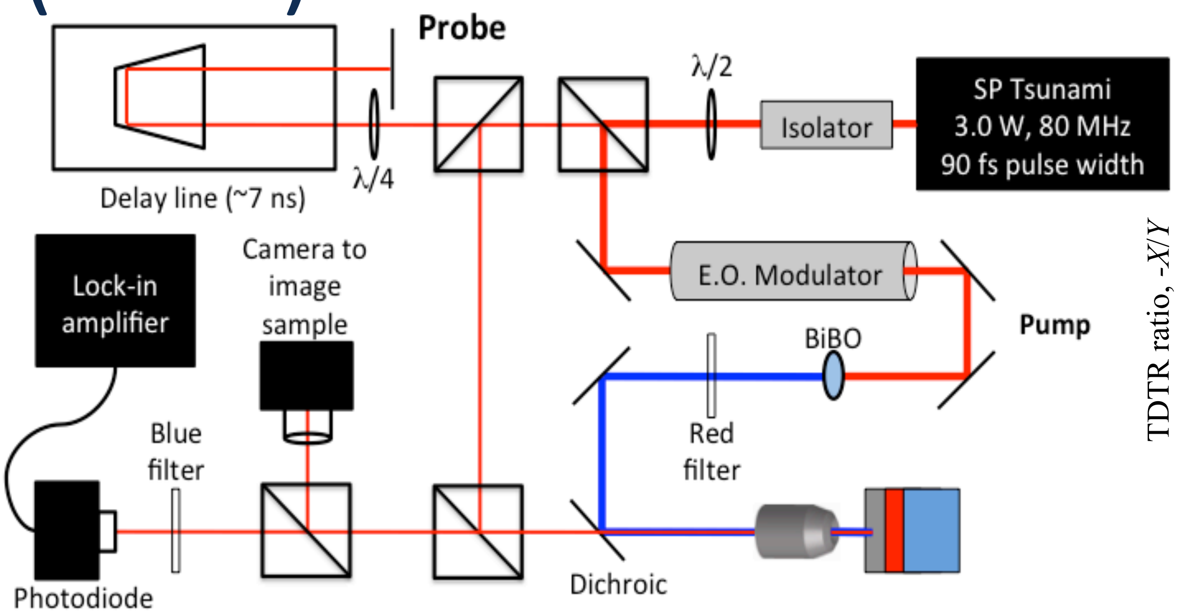
Thermal Conductivity of Ferroelectrics

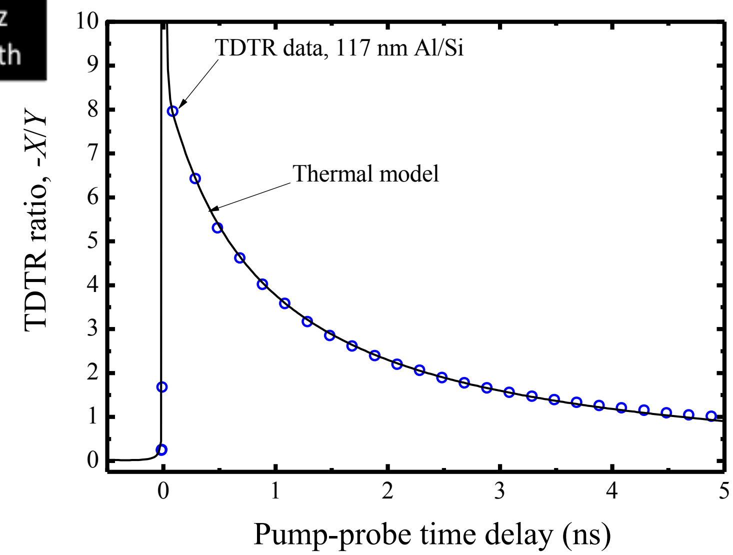
- Ferroelectrics and related materials can have low thermal conductivities
  - Complex phonon spectra
  - Soft modes
  - Anisotropy
- What about the role of boundaries?
  - Grain boundaries
  - Weakly bound interfaces
  - Domain boundaries

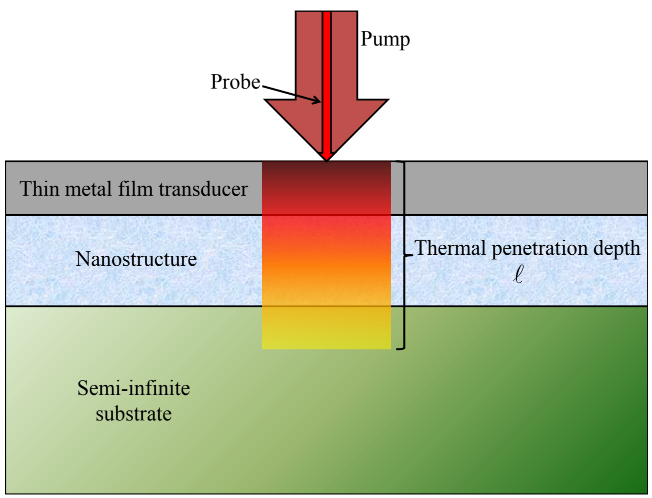
Thermal Conductivity of Ferroelectric Single Crystals



Time Domain ThermoReflectance (TDTR)

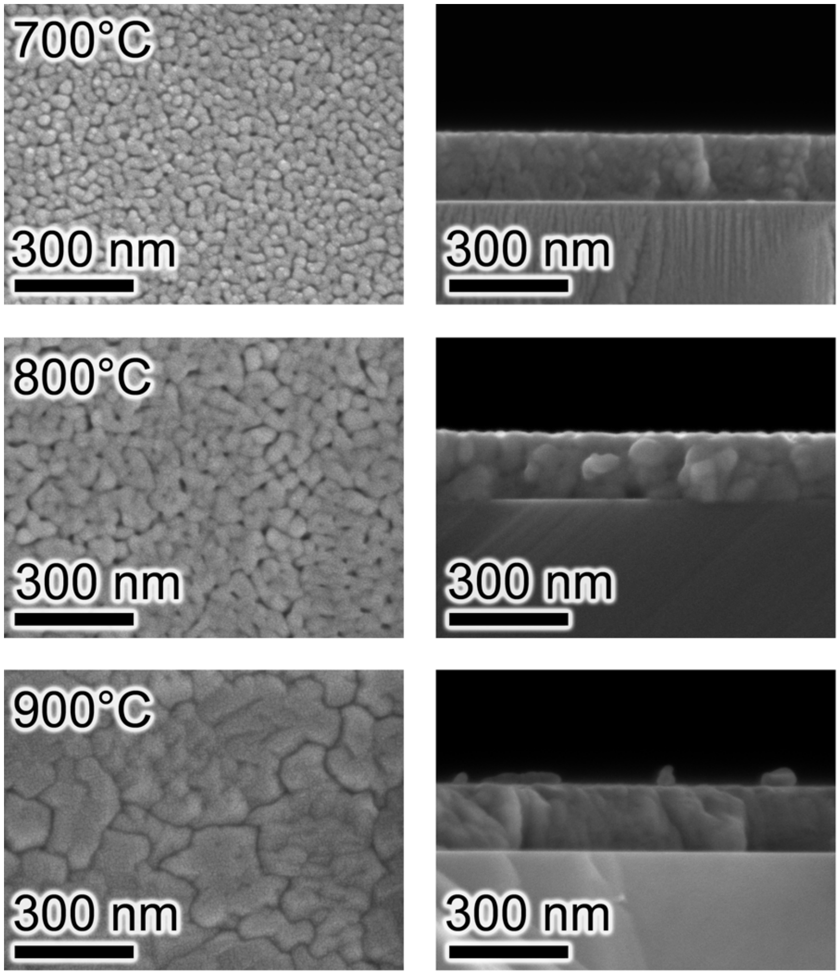


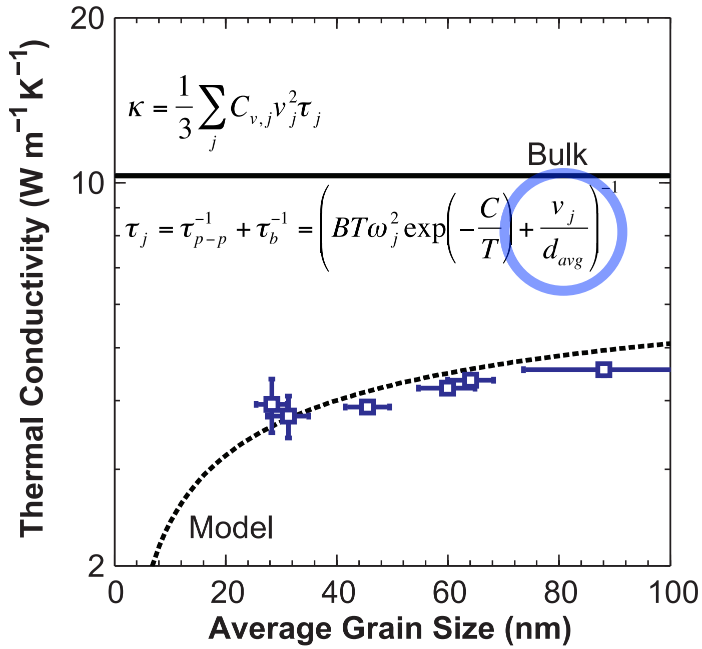




- Can measure thermal conductivity of thin films and substrates (k) separately from thermal boundary conductance (h_K)
- Nanometer spatial resolution (~10's of nm)
- Femtosecond to nanosecond temporal resolution
- Noncontact

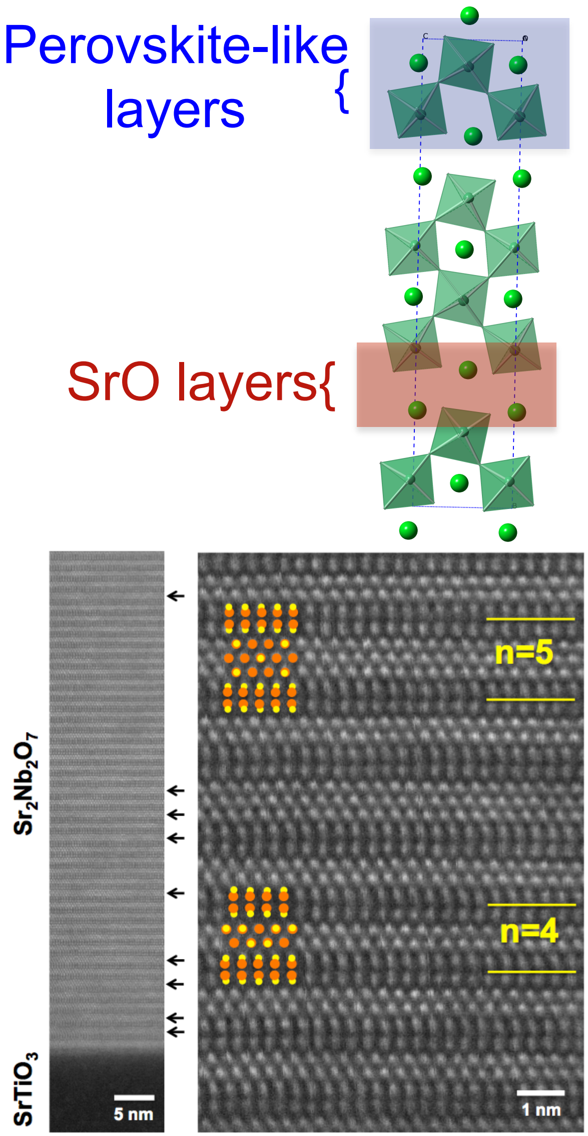
Grain Boundaries: $SrTiO_3$

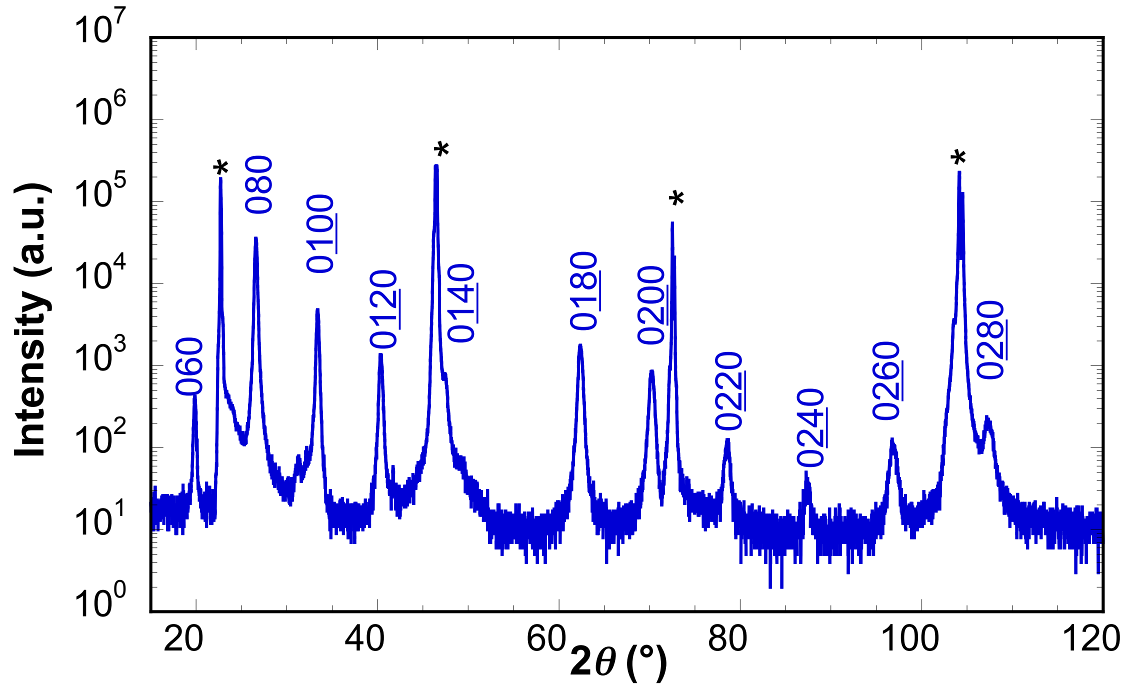




- Grain size series of $SrTiO_3$ prepared via CSD and altering processing temperature
- 3X reduction in thermal conductivity from single crystal value via nano-grain formation
- ***Grain boundary scattering dominates at fine sizes***

Coherent "Interfaces:" $Sr_2Nb_2O_7$

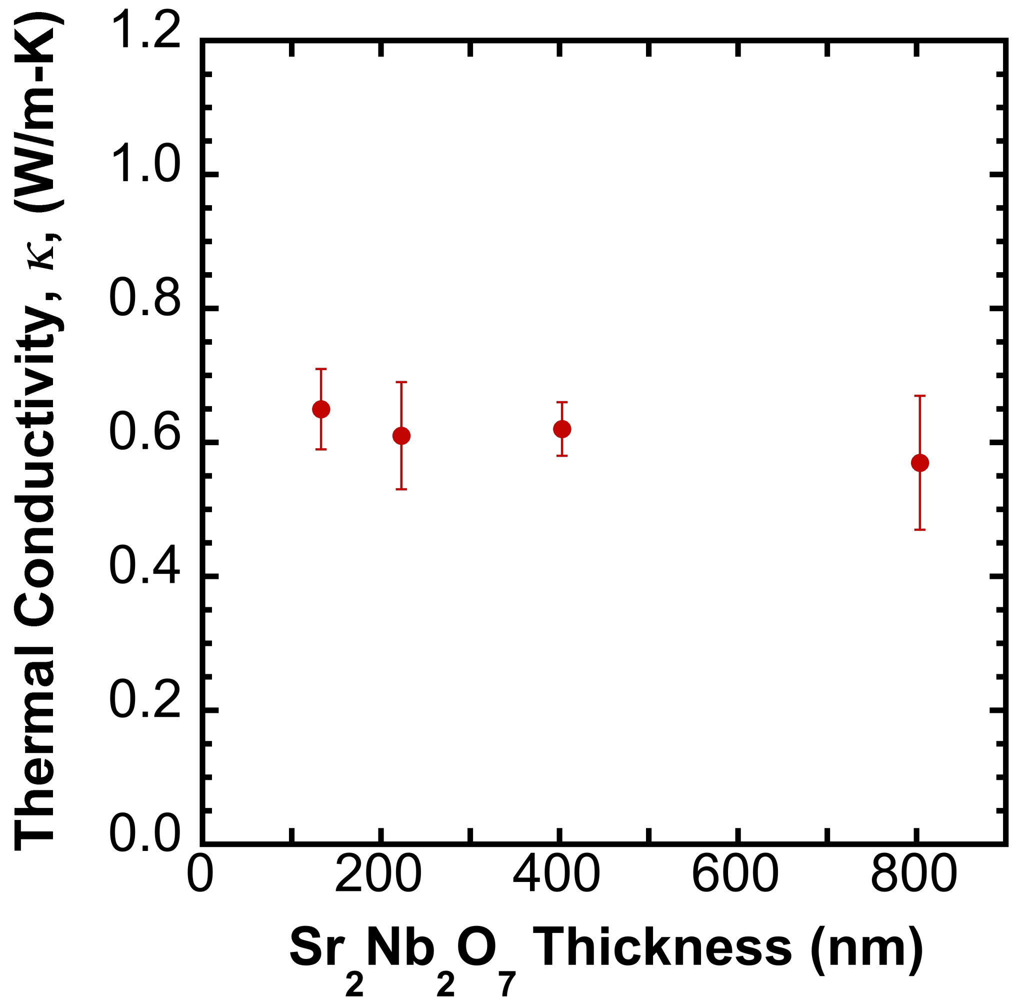




- CSD-derived thin films
- Forms *b*-axis oriented fiber texture on a variety of substrates
  - (001) $SrTiO_3$, *c*-plane Sapphire, polycrystalline Al_2O_3

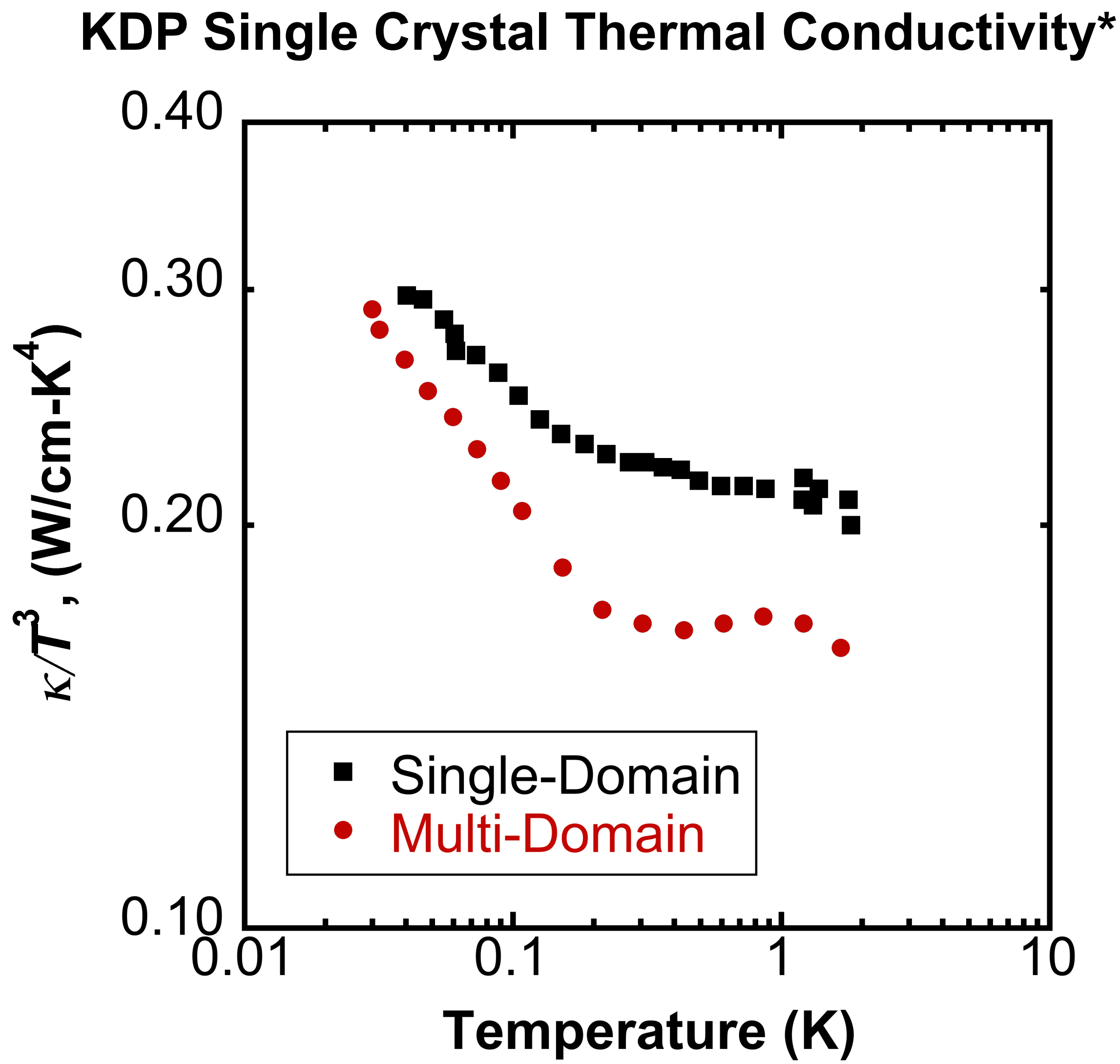
Coherent "Interfaces:" $Sr_2Nb_2O_7$

- Cross-plane thermal conductivity ~ 0.6 W/m-K
- Low thermal conductivity can be attributed to phonon scattering at the weakly bound SrO-SrO layers
- Substantially lower conductivity value than hot-forged ceramics*
  - Much greater degree of texture in thin films than ceramic counterparts (~1W/m-K)
- ***What about other coherent interfaces?***

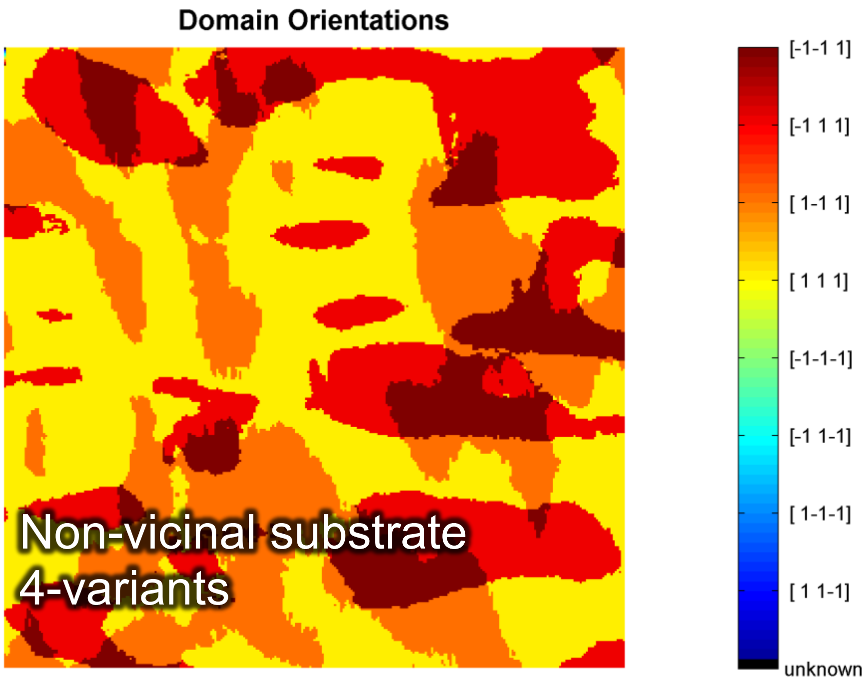


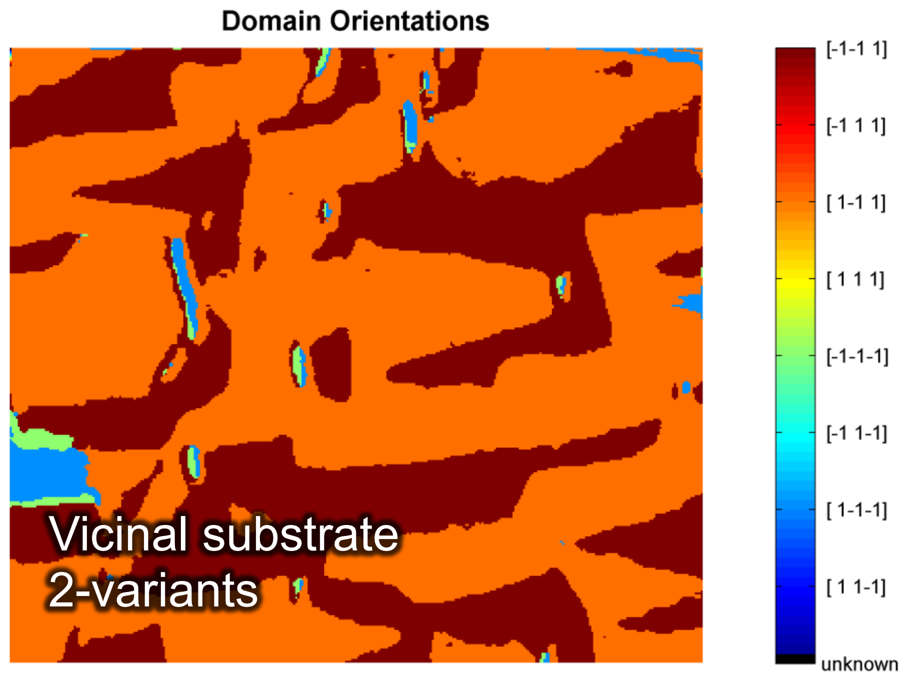
Coherent Interfaces: Domain Boundaries

- Strain and orientation changes across coherent interfaces are known to affect thermal conduction
- These two features both exist at ferroelastic domain walls
- We would therefore anticipate that ***domain boundaries can scatter phonons***
- What about domains in thin films?



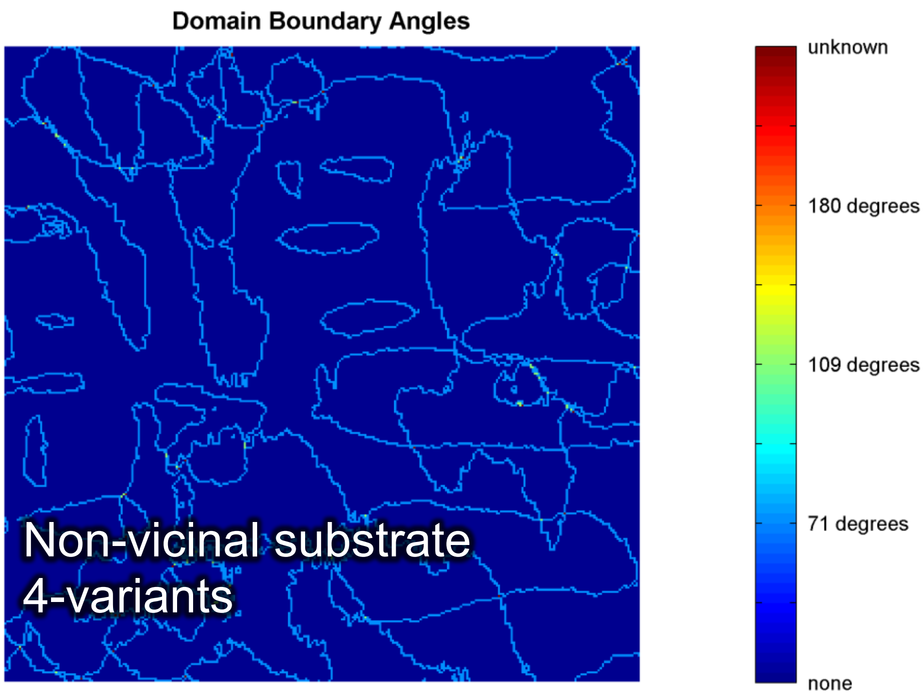
Domain Engineered $BiFeO_3$ Samples

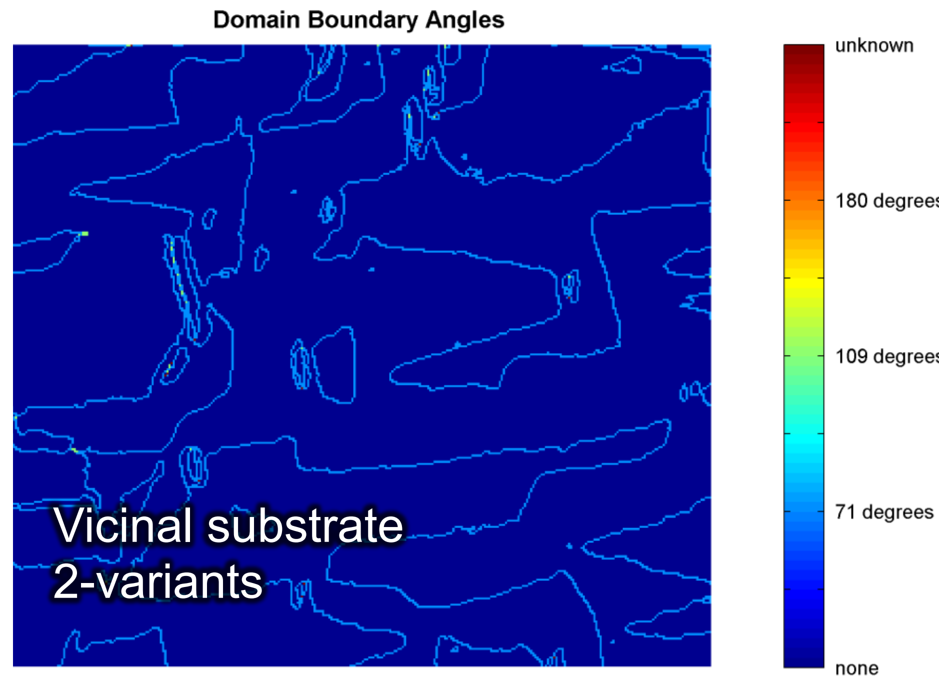




- 30 nm thick $BiFeO_3$ grown on non-vicinal and vicinal (001)-oriented $SrTiO_3$ substrates via reactive molecular-beam epitaxy
- Less complex domain assemblage for vicinal cuts
- Apparently fewer domain walls/area

Domain boundary quantification

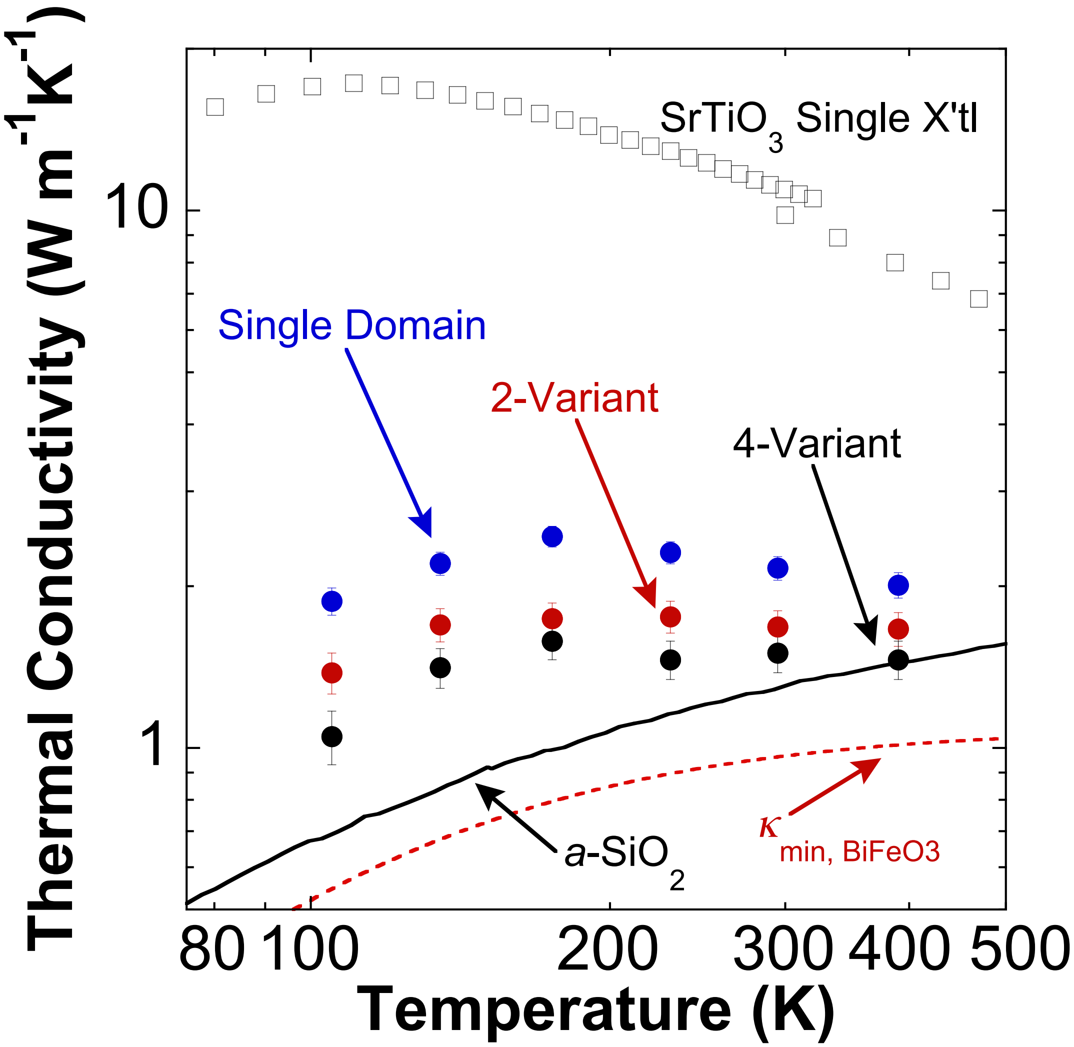




- Vector-Resolved PFM Characterization
  - Virtually all 71° domain walls
  - ***4-variant: 16 µm domain wall/μm^2***
  - ***2-variant: 11 µm domain wall/μm^2***
  - ***1-variant: no observable domain walls***

Thermal Conductivity of $BiFeO_3$

- 90 nm Platinum transducer patterned on films
- Effective thermal conductivities of $BiFeO_3$ <2.5 W/m-K
- Presence of domain walls reduces κ by ~30%.
- ***Domain walls appear to be scattering phonons***

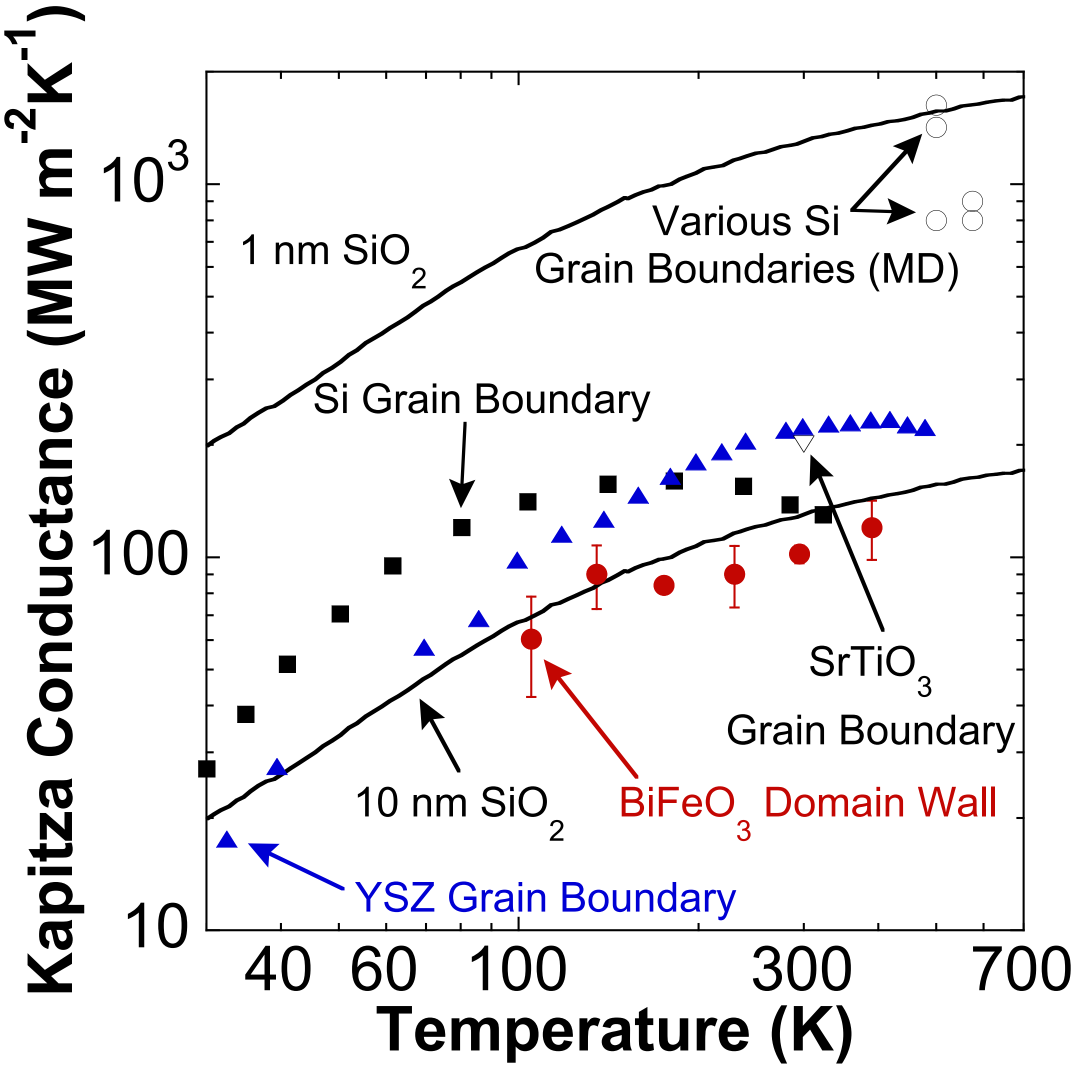


Domain Wall Kapitza Conductance

- Domain wall Kapitza conductance calculated from thermal conductivity data:

$$h_k = \frac{\kappa_0}{d\left(\frac{\kappa_0}{\kappa} - 1\right)}$$

- 71° $BiFeO_3$ domain walls have resistances greater than grain boundaries in similar materials



Summary

- In addition to grain boundaries, coherent interfaces including weakly bound layers and domain boundaries also scatter phonons
- Domain boundaries can scatter phonons even at room temperature
- We have developed a means to image domain structure *under applied field*
- We believe we have demonstrated the first room temperature thermal switch without utilizing a phase transition or physical separation