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Controlling thermal boundary conductance with structure: From single interfaces to superlattices

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Harry S. Truman Fellowship Program

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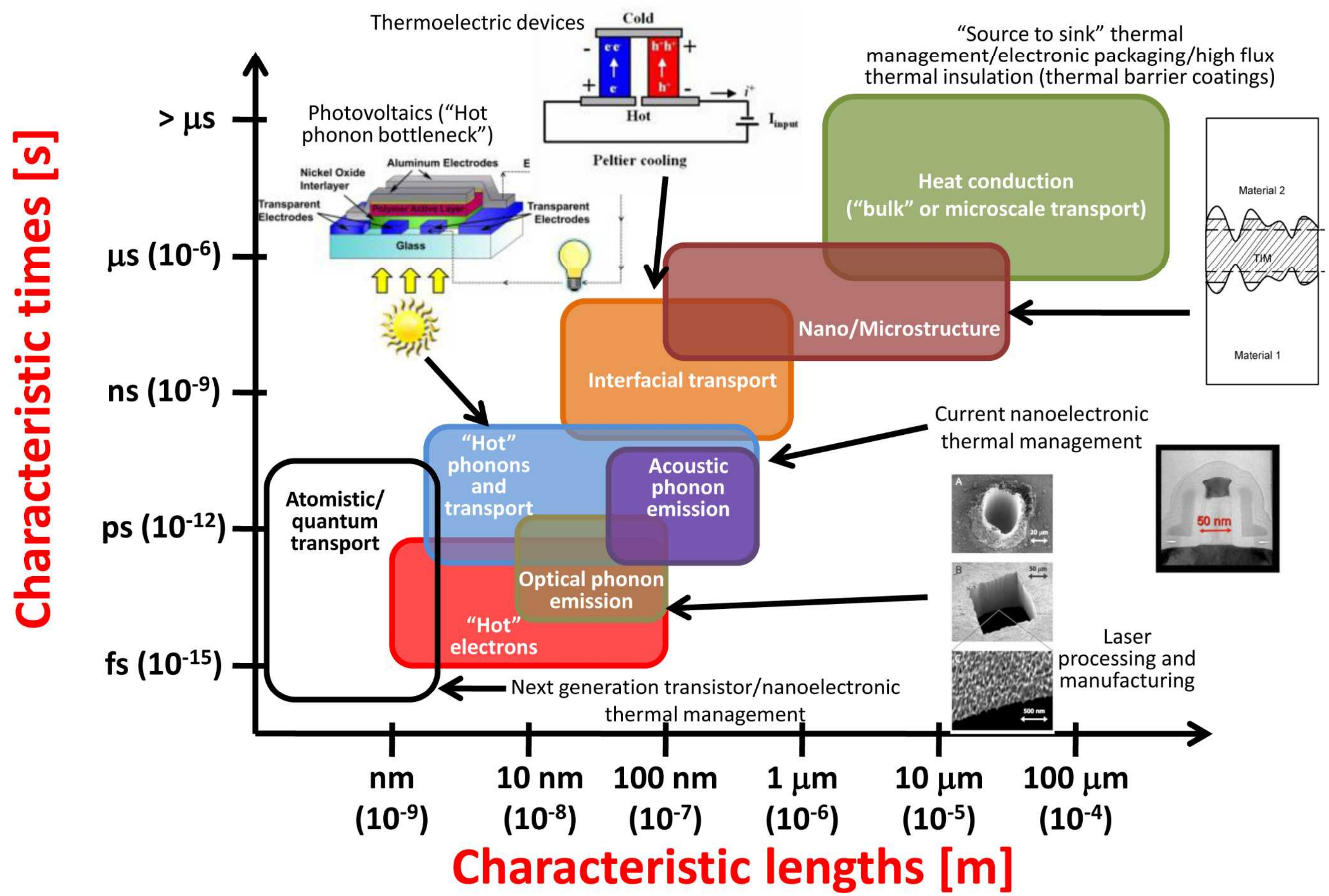
Thermal transport regimes

Need to understand the "bottom" to engineer "up"



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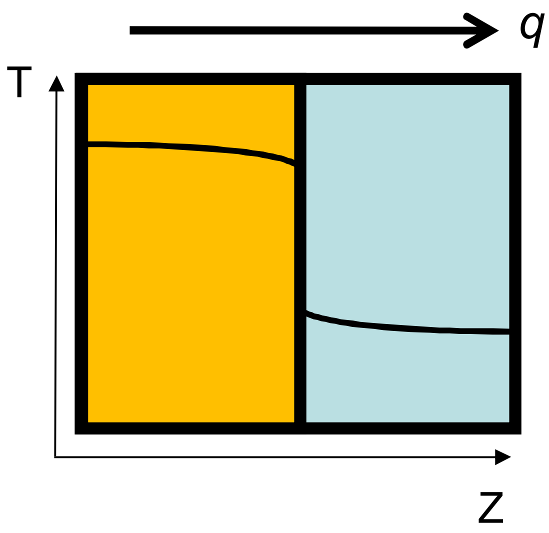
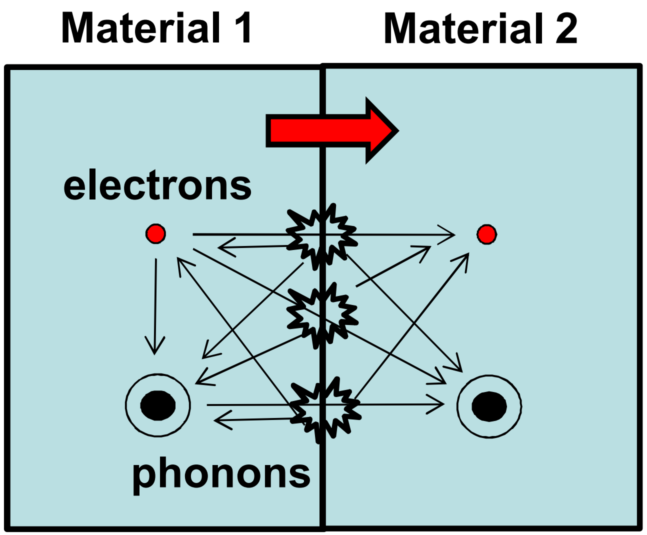
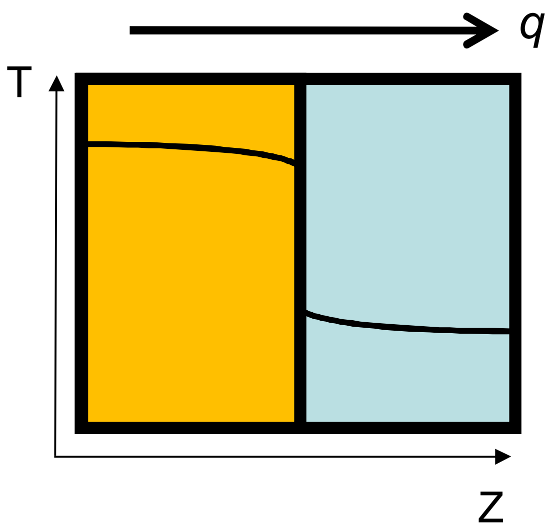
Thermal boundary conductance

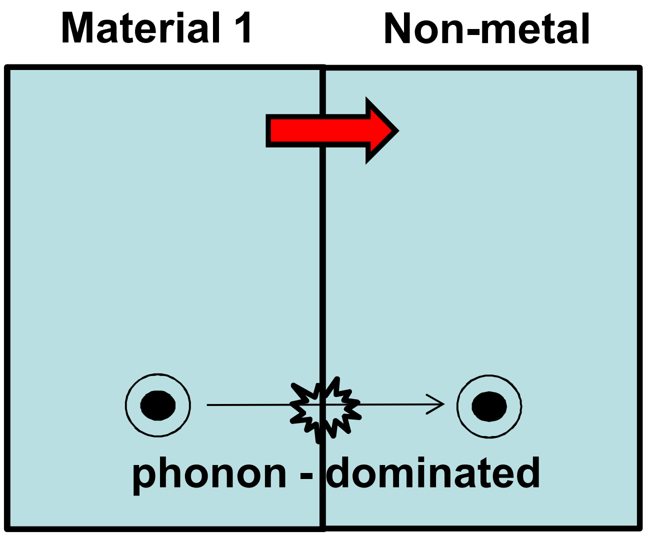




$$q = h_{\mathrm{K}} \Delta T = \frac{1}{R_{\mathrm{K}}} \Delta T$$

Thermal boundary conductance





$$q = h_{\mathrm{K}} \Delta T = \frac{1}{R_{\mathrm{K}}} \Delta T$$

Outline

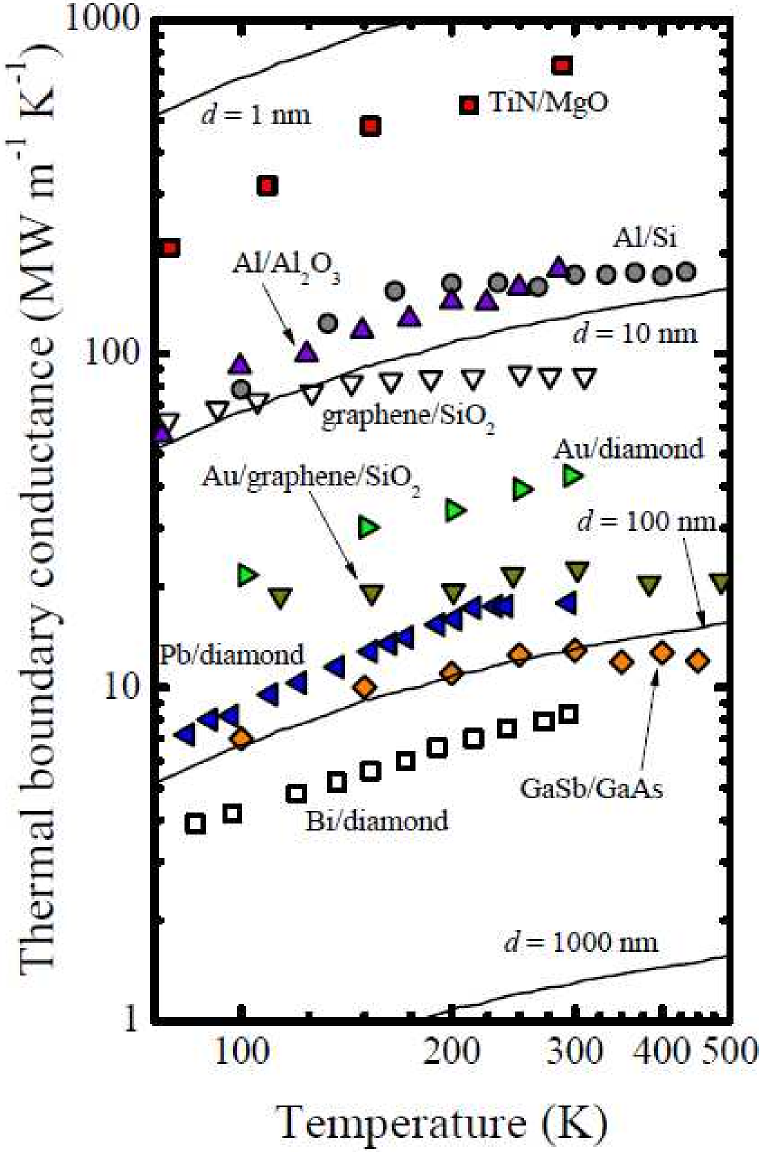
- Thermal boundary conductance: background

- Time domain thermoreflectance (TDTR)

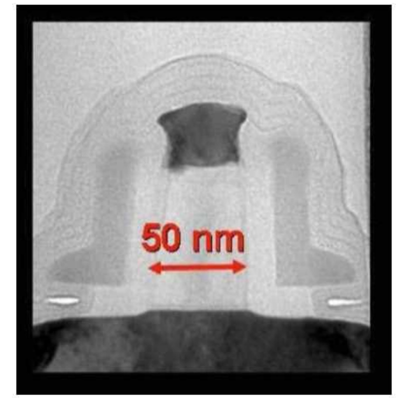
- Controlling h_K with structure and quantum dots
  - Collaborators: John Duda, Chris Petz, Jerry Floro (U. Virginia)

- Work in progress: Thermal transport in STO/CTO superlattices with structurally variant interfaces
  - Collaborators: Jayakanth, Pim, Ramesh, Arun (this group – Berkeley)

Thermal boundary conductance



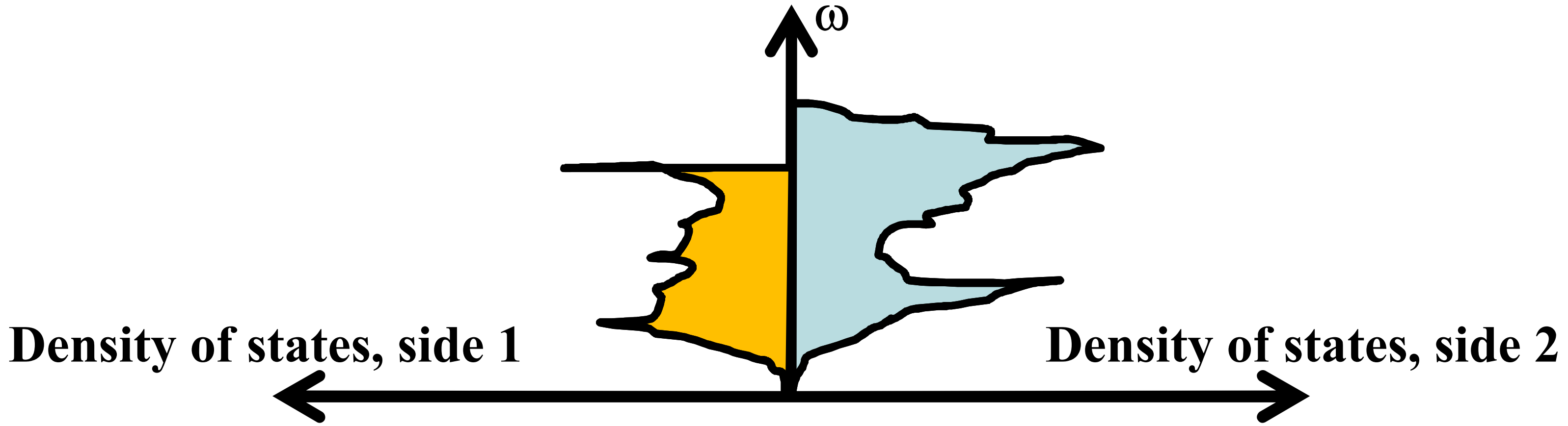
Nanoelectronic design



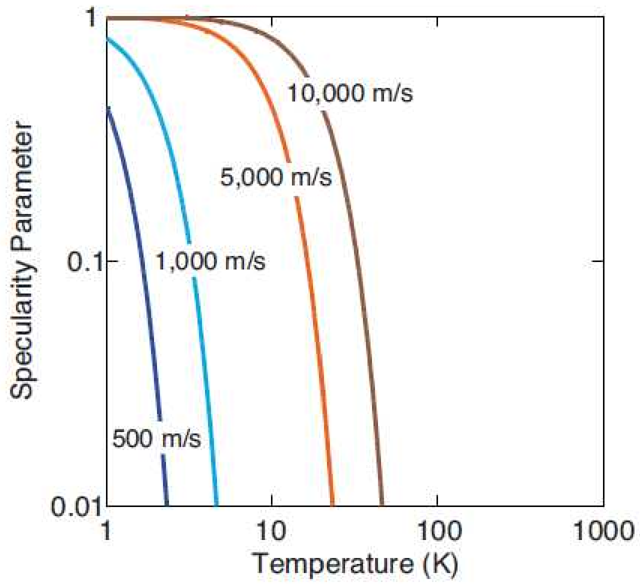
Thermoelectric nanomaterials

$$ZT = \frac{S^2 \sigma T}{\kappa}$$

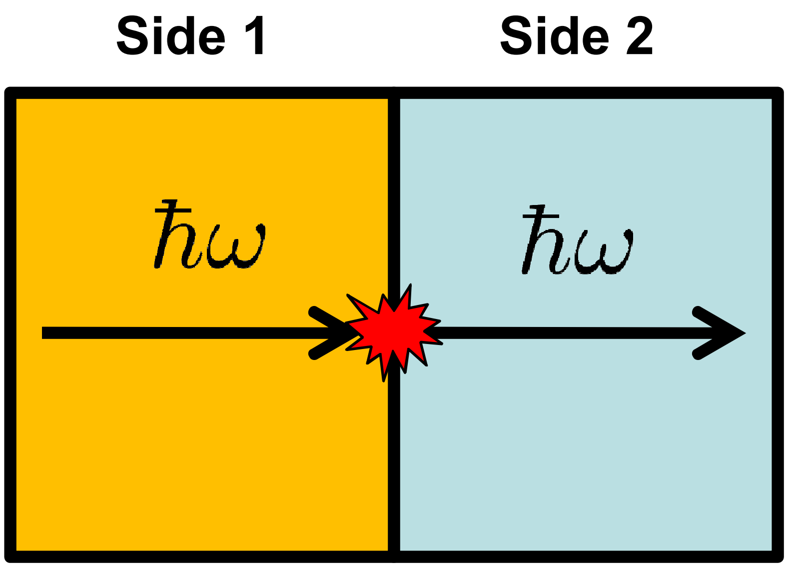
Diffuse mismatch model (DMM)



Diffuse assumption (specularity)

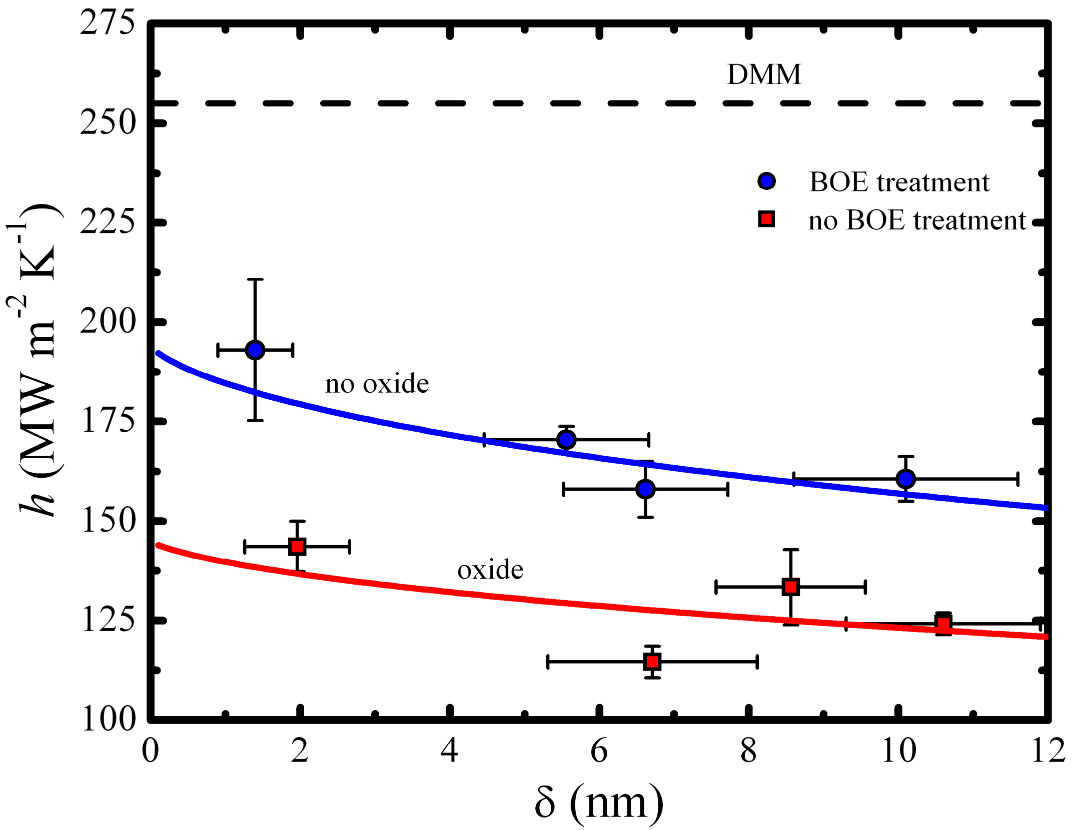


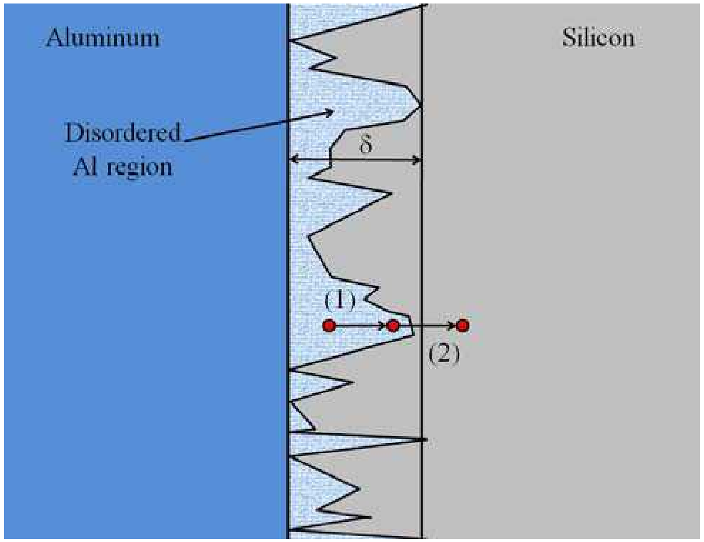
Two phonon scattering (elastic)



Hopkins, *J. Appl. Phys.* 106, 013528 (2009)

Chemically roughened Al/Si interfaces





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Hopkins *et al.*, *Phys. Rev. B* 82, 085307 (2010)

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- **Controlling h_K with structure and quantum dots**
  - **Collaborators: John Duda, Chris Petz, Jerry Floro (U. Virginia)**
- **Work in progress: Thermal transport in STO/CTO superlattices with structurally variant interfaces**
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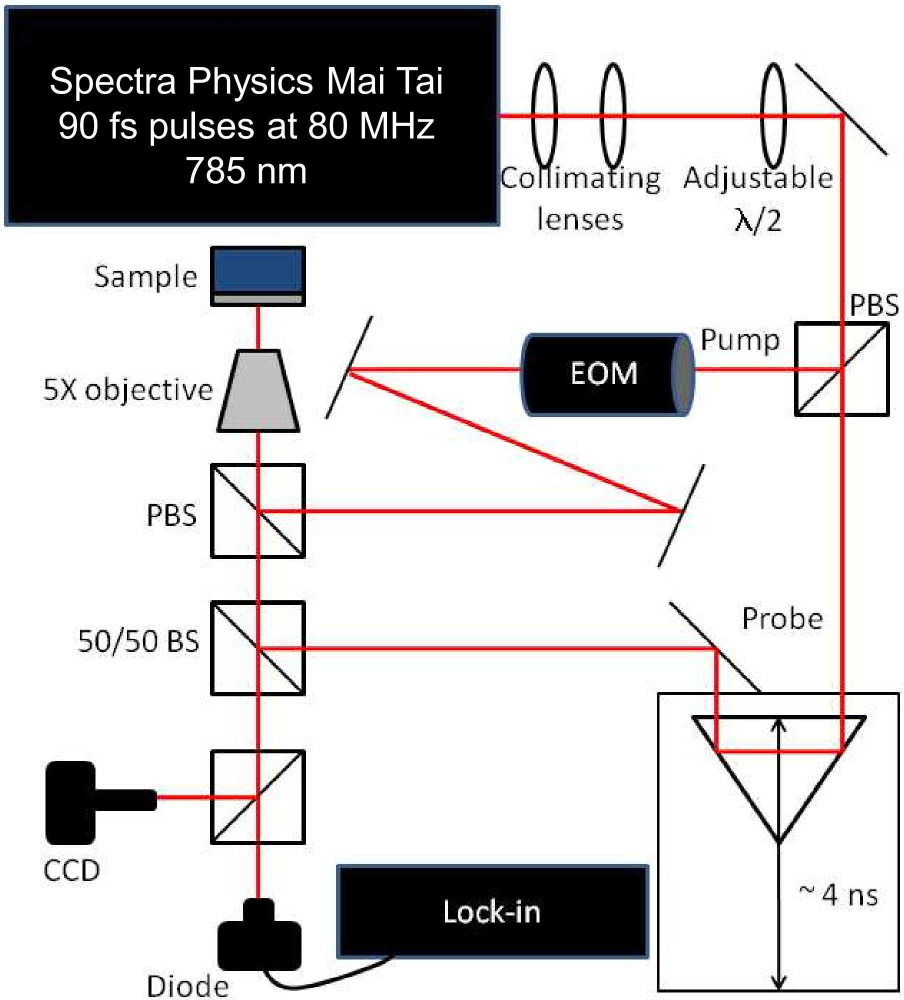
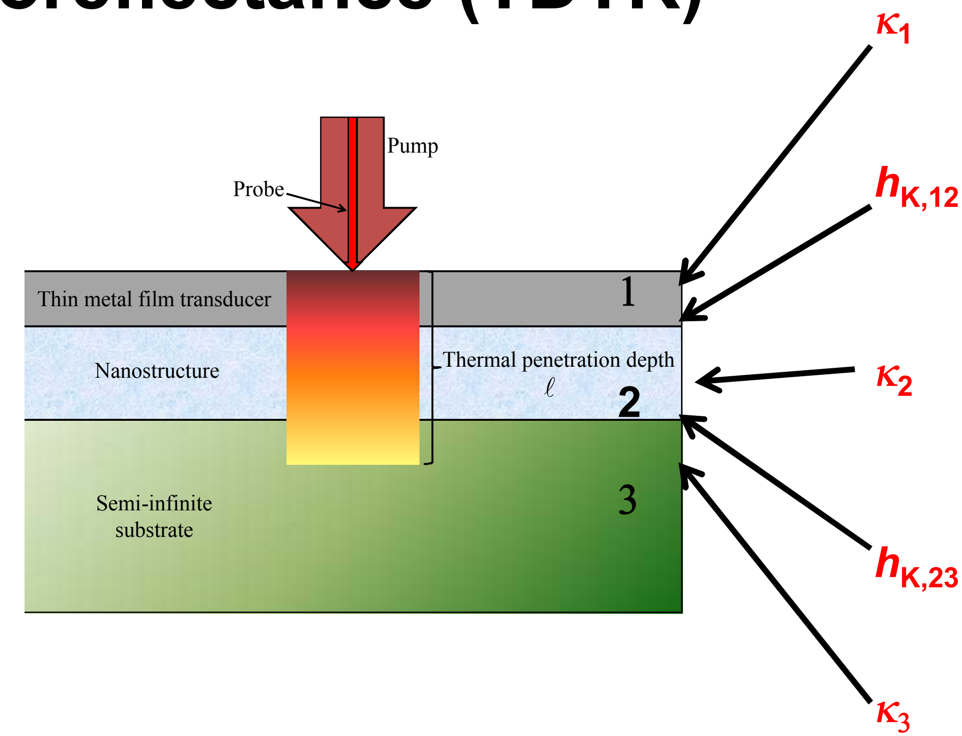
Time domain thermoreflectance (TDTR)





- 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

Hopkins, *et al.*, *J. Heat Trans.* 132, 081302 (2010)

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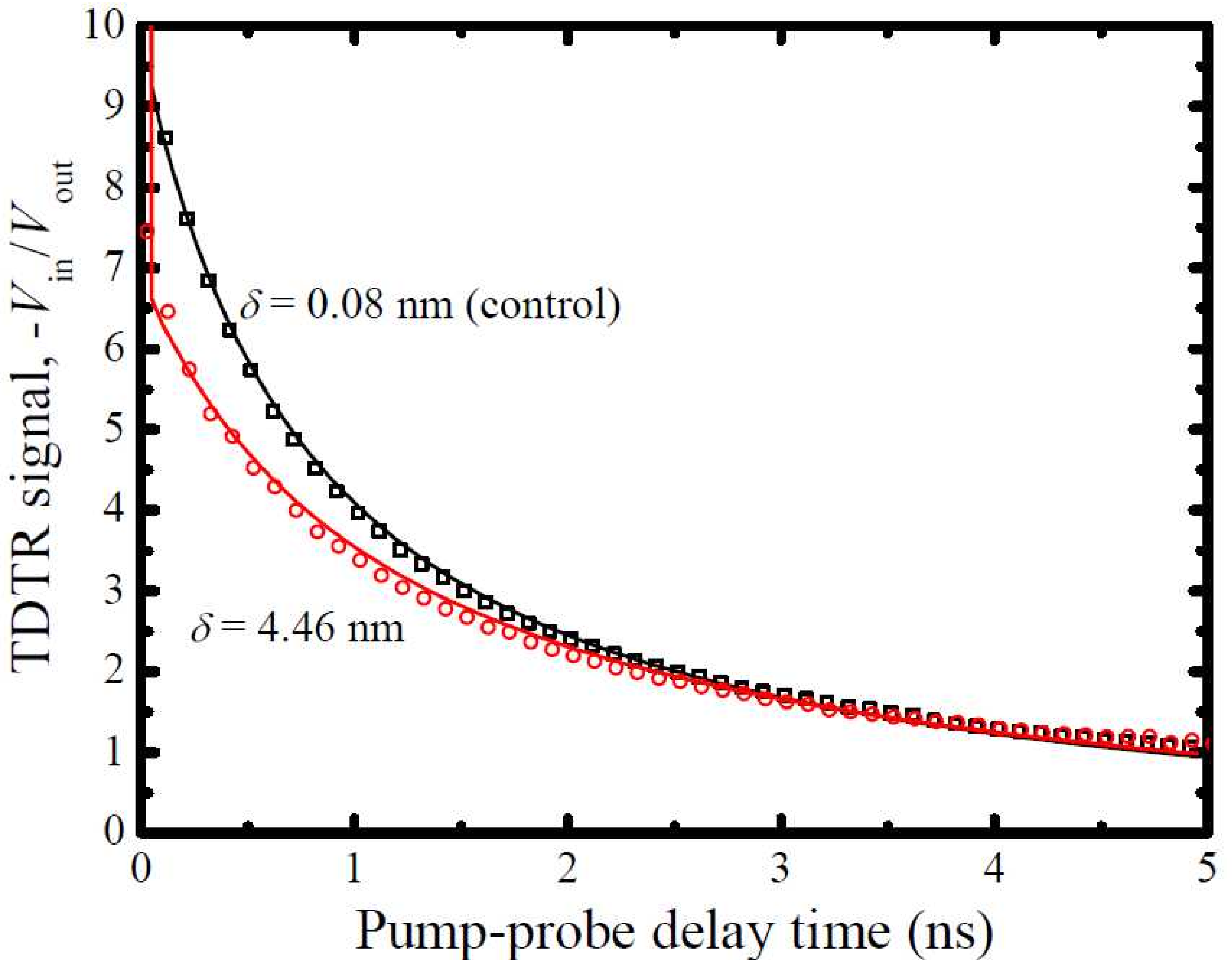
Time domain thermoreflectance (TDTR)



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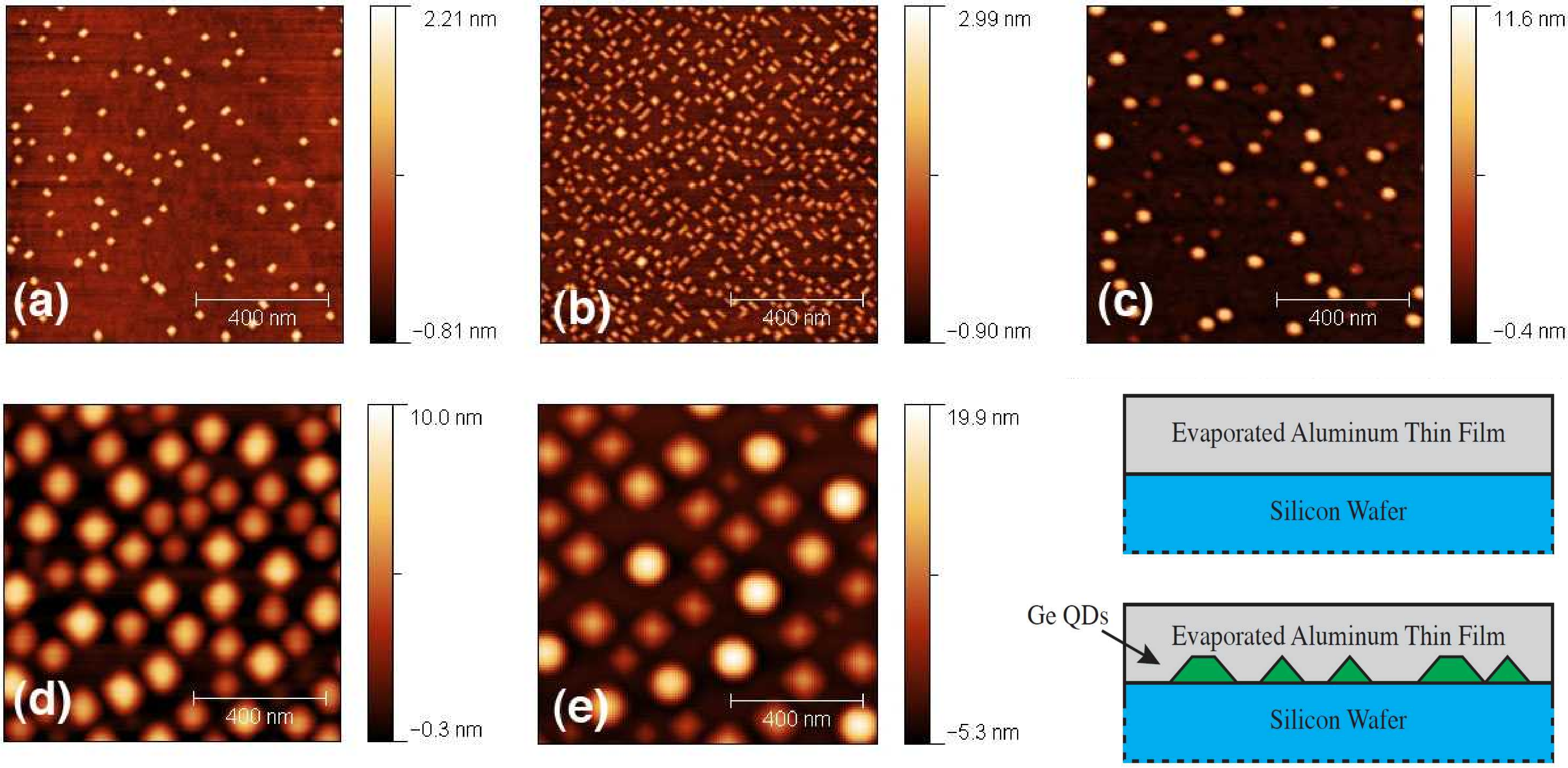
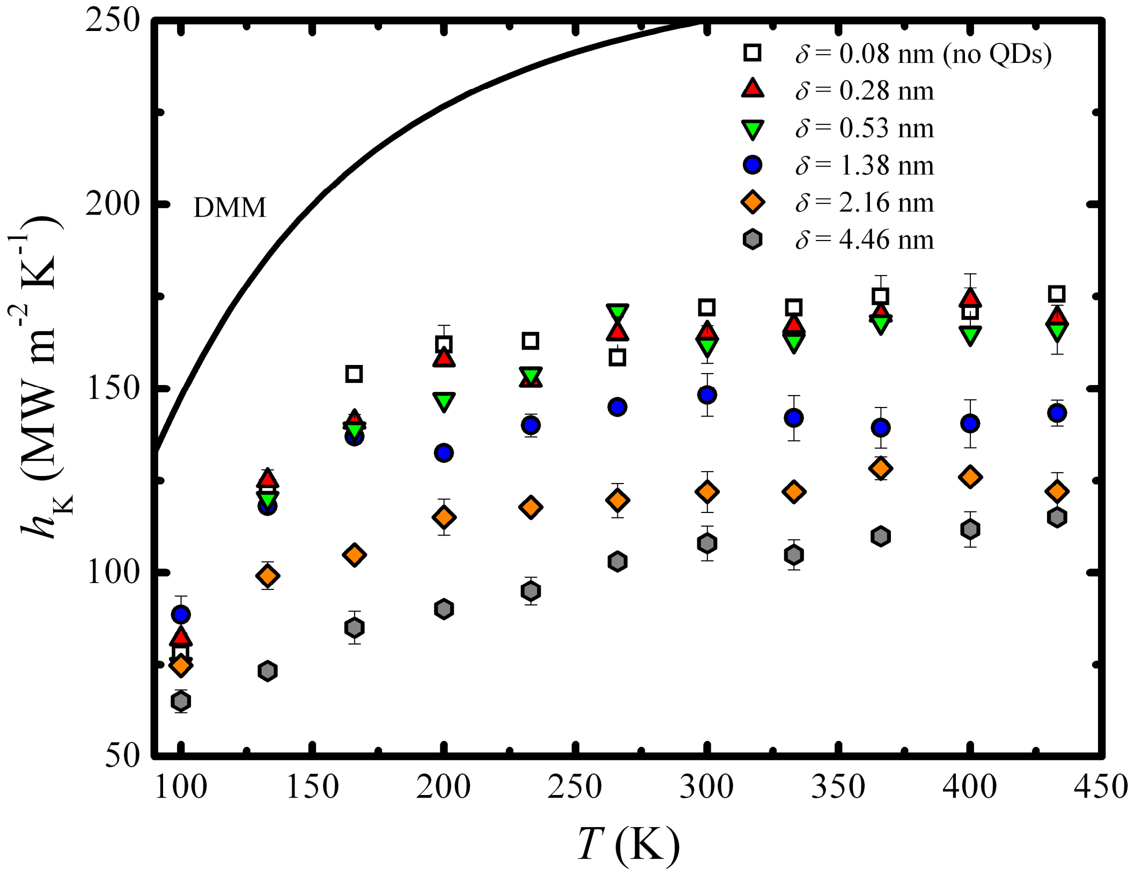
Using QDs to control interface roughness

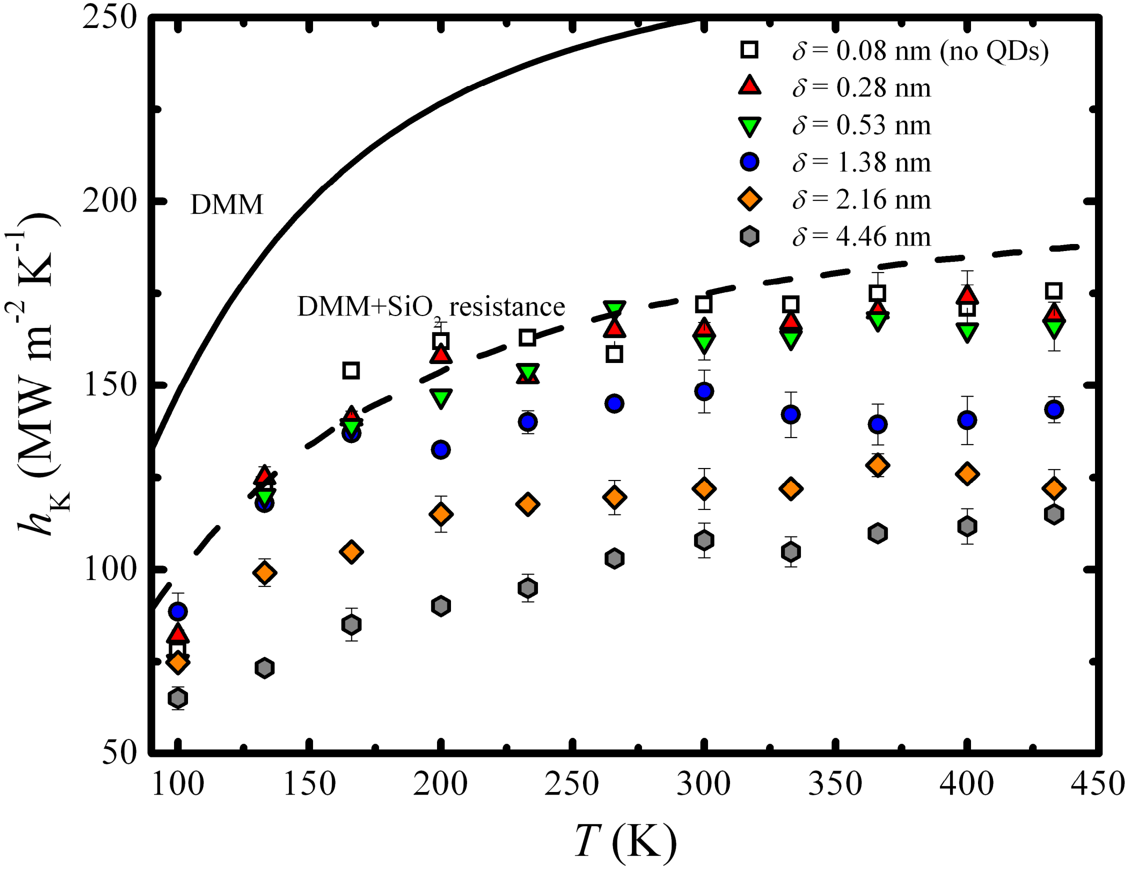


Thermal boundary conductance of QD patterned interfaces



Thermal boundary conductance of QD patterned interfaces

$$h_{\text{total}} = \left(\frac{1}{h_{\text{DMM}}} + \frac{1}{h_{\text{oxide}}}\right)^{-1} = \left(\frac{1}{h_{\text{DMM}}} + \frac{d_{\text{oxide}}}{\kappa_{\text{SiO}_2}}\right)^{-1}$$



Phonon attenuation

Beer's law for photon attenuation

$$I = I_0 \exp\left[\frac{-4\pi\beta}{\lambda} d\right]$$

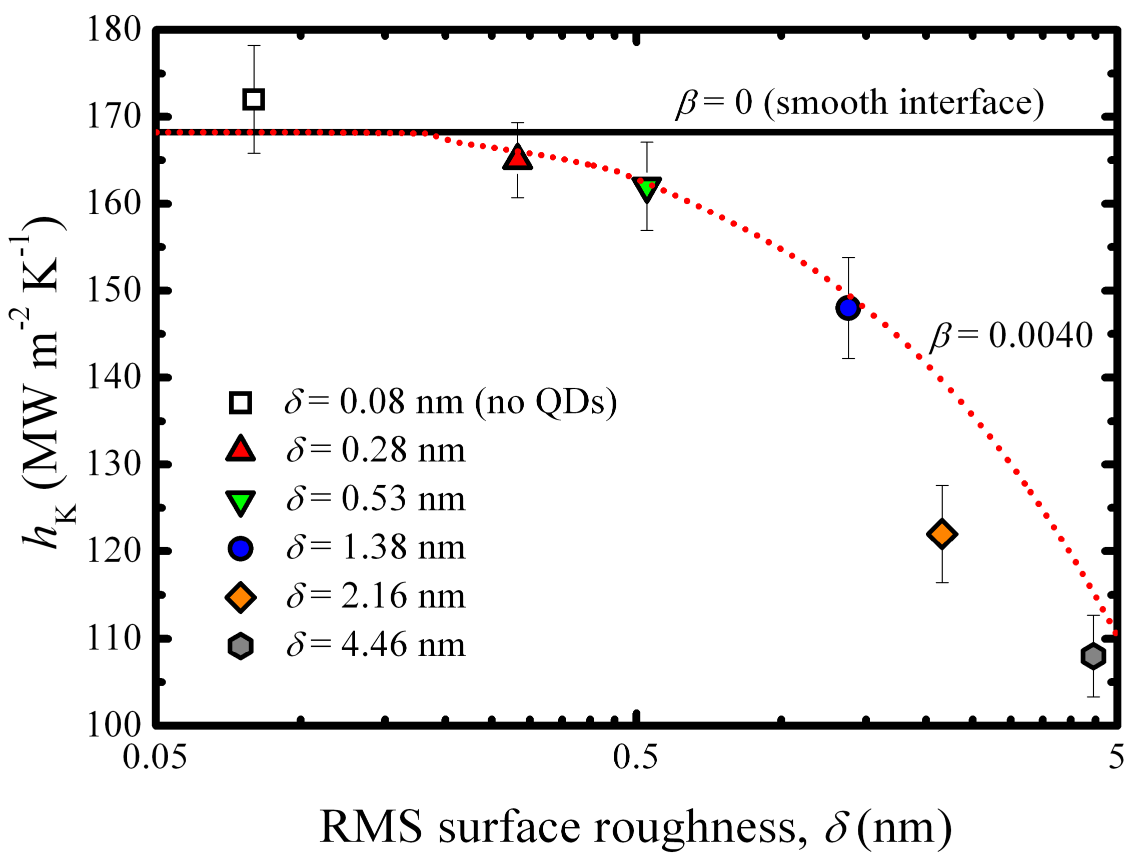
Parallel for phonon attenuation around rough interfaces

$$I = I_0 \exp\left[\frac{-4\pi\beta}{\lambda} \delta\right]$$

Thermal boundary conductance with attenuation

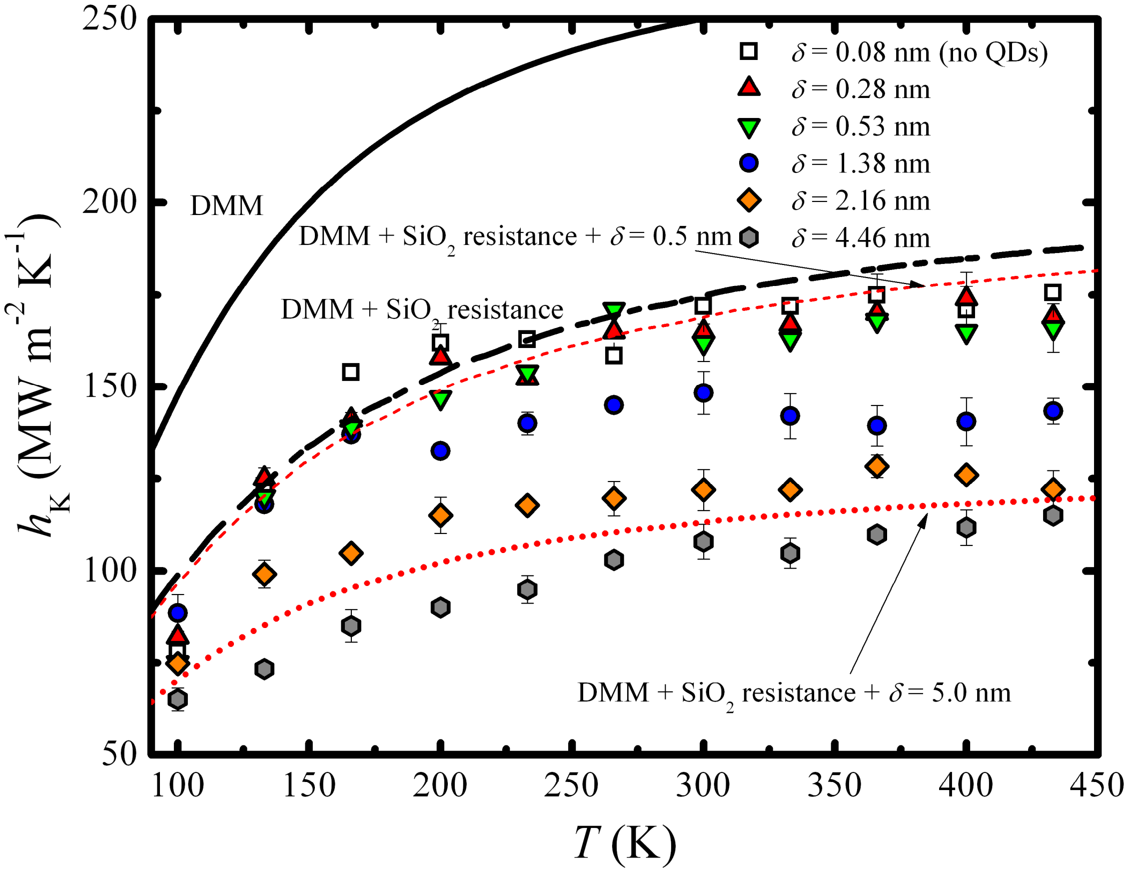
$$h_{\mathrm{K}} = \begin{cases} h_{\mathrm{DMM}} & \lambda > \delta \\ h_{\mathrm{DMM}}\left(\exp\left[-\left(\frac{4\pi\beta}{\lambda}\right)\delta\right]\right) & \lambda < \delta \end{cases}$$

Room temperature trends in thermal boundary conductance at QD patterned interfaces



Long wavelength "phonon filtering" at QD patterned interfaces

$$h_{\mathrm{K}} = \begin{cases} h_{\mathrm{DMM}} & \lambda > \delta \\ h_{\mathrm{DMM}}\left(\exp\left[-\left(\frac{4\pi\beta}{\lambda}\right)\delta\right]\right) & \lambda < \delta \end{cases}$$



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$CaTiO_3$–$SrTiO_3$ superlattices on $SrTiO_3$ substrates

Jayakanth and Pim

Well defined series			
Sample name	desired super lattice CaTiO3 + SrTiO3 (monolayers)	average doublelayer thickness (nm)	estimated total thickness (nm)
PR281	(4+4) x 65	3.1	205
PR282	(9+9) x 29	7.2	201
PR285	(29+28) x 9	22.6	204
PR286	(89+87) x 3	72.5	217

Less defined series			
Sample name	desired super lattice CaTiO3 + SrTiO3 (monolayers)	average doublelayer thickness (nm)	estimated total thickness (nm)
PR280	(4+4) x 65	3.3	214
110110B	(4+4) x 65	3	195
PR279	(9+9) x 29	7	204
110106	(29+28) x 9	24	216
110104	(89+87) x 3	70	210

Extra samples			
Sample name	desired super lattice CaTiO3 + SrTiO3 (monolayers)	average doublelayer thickness (nm)	estimated total thickness (nm)
PR316 - Bad*	(2+2) x 130	NA**	150
PR317 - Good	(2+2) x 130	NA**	200
PR318	alloy	NA***	189

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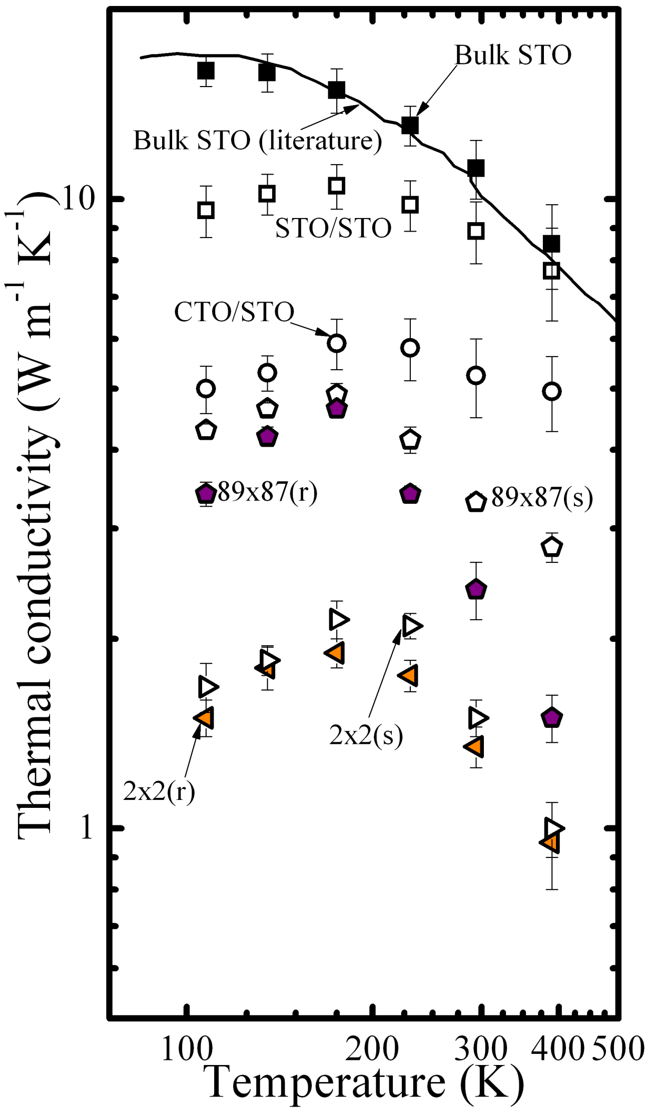
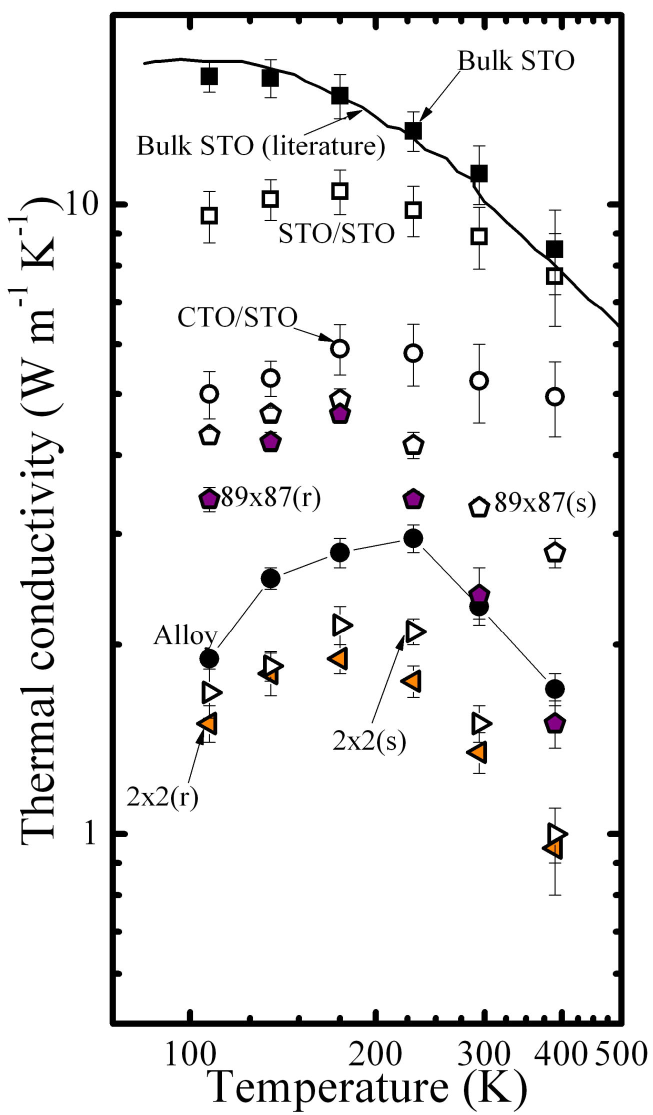
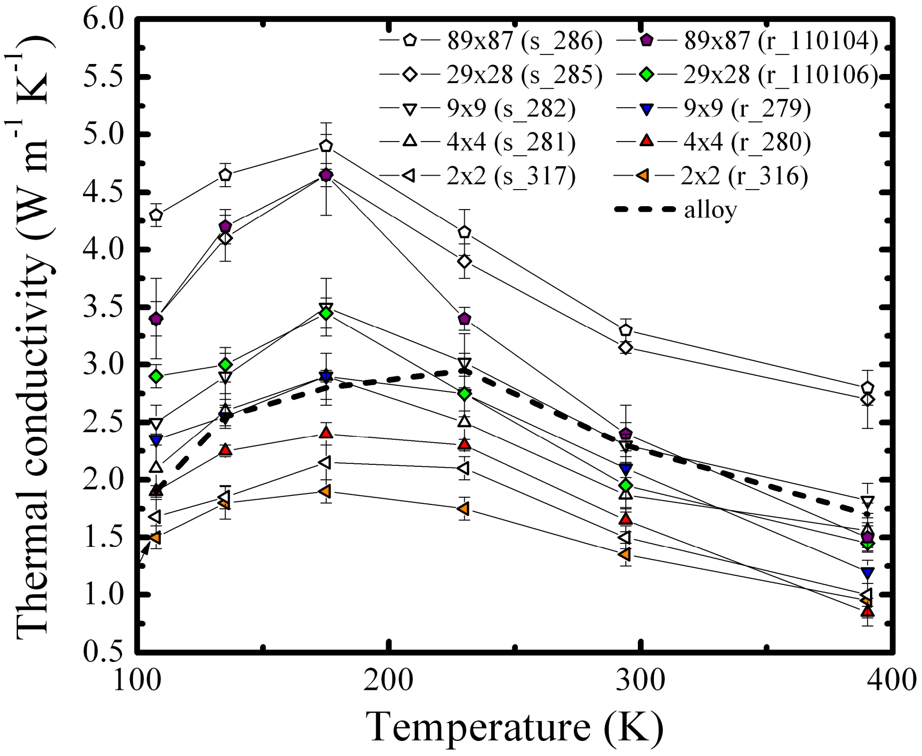
Thermal conductivity of STO/CTO superlattices

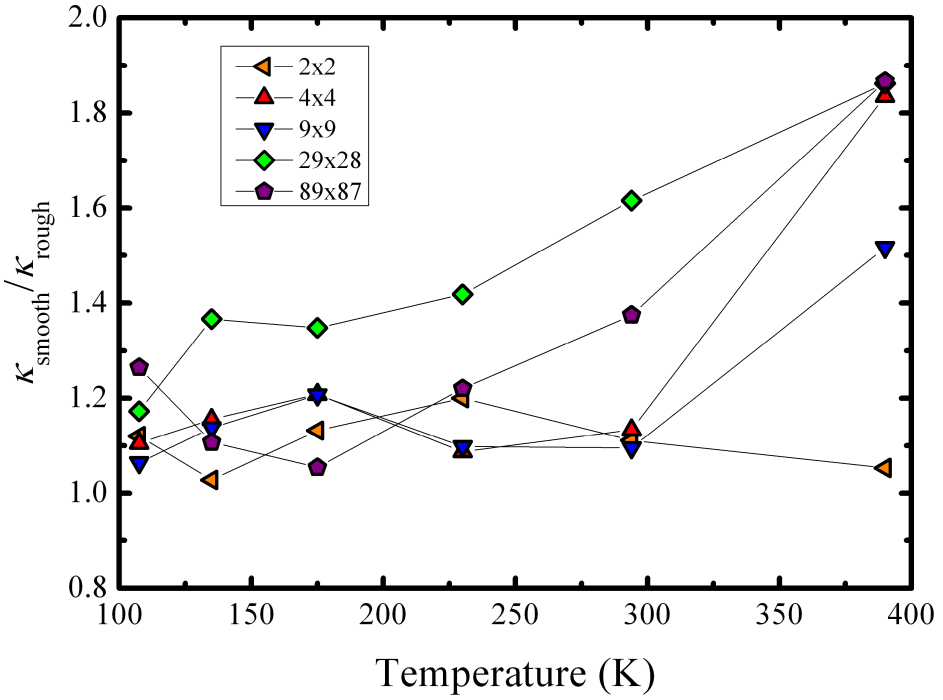


Thermal conductivity of STO/CTO superlattices

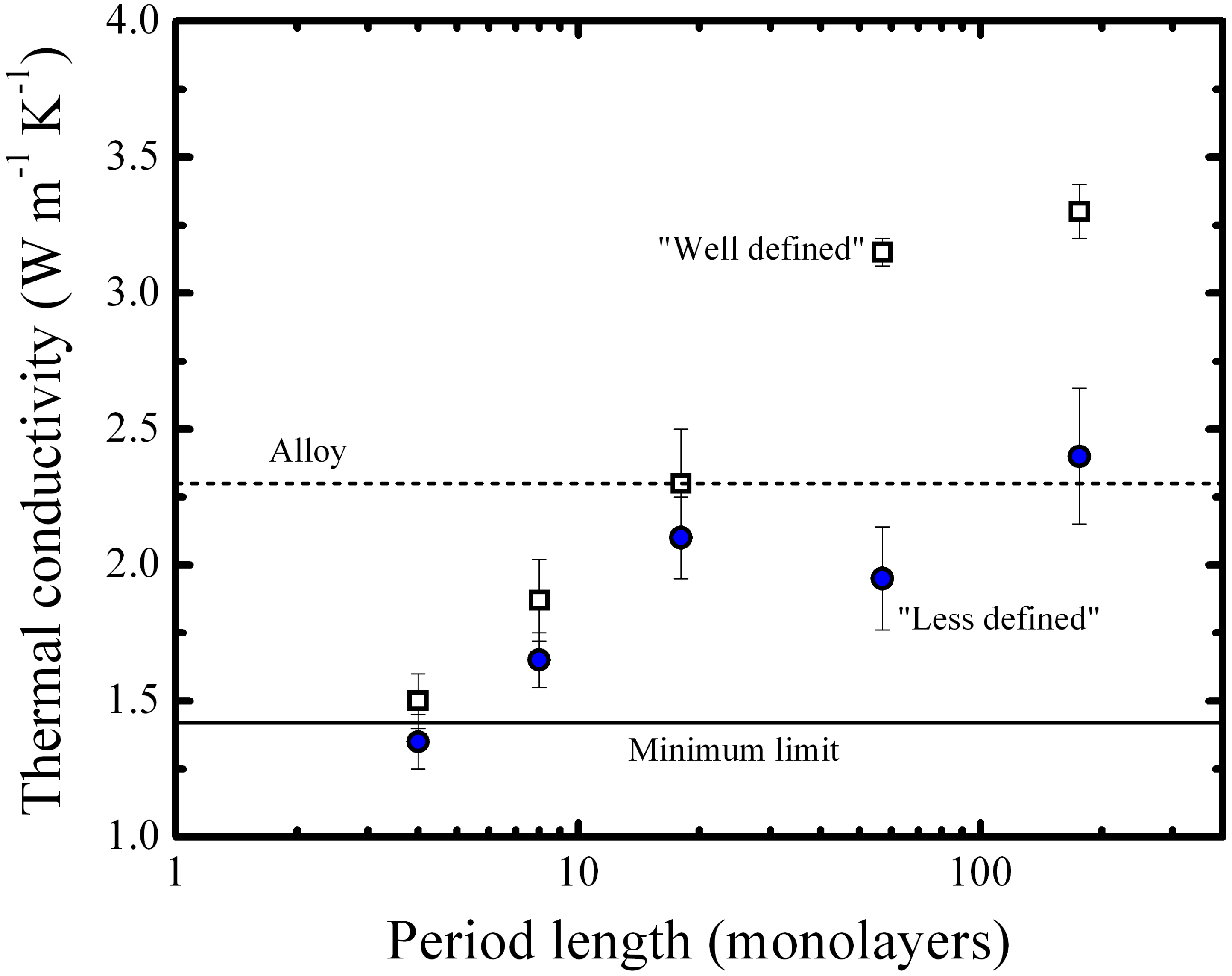


Thermal conductivity of STO/CTO superlattices





Approaching the minimum limit



Summary

Controlling thermal boundary conductance with structure: From single interfaces to superlattices

- Thermal resistances at interfaces can pose a dominant resistance in nanosystems

- TDTR is an effective technique to measure thermal resistances in nanosystems

- Quantum dots can be used to control interfacial roughness, and therefore thermal boundary conductance

- Roughening in STO/CTO superlattices can effectively reduce the thermal conductivity (close to theoretical minimum for STO)

Thanks to funding from the Harry S. Truman Fellowship Program through the LDRD office at Sandia.

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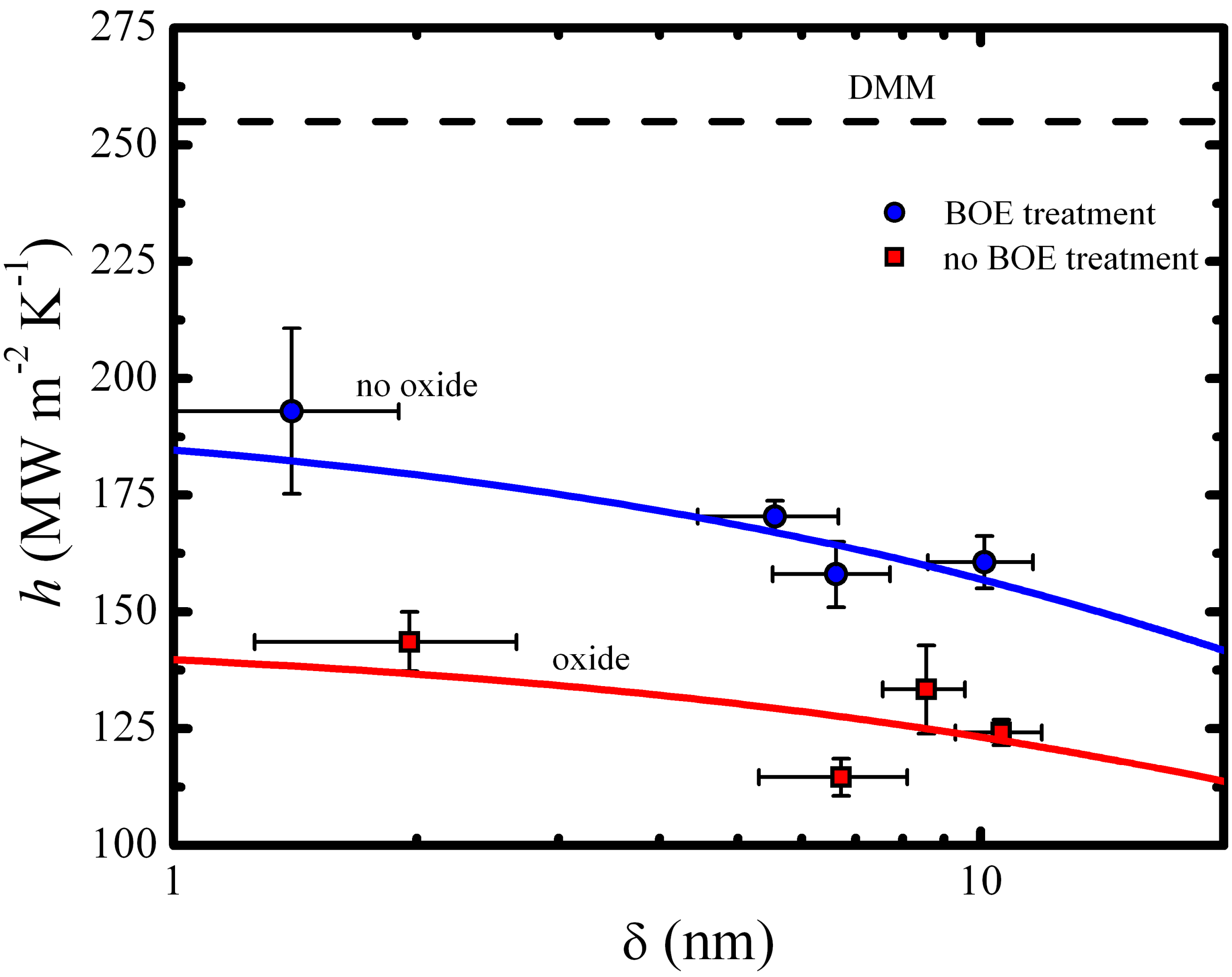

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