UNIVERSITY of VIRGINIA | SCHOOL of ENGINEERING & APPLIED SCIENCE

Thermal conductivity and heat capacity of dielectric and ferroelectric hafnium zirconium oxide thin films

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APPLIED PHYSICS LETTERS **113**, 192901 (2018)

Thermal resistance and heat capacity in hafnium zirconium oxide ($Hf_{1-x}Zr_xO_2$) dielectrics and ferroelectric thin films

Ethan A. Scott,[1] Sean W. Smith,[2] M. David Henry,[2] Christina M. Rost,[1] Ashutosh Giri,[1] John T. Gaskins,[1] Shelby S. Fields,[3] Samantha T. Jaszewski,[3] Jon F. Ihlefeld,[3,4] and Patrick E. Hopkins[1,3,5,a)]

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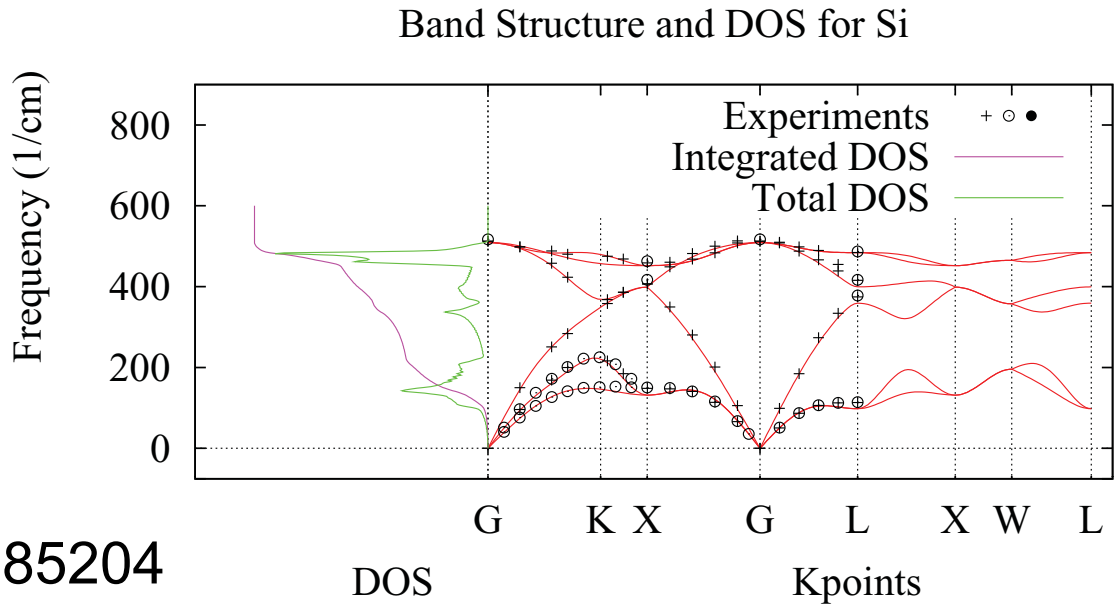
Thermal conductivity of materials - nanoscopic

$$\kappa = \frac{1}{3} C v \lambda = \frac{1}{3} C v_g^2 \tau$$

Heat capacity
(energy density of carriers)

Velocity
(how fast they move)

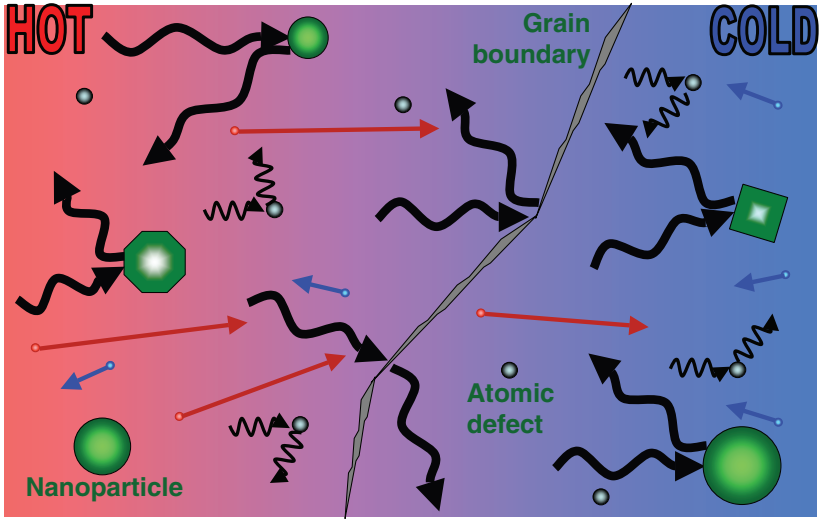


PRB **84**, 085204

Thermal conductivity of materials - nanoscopic

$$\kappa = \frac{1}{3} C v \lambda = \frac{1}{3} C v_g^2 \tau$$

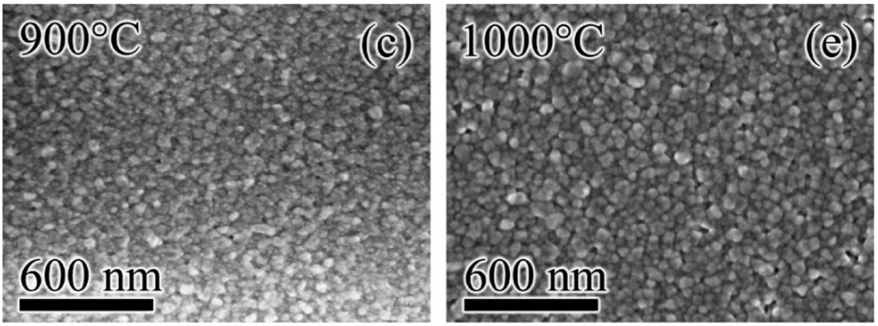
Mean free path/scattering time
(how often energy carriers scatter and lose energy)

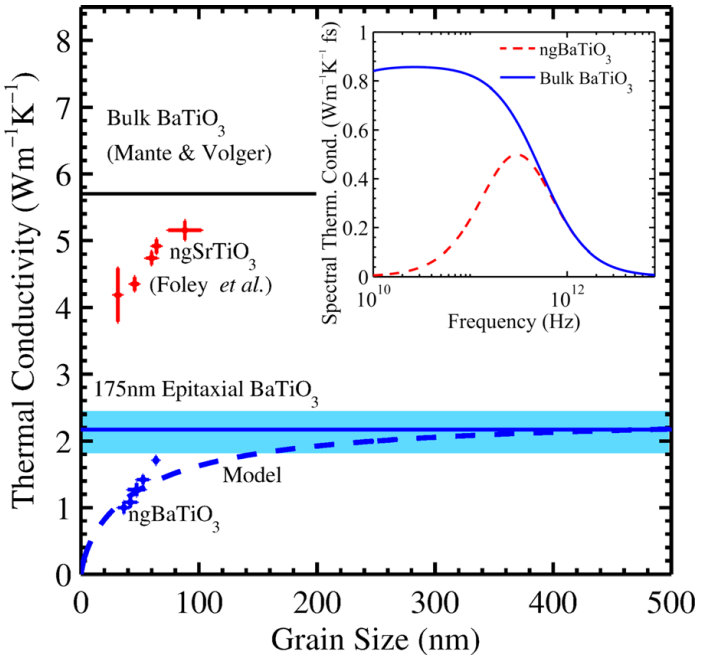


Adv. Mat. **22**, 3970

Classic example: Phonon boundary scattering and reduced κ

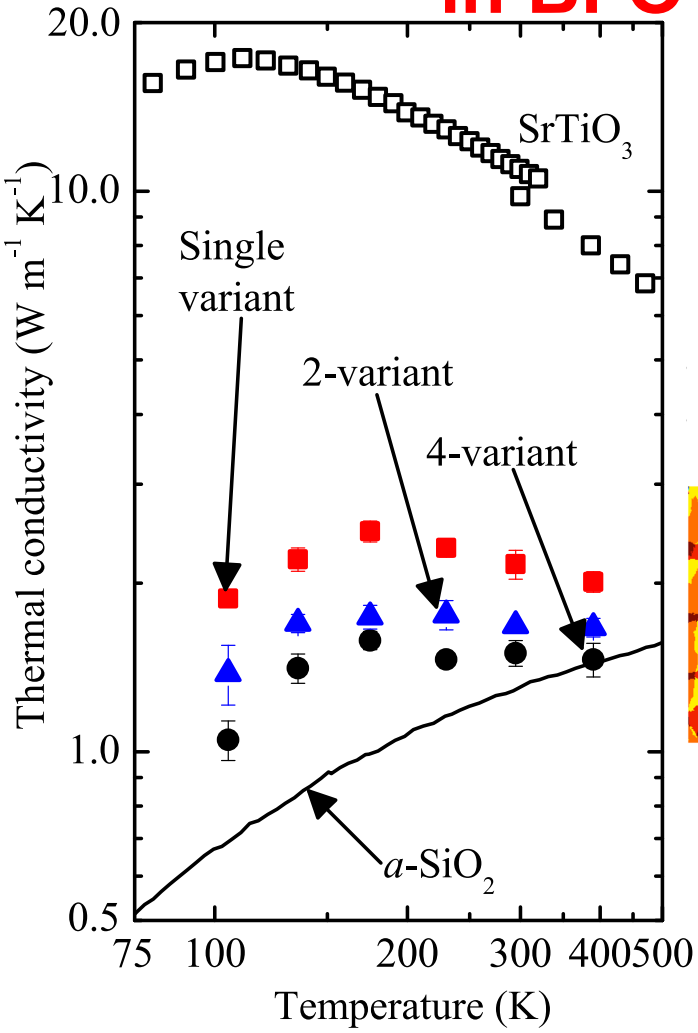
Grain boundaries in BTO

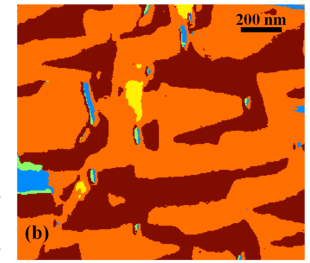




APL **105**, 082907

FE Domain boundaries in BFO

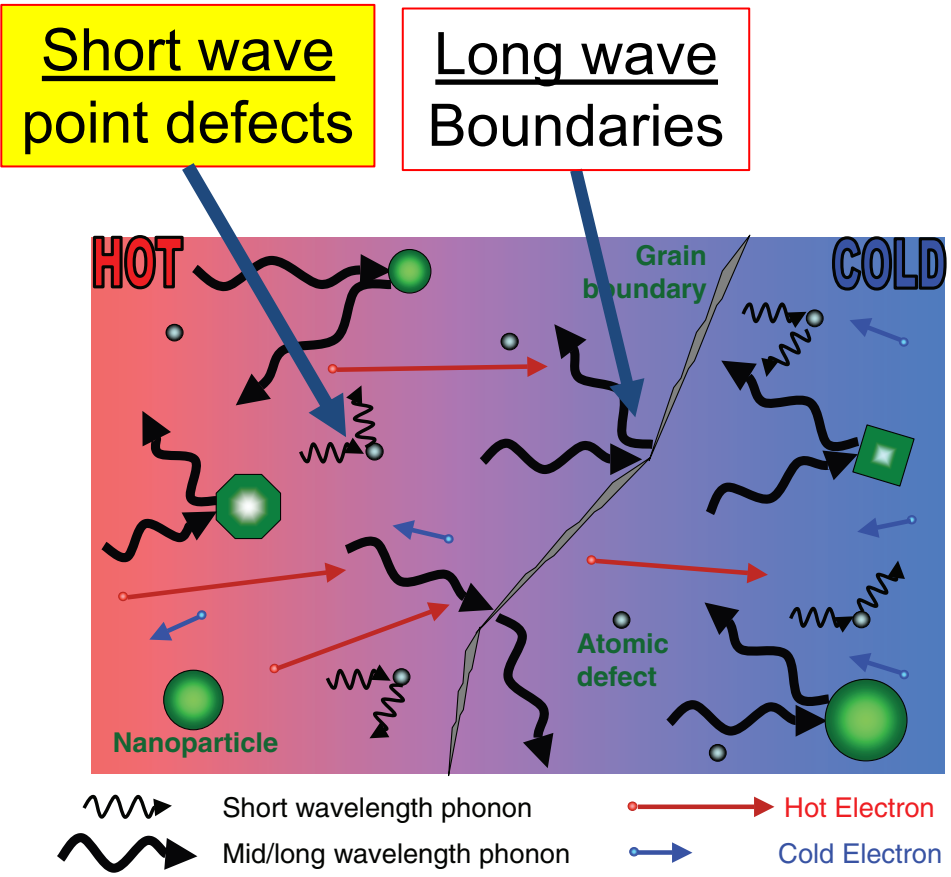




APL **102**, 121903

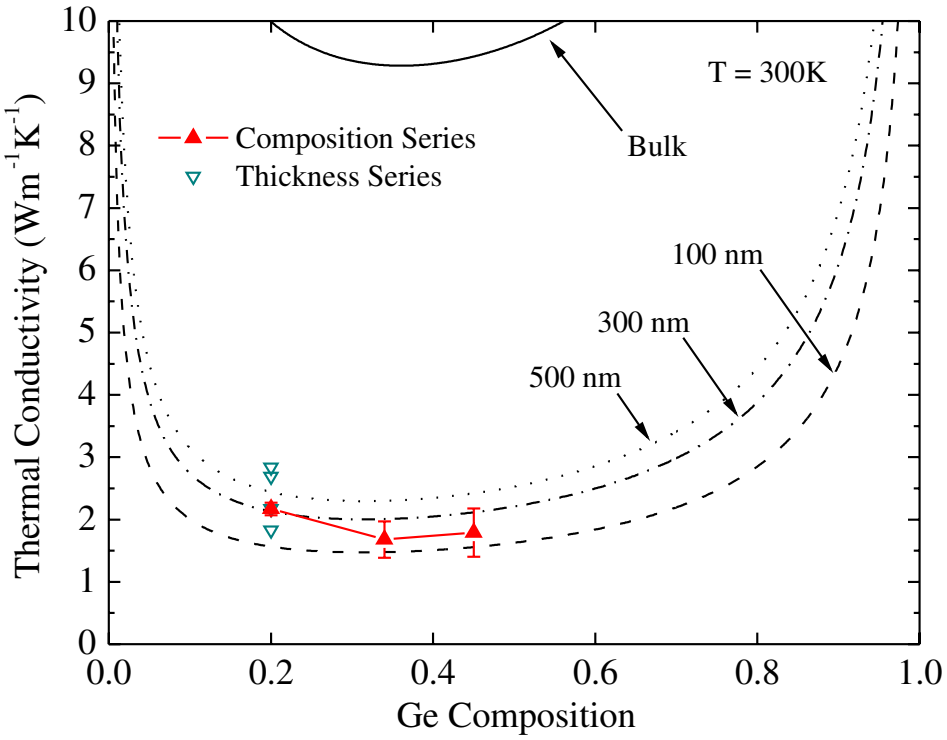
Spectral phonon transport in alloys

How do defects and interfaces play a role?



Adv. Mat. **22**, 3970

Thermal conductivity $Si_{1-x}Ge_x$ alloys



Phys. Rev. Lett. **109**, 195901

Spectral phonon transport in alloys

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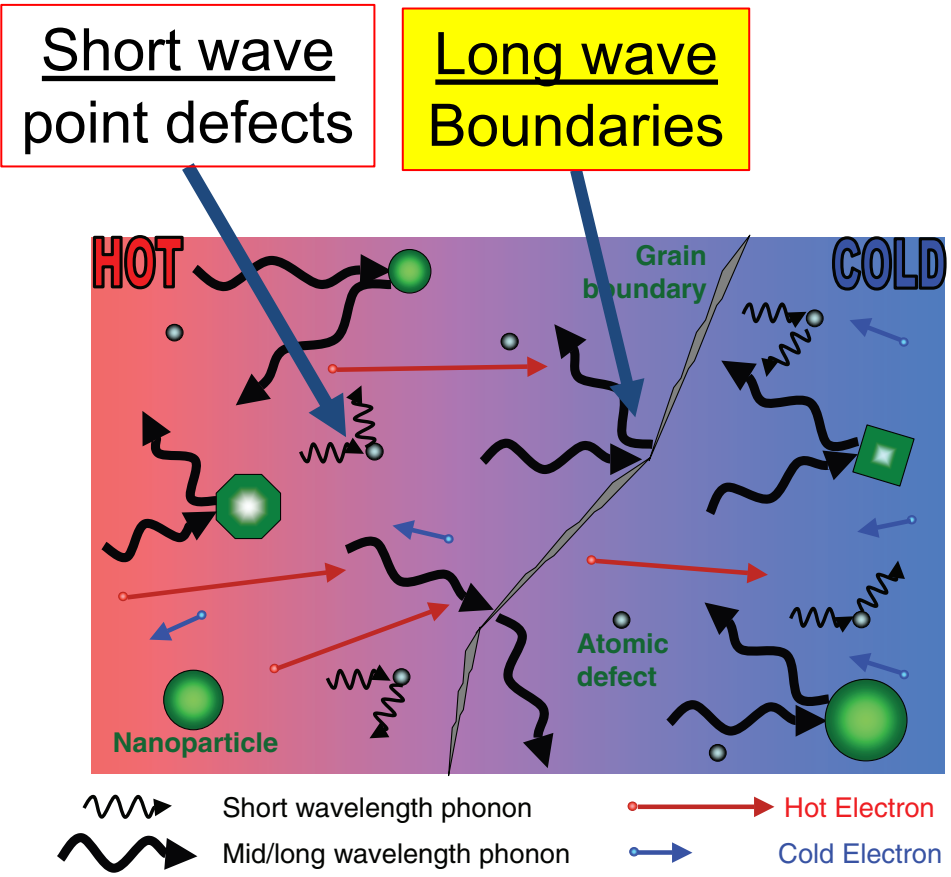
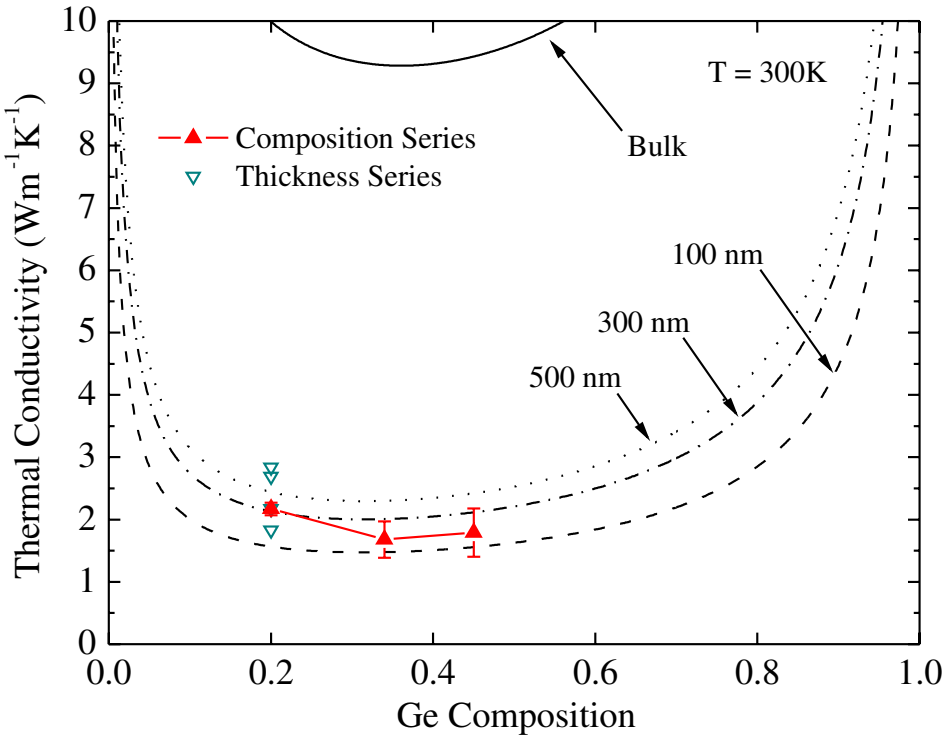


Adv. Mat. **22**, 3970

Thermal conductivity $Si_{1-x}Ge_x$ alloys



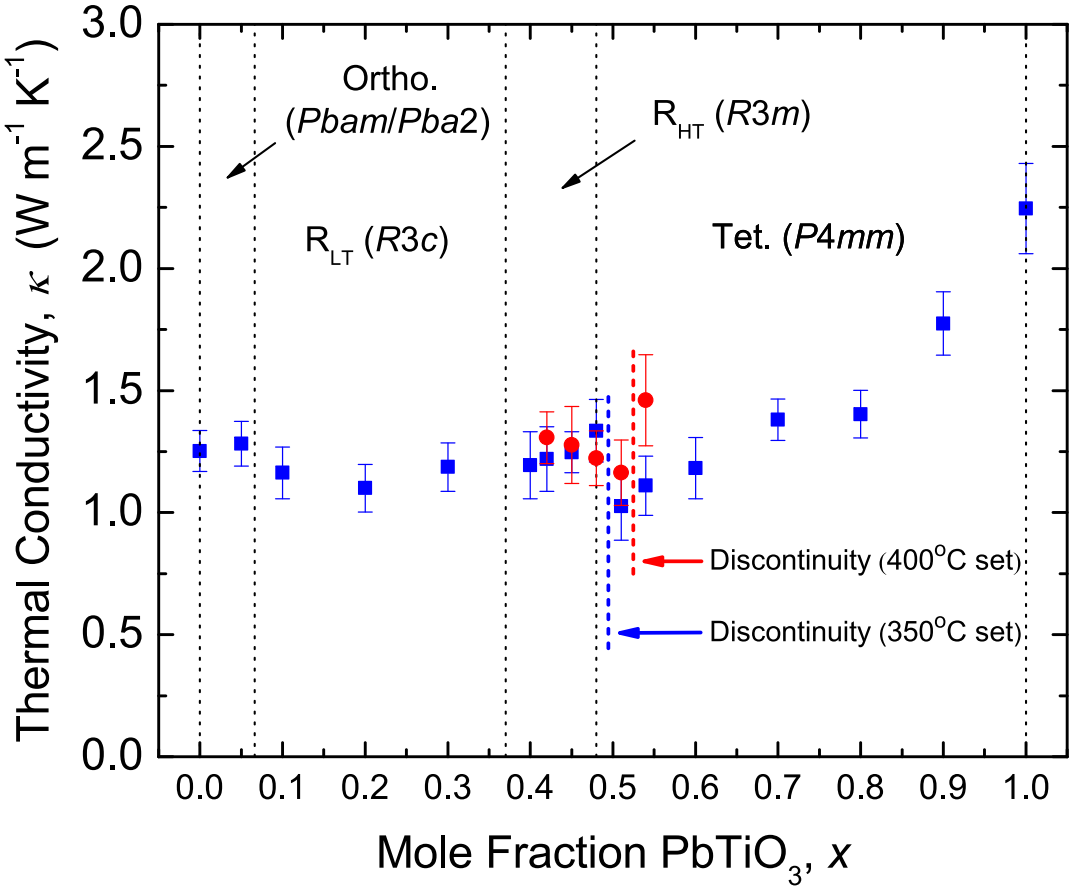
Phys. Rev. Lett. **109**, 195901

Spectral phonon transport in ferroelectric solid solutions

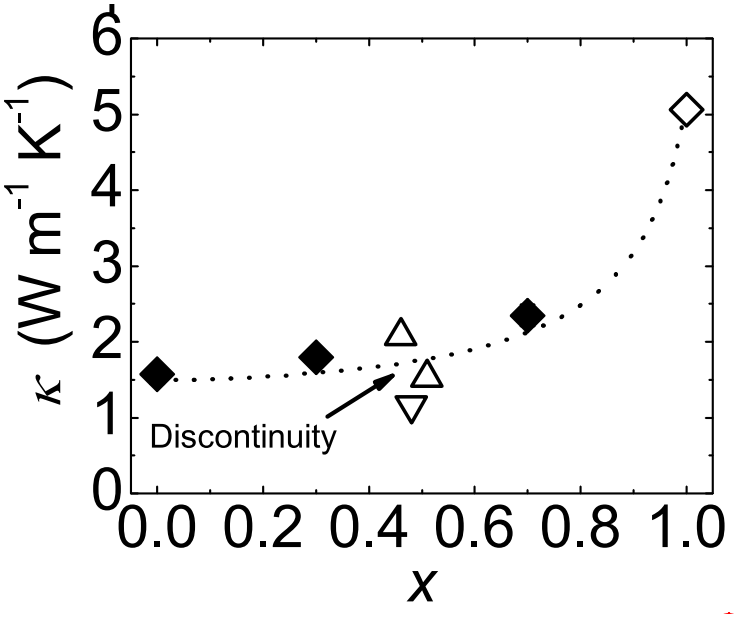
How do defects and interfaces play a role?

Thermal conductivity of PZT thin films

Thin film

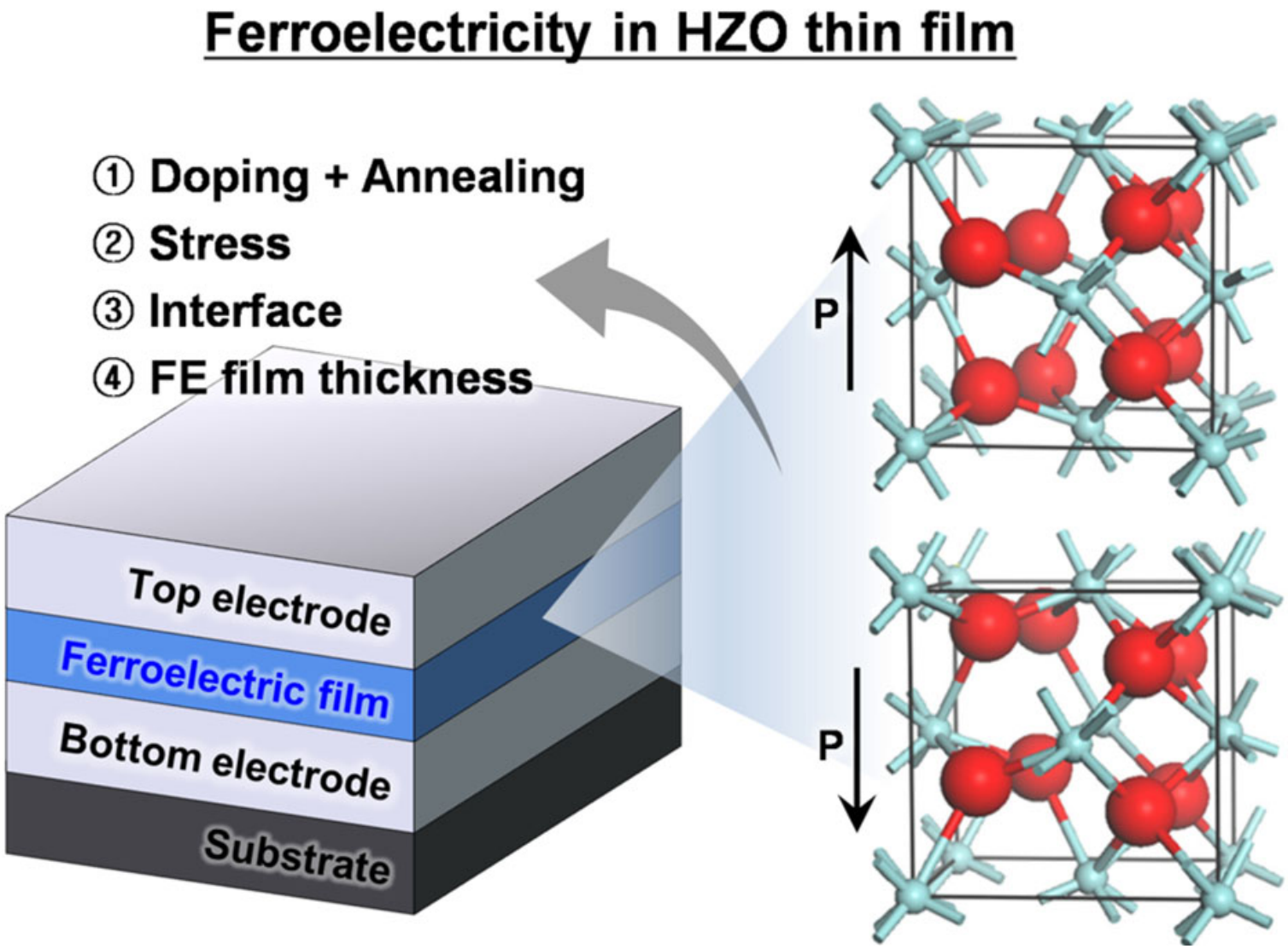


Bulk



J. Appl. Phys. **121**, 205104

This talk: Hafnium zirconium oxide thin films



JOM **71**, 246

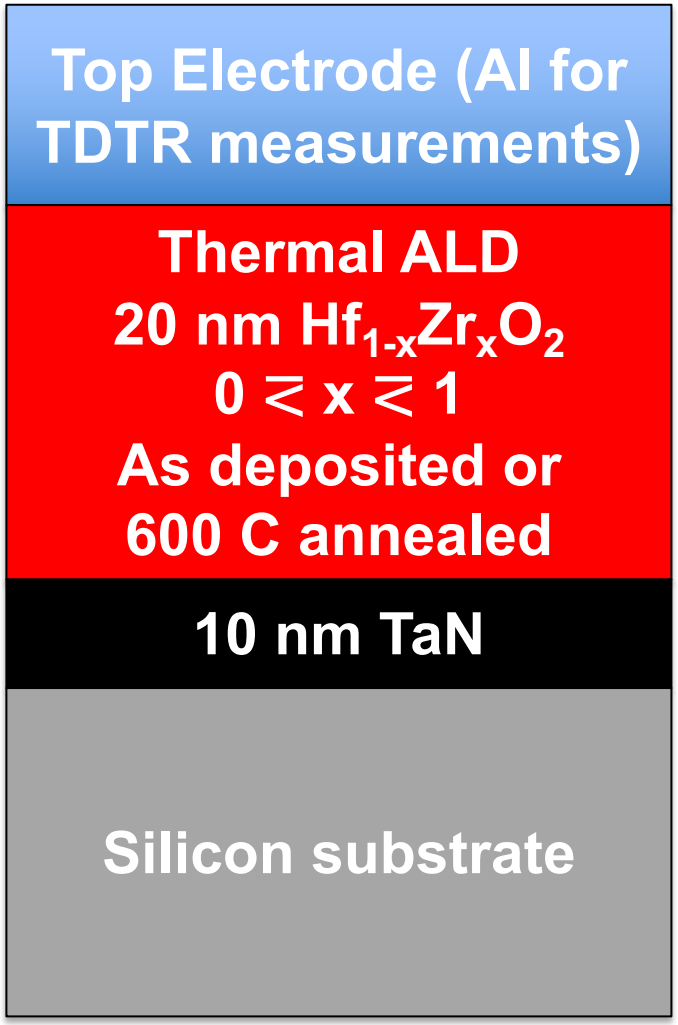
This talk: Hafnium zirconium oxide thin films

What are the phonon thermal transport mechanisms dictating the thermal conductivity of HZO thin films?

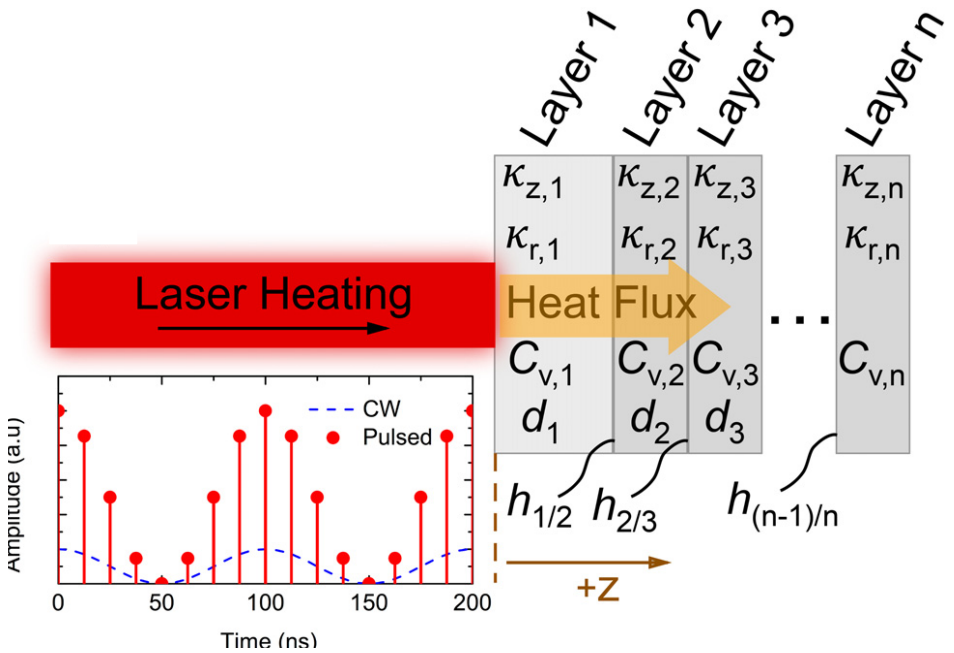
Interplay among:

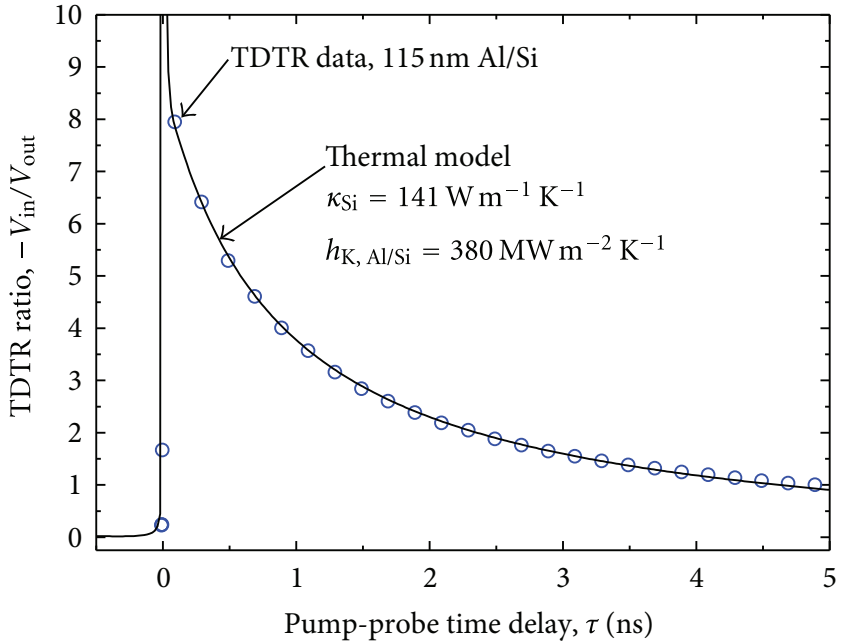
- Boundary scattering
- "Alloy" scattering (Hf and Zr masses)
- Crystalline (FE phase) vs. amorphous effects

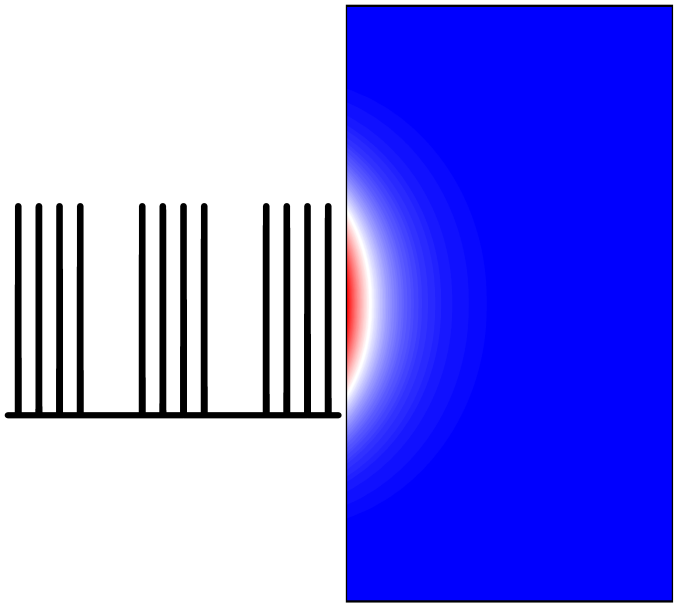
Can we measure heat capacity of 20 nm thick HZO film?



Measuring thermal conductivity in thin films: TDTR







TDTR Reviews and Analyses

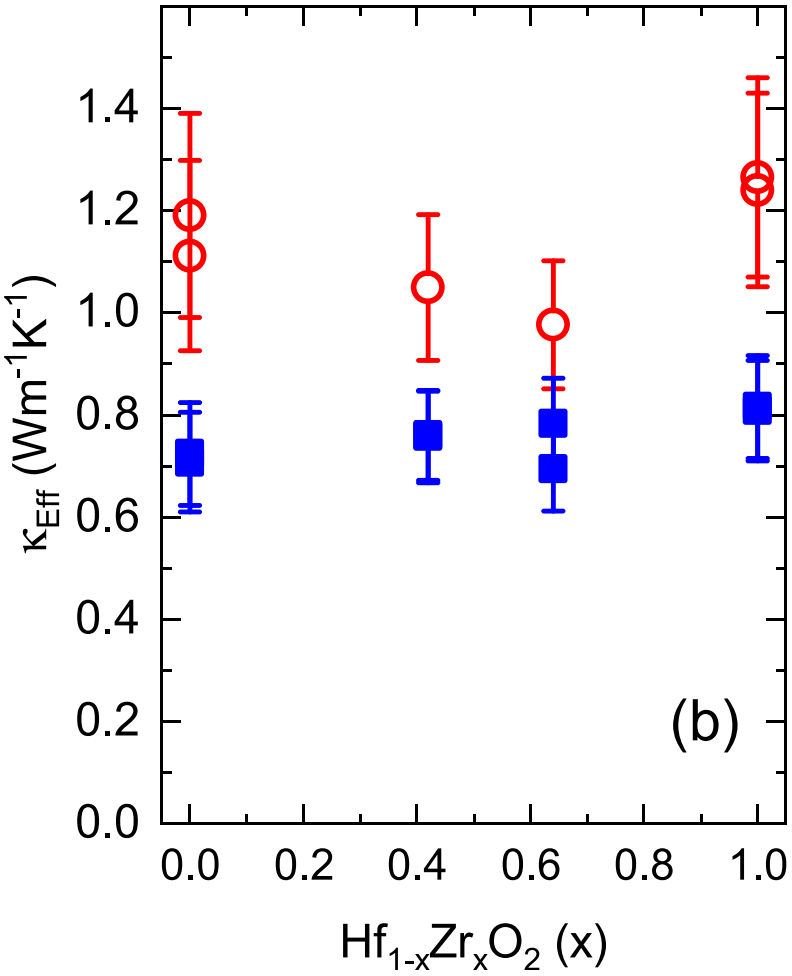
Rev. Sci. Instr. **75**, 5119

Rev. Sci. Instr. **79**, 114902

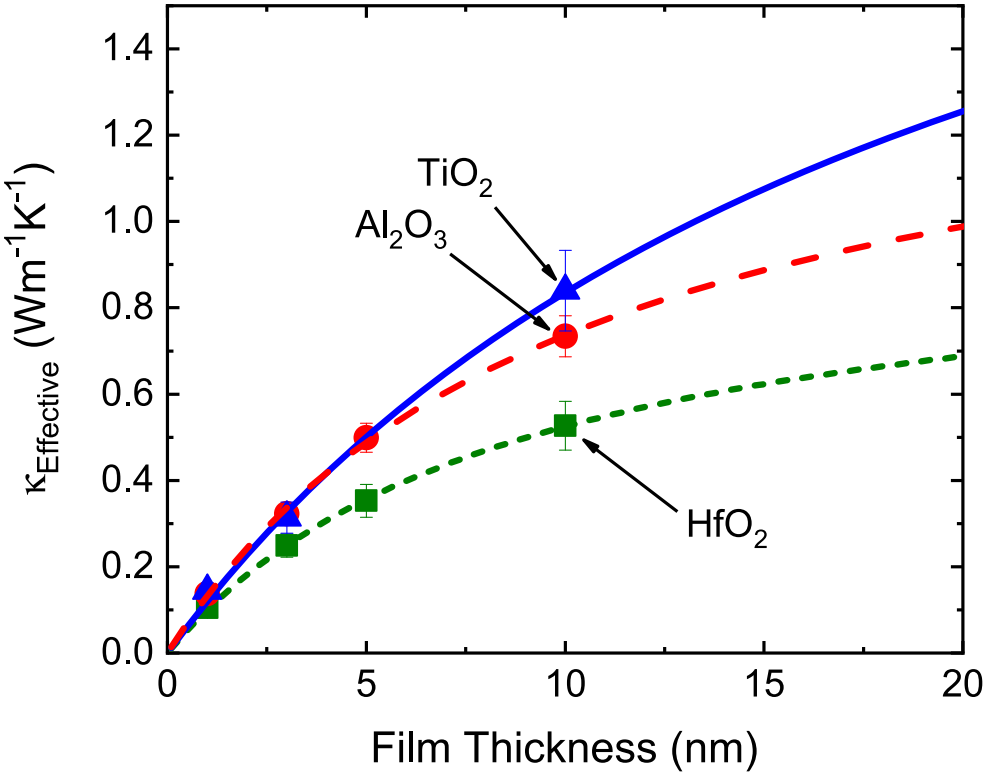
J. Heat Trans. **132**, 081302

Ann. Rev. Heat Trans. **16**, 159

Thermal conductivity of HZO thin films



- Increase in k due to crystallization
- Most likely boundary scattering limited
- Values similar to other ALD grown films



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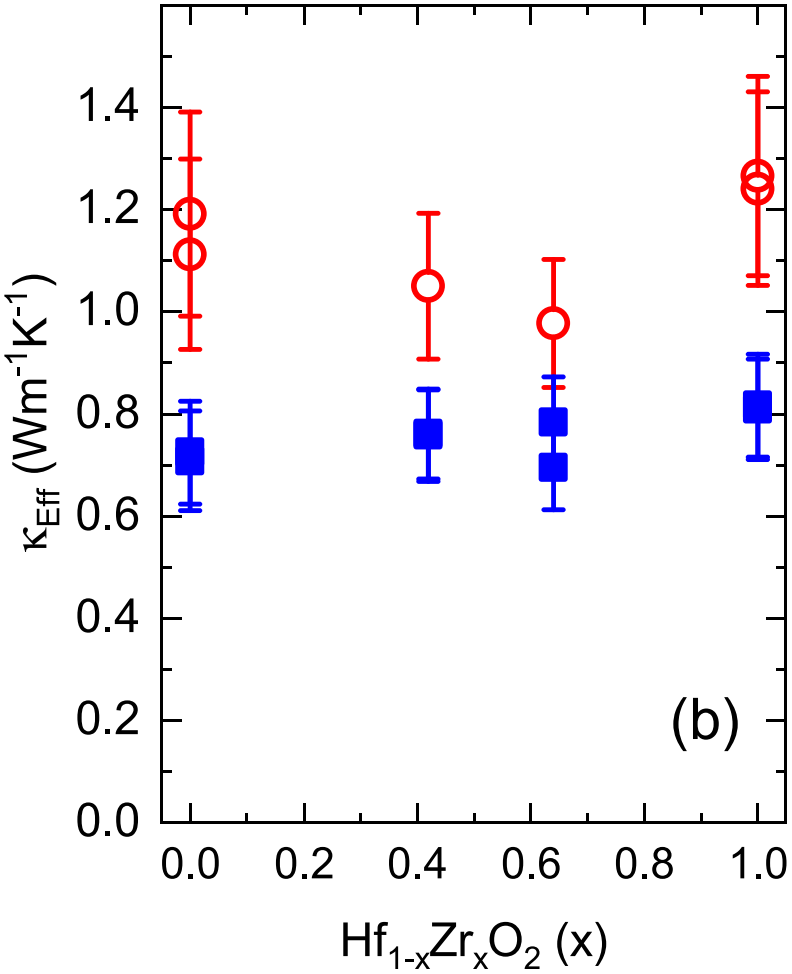
APL Materials **6**, 058302

Thermal conductivity of HZO thin films



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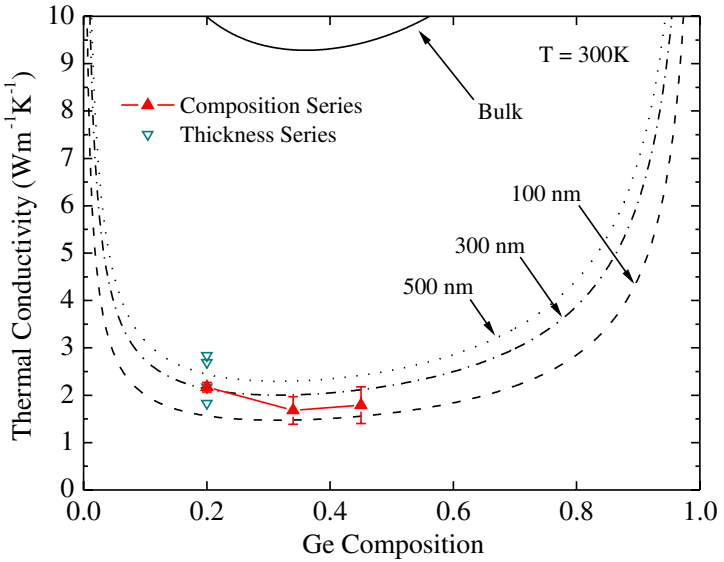
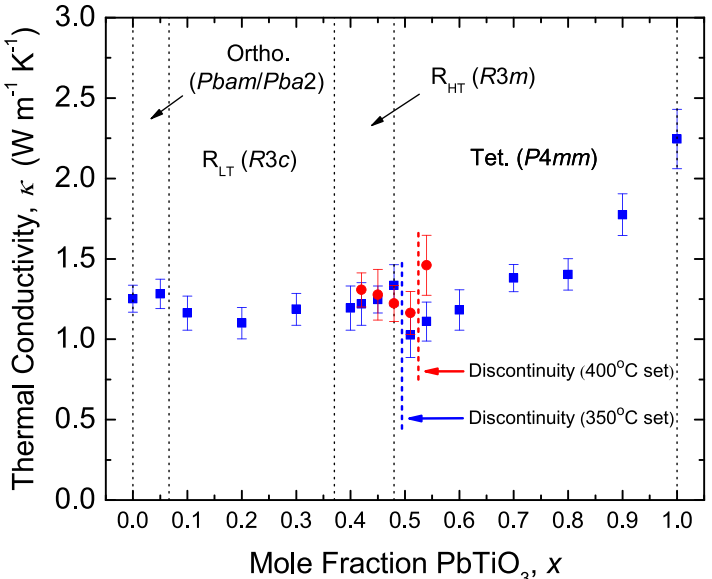
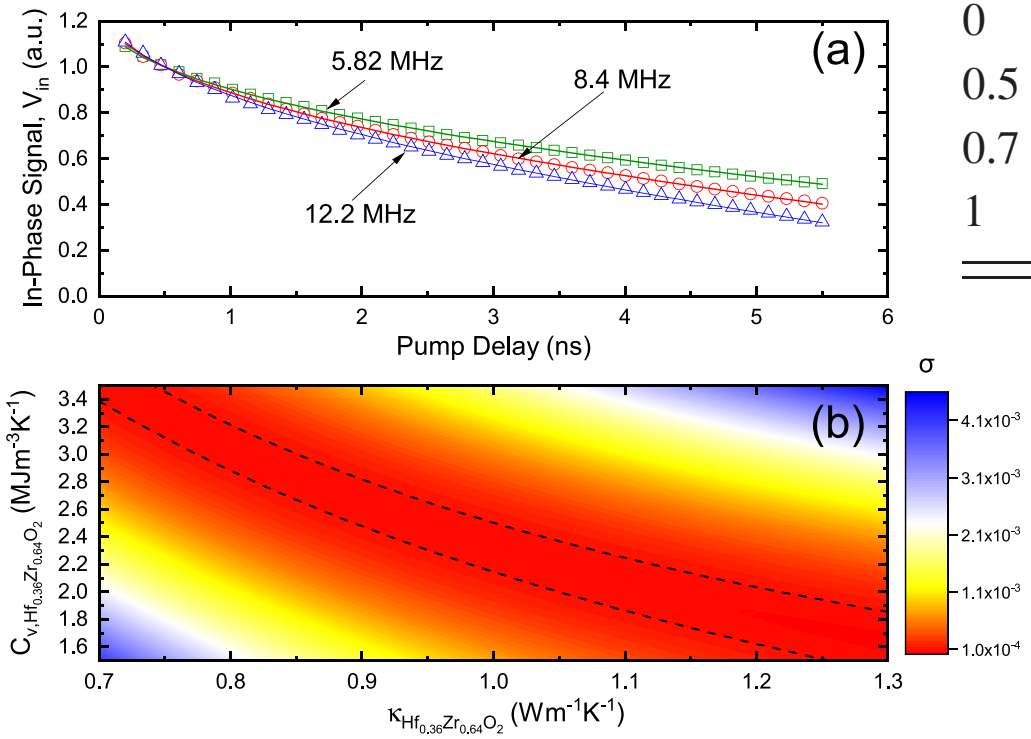
SiGe: *Phys. Rev. Lett.* **109**, 195901



PZT: *J. Appl. Phys.* **121**, 205104

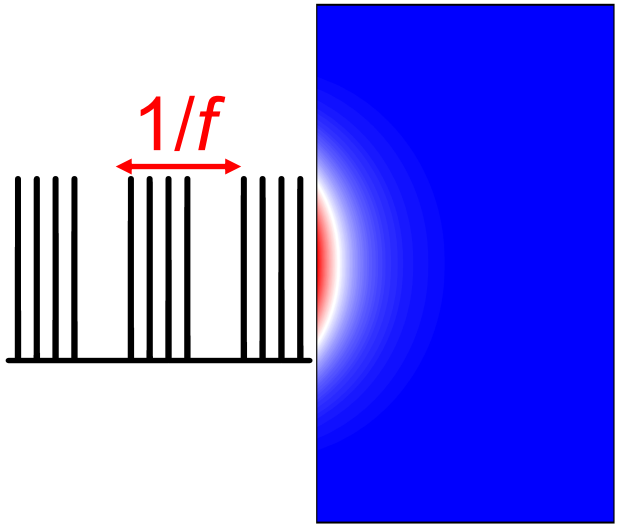


Heat capacity of HZO thin films



$Hf_{1-x}Zr_xO_2$ (x)	C_v (MJ m^{-3} K^{-1})
0	2.63–2.77
0.5	2.18 ± 0.56
0.7	2.64 ± 0.53
1	2.56–2.60

Modulate at different frequencies, ***f***, to change sensitivity to C and κ



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Thermal conductivity of ferroelectric HZO shows strong influence from boundary scattering for 20 nm films

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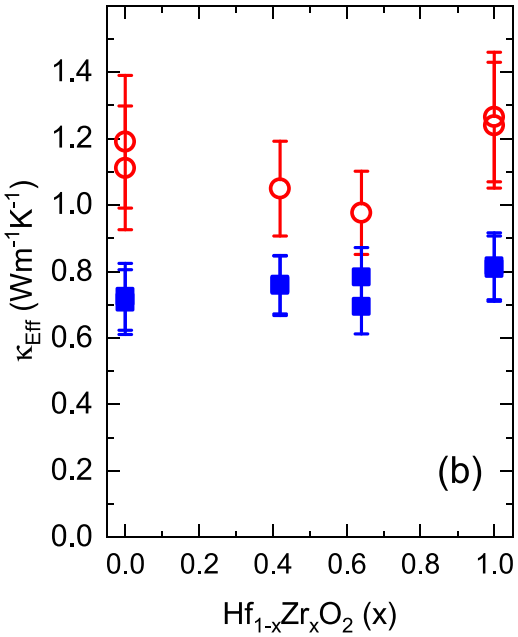

$Hf_{1-x}Zr_xO_2$ (x)	C_v (MJ m^{-3} K^{-1})
0	2.63–2.77
0.5	2.18 ± 0.56
0.7	2.64 ± 0.53
1	2.56–2.60

As-deposited – amorphous

Annealed – Monoclinic or mixed tetragonal/orthorhombic

HfO_2 – Monoclinic, ZrO_2 - tetragonal