SCHOOL of ENGINEERING & APPLIED SCIENCE
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Ballistic transport of long wavelength phonons in superlattices and nanograined alloys

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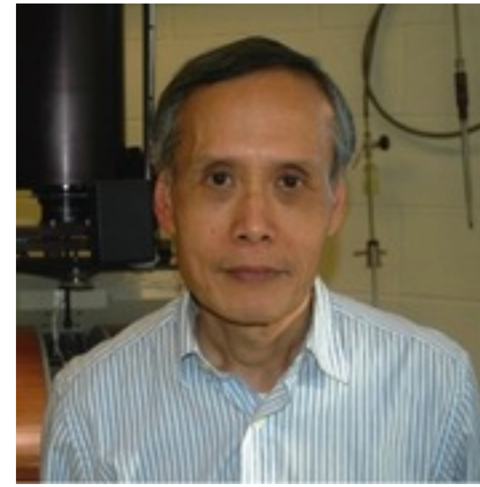
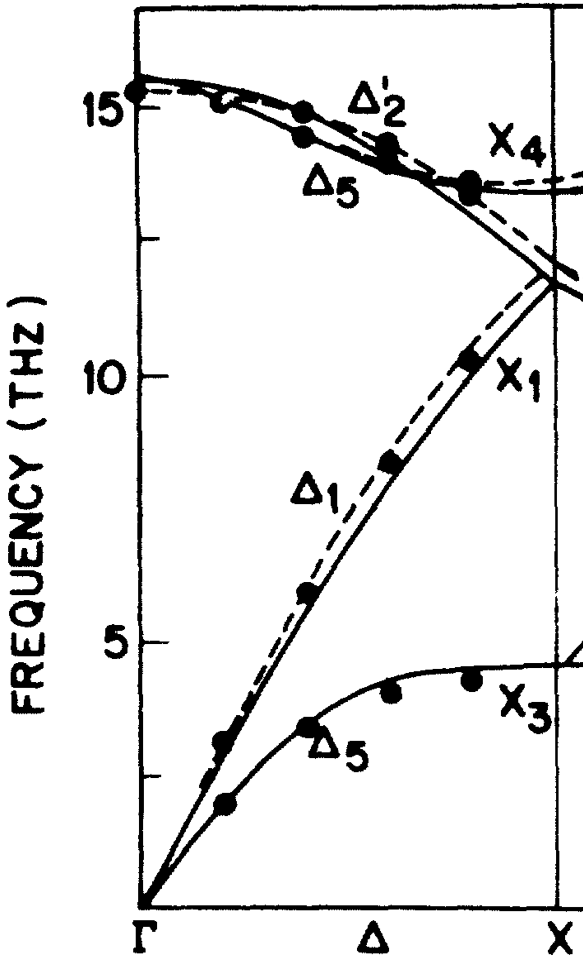


Prof. Avik Ghosh (UVA)

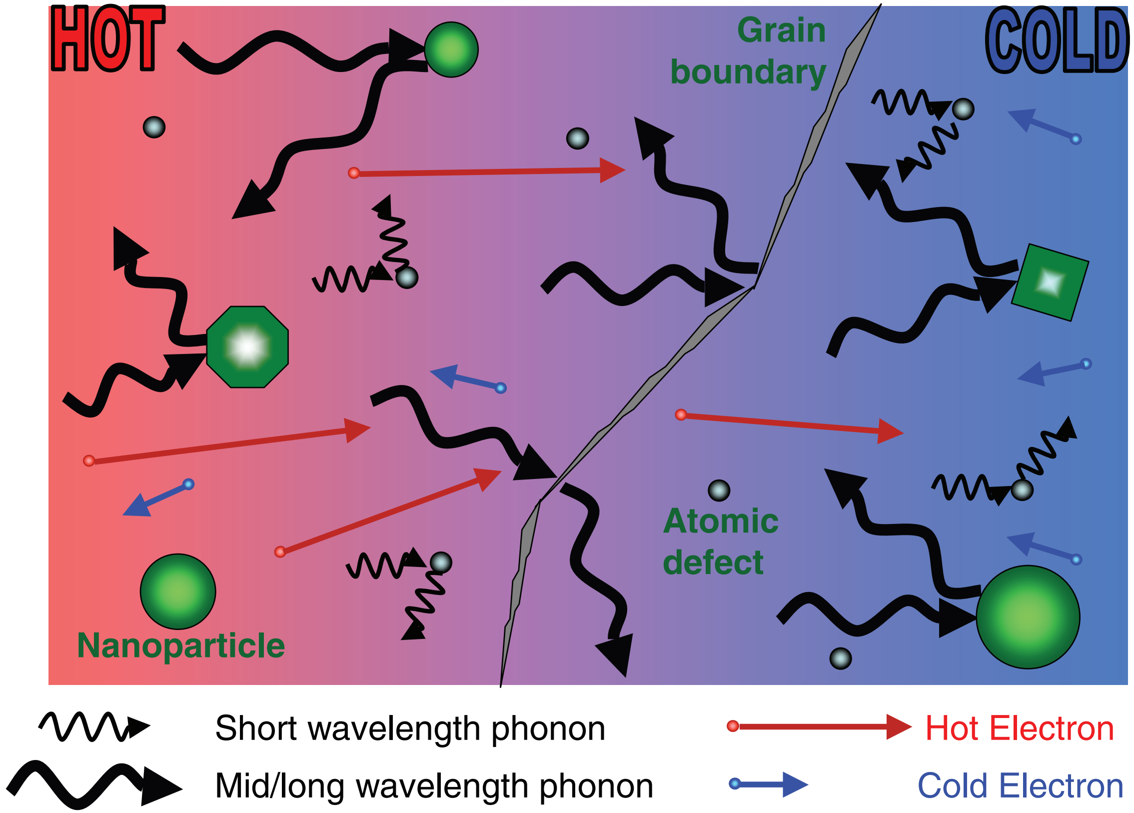
Designing phonon transport on the nanoscale

Silicon phonon dispersion



from *PRB* **15**, 4789 (1977)

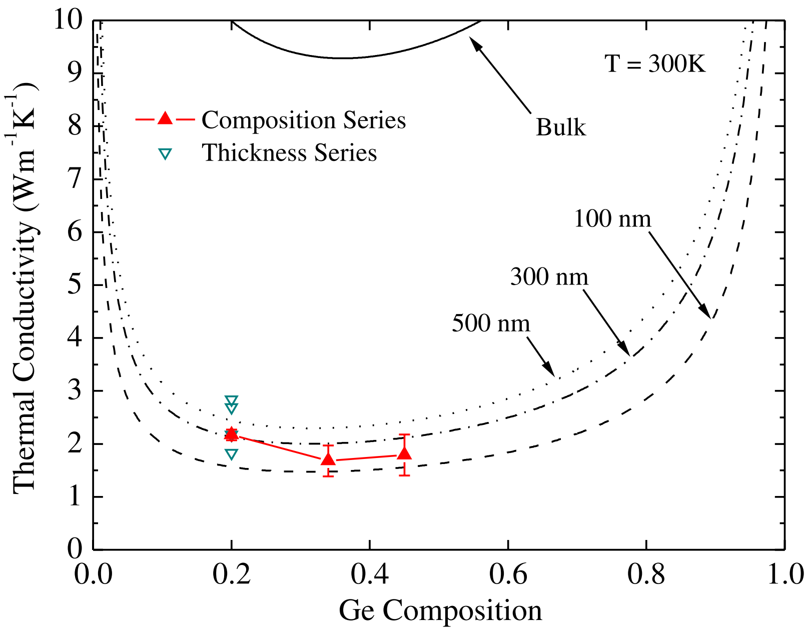
$$\kappa = \frac{1}{3}Cv\lambda = \frac{1}{3}Cv_g^2\tau$$

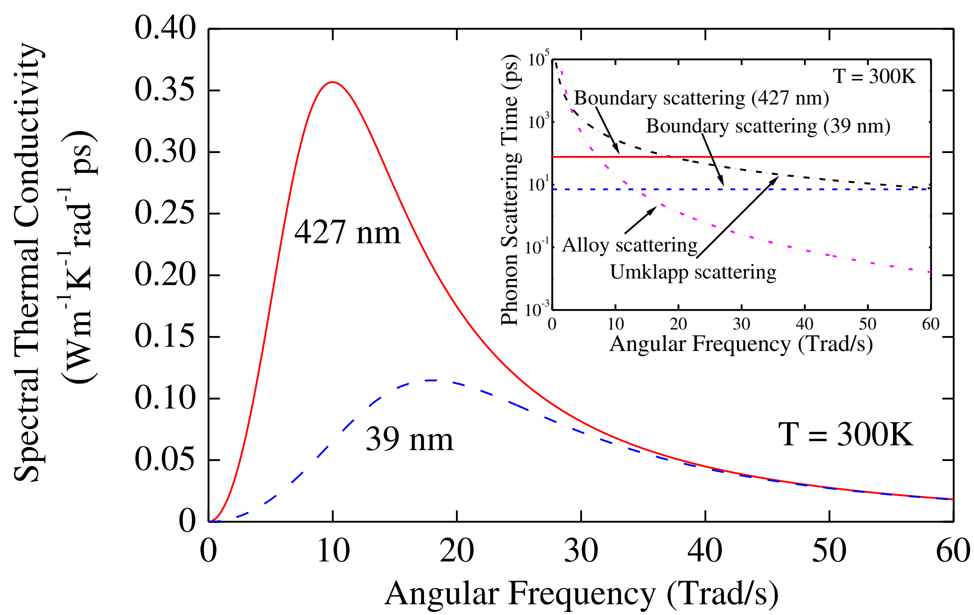


from *Adv. Mat.* **22**, 3970 (2010)

Thin film alloys: short vs. long wavelength phonons

Short wavelength phonons: defect scattering
Long wavelength phonons: limited by film thickness
Example: SiGe alloy thin films





Cheaito et al, *PRL* **109**, 195901 (2012)

Thin film alloys: short vs. long wavelength phonons

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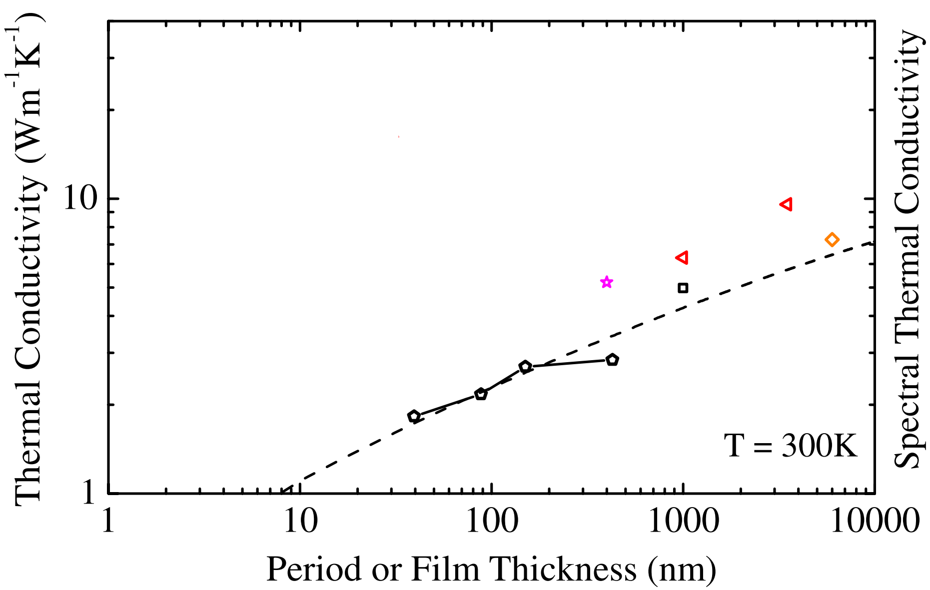
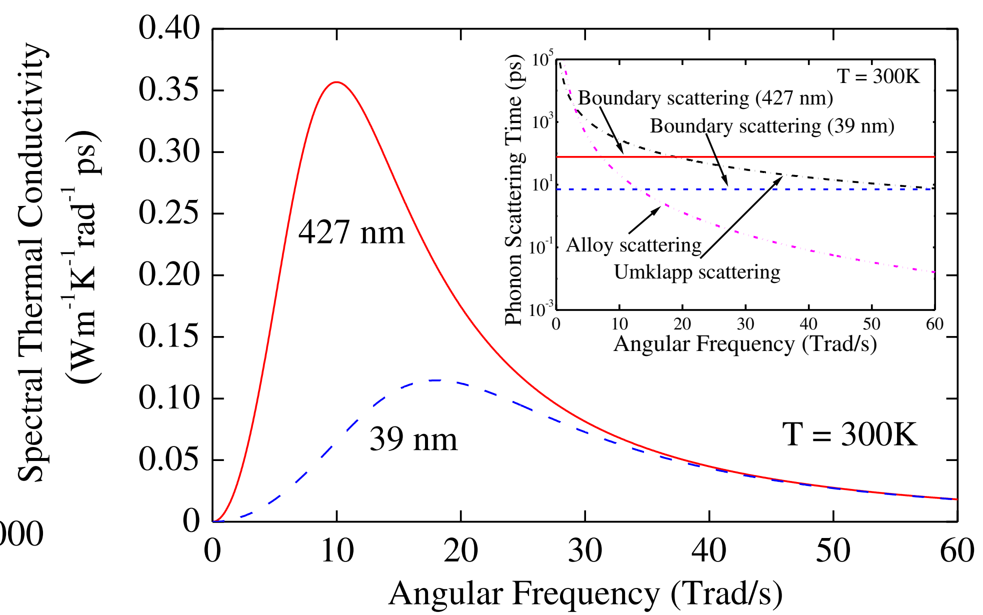
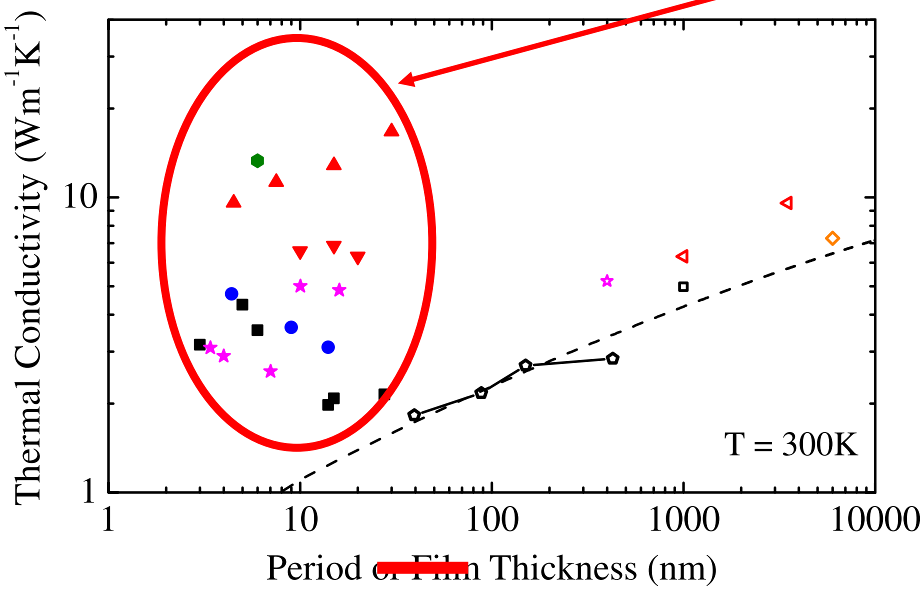


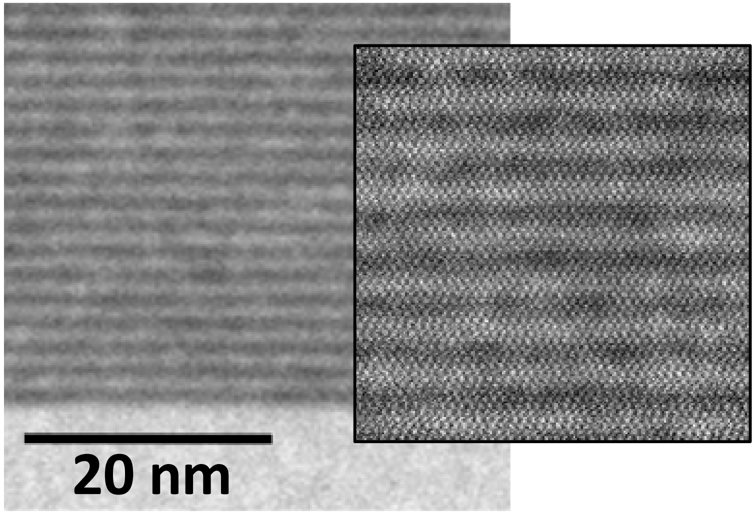


Cheaito et al, *PRL* **109**, 195901 (2012)

Boundary scattering in superlattices

Short wavelength phonons: defect scattering
Long wavelength phonons: limited by film thickness
What about superlattices?





d_{SL} = 2 nm

Cheaito et al, *PRL* **109**, 195901 (2012)

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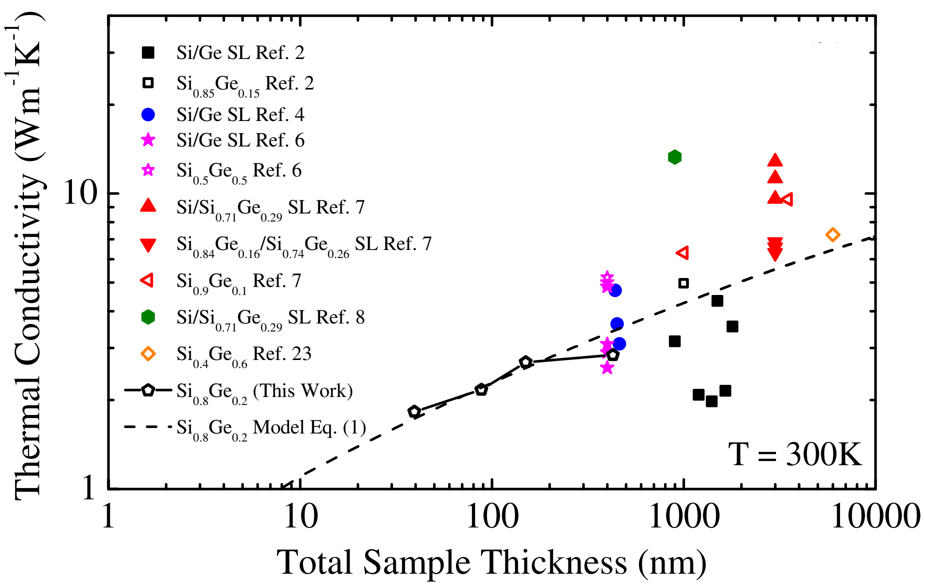
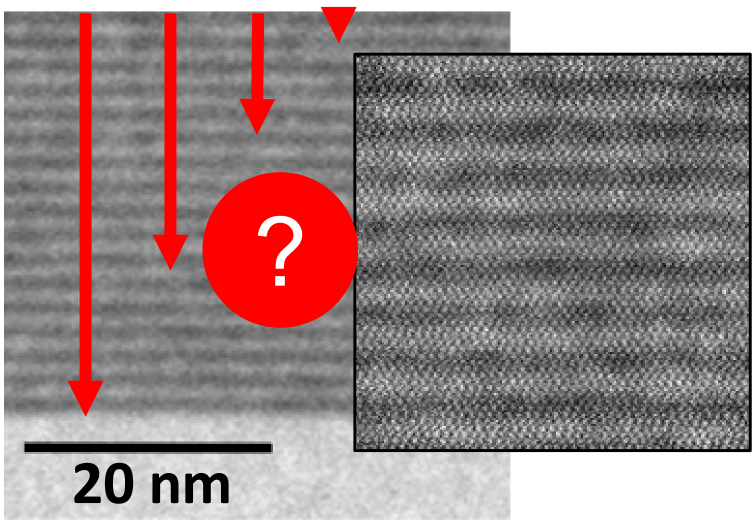




d_{SL} = 2 nm

Cheaito et al, *PRL* **109**, 195901 (2012)

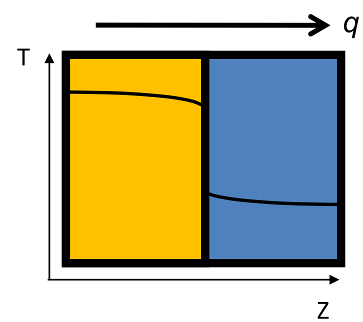
Outline

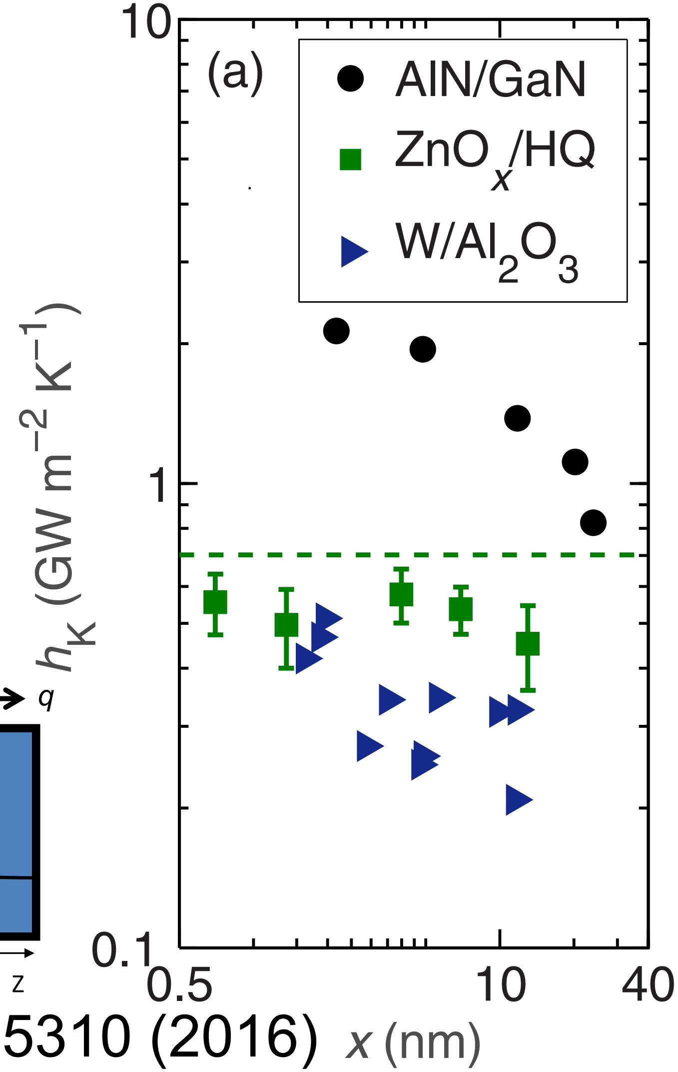
Question: Do phonons "see" interfaces spectrally in superlattices and nanocomposites?

Outline

- Period vs. sample thickness boundary scattering in thermal conductivity of SLs

- Spectral thermal conductivity in nano-grained silicon-germanium

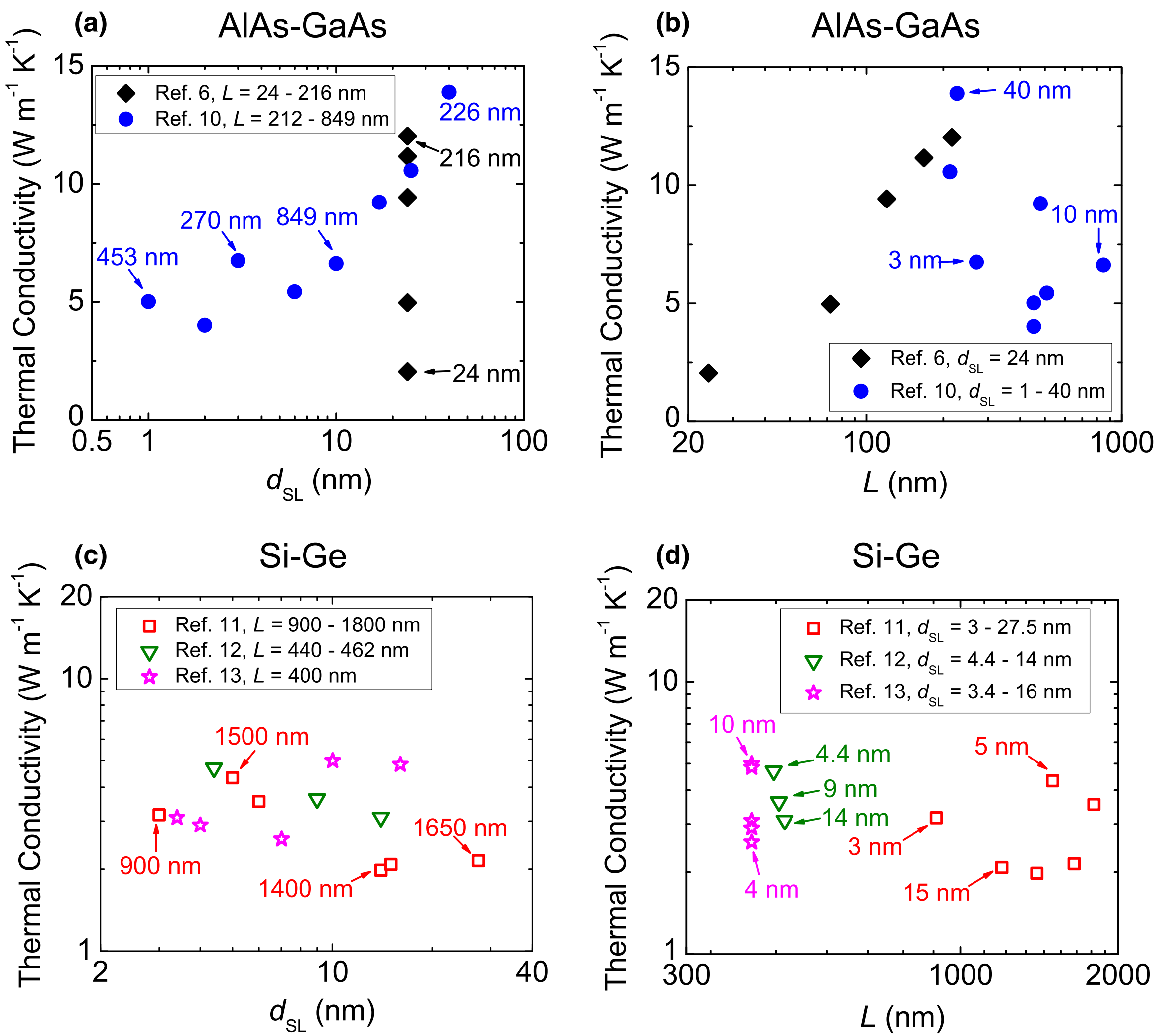




Giri et al, *PRB* **93**, 115310 (2016)

Superlattices: Period vs. sample thickness effects

Why has this not been observed before?
Inconsistent comparisons, must control sample and period



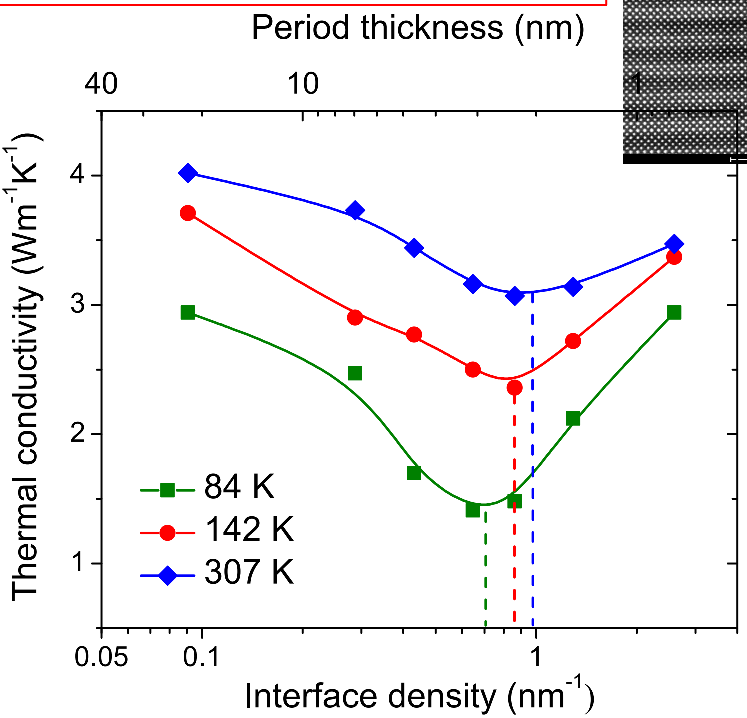
Cheaito et al, *PRB* **97**, 085306 (2018)

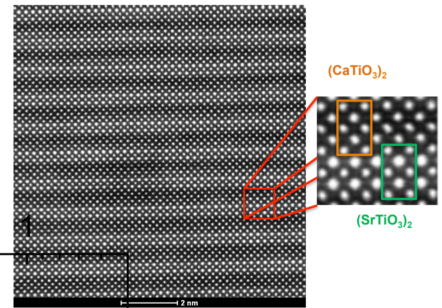
Superlattices: Period vs. sample thickness effects

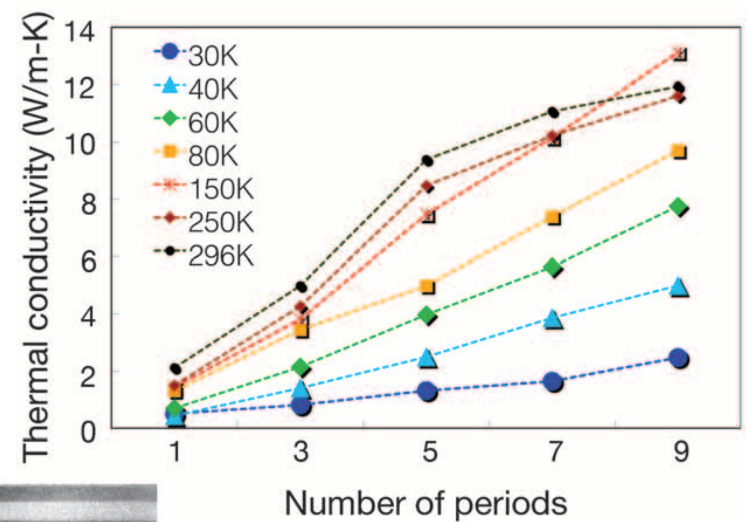
Must study both to understand novel phonon transport mechanisms: e.g., coherent vs. ballistic vs. incoherent

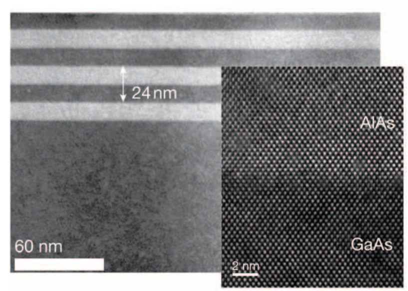
CTO/STO
Sample constant
Period variable

GaAs/AlAs
Sample variable
Period constant





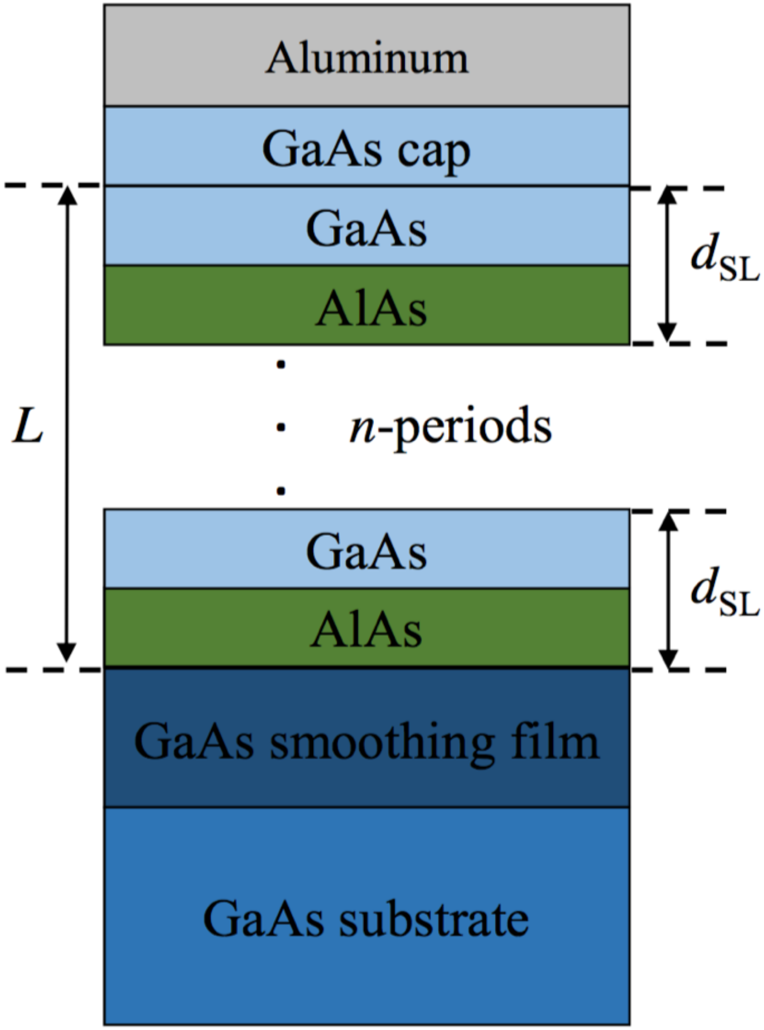


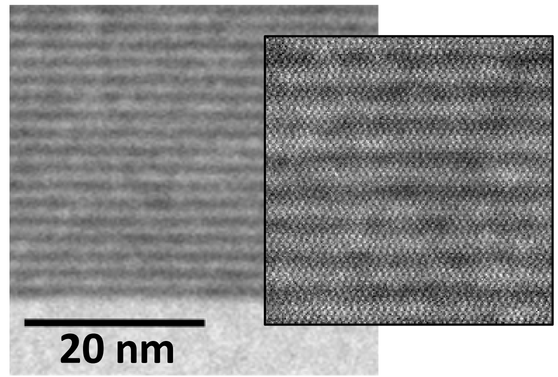


Nat. Mat. **13**, 168 (2013)

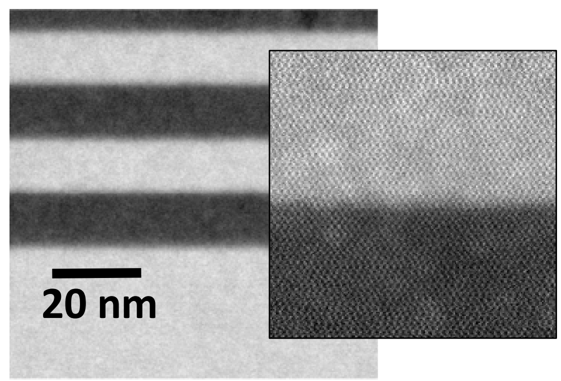
Science **338**, 936 (2012)

Sample matrix of GaAs/AlAs superlattices





d_{SL} = 2 nm

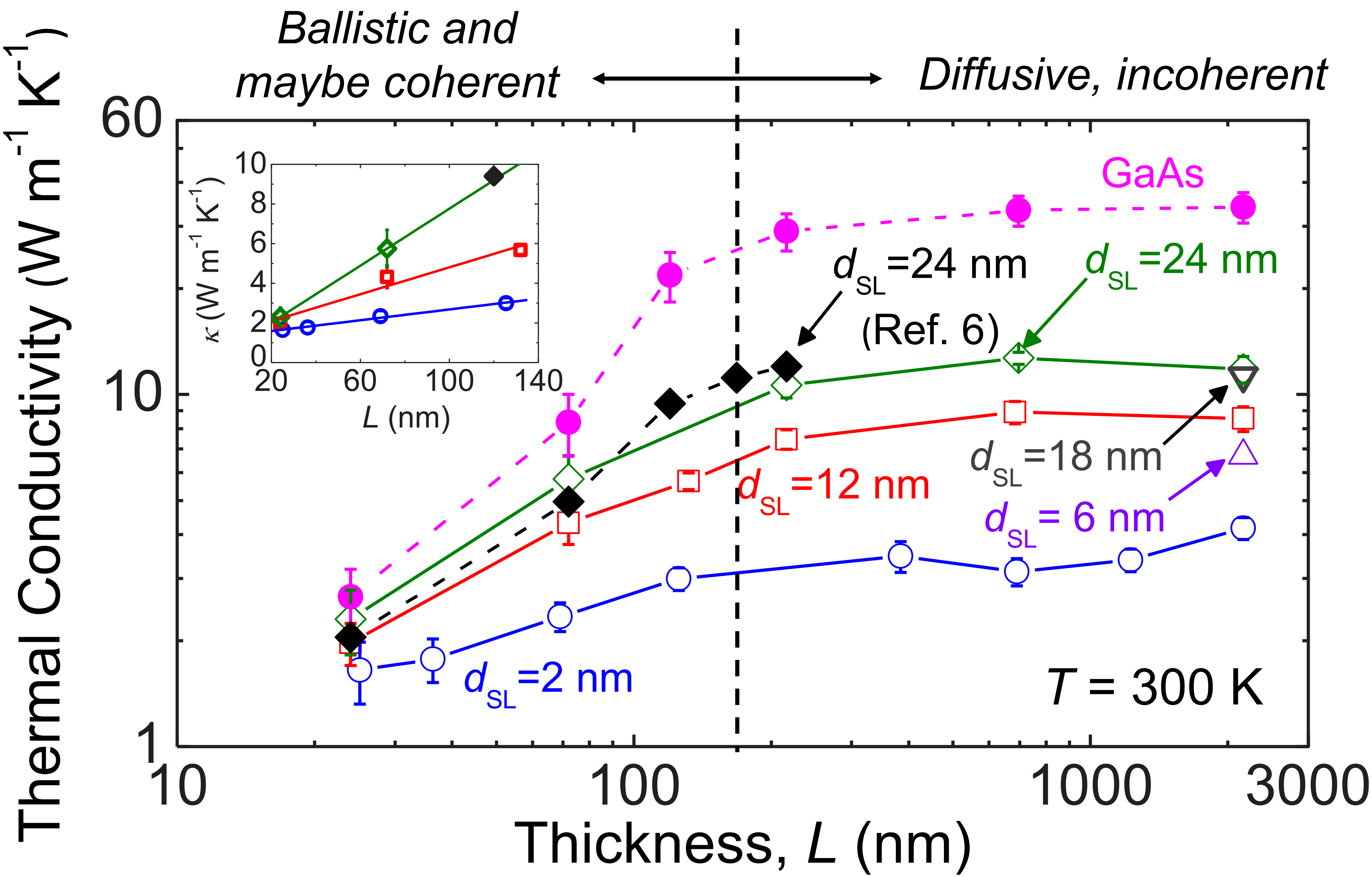


d_{SL} = 24 nm

	Sample Code	d_{SL} (nm)	L (nm)
Superlattices:			
	R13-20	2	20.1
	R13-25	2	31.3
	R13-24	2	64
	R13-21	2	120.5
	R13-27	2	384
	R13-22	2	685.4
	R13-23	2	1,220
	R13-26	2	2,160
	R14-125	12	24
	R14-126	12	72
	R14-127	12	132
	R14-128	12	216
	R14-129	12	684
	R13-111	12	2,160
	R14-121	24	24
	R14-122	24	72
	R14-123	24	216
	R14-124	24	696
	R13-109	24	2,160
	R13-112	6.0	2,160
	R13-110	18.0	2,160

Cheaito et al, *PRB* **97**, 085306 (2018)

Thermal conductivity of GaAs/AlAs SLs



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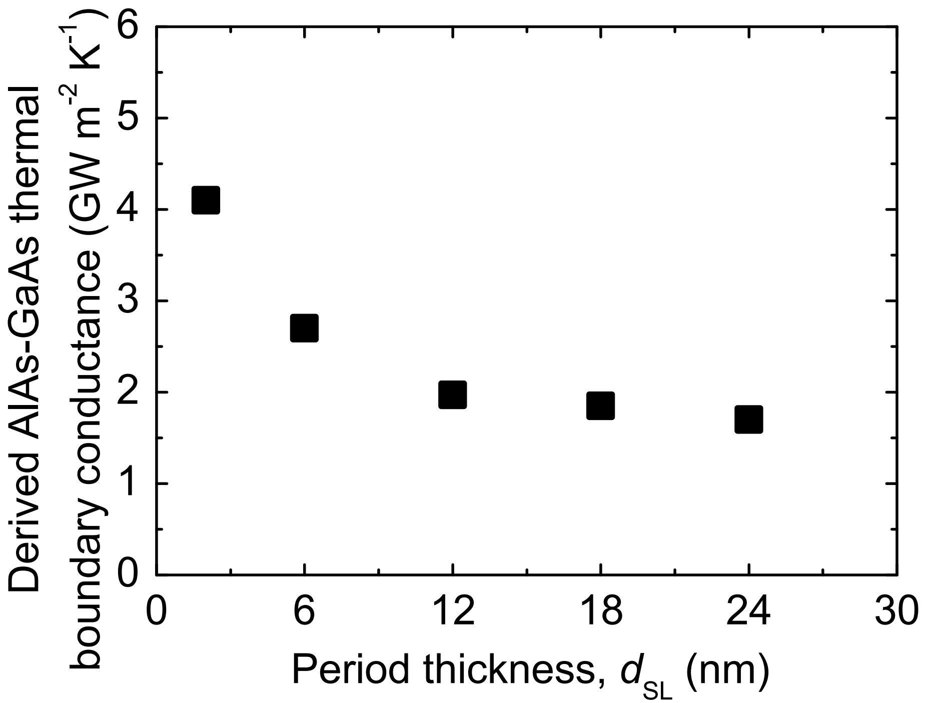
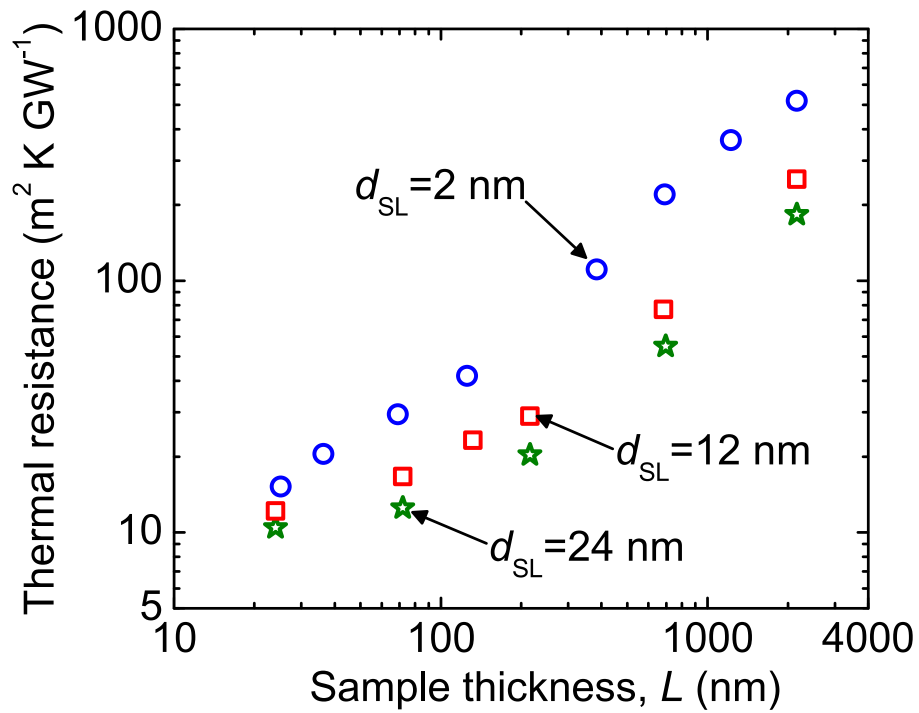
Known: can control thermal resistance with L and d_{SL}

Long and short wavelength phonons "see" boundaries differently, based on length scale and wavelength

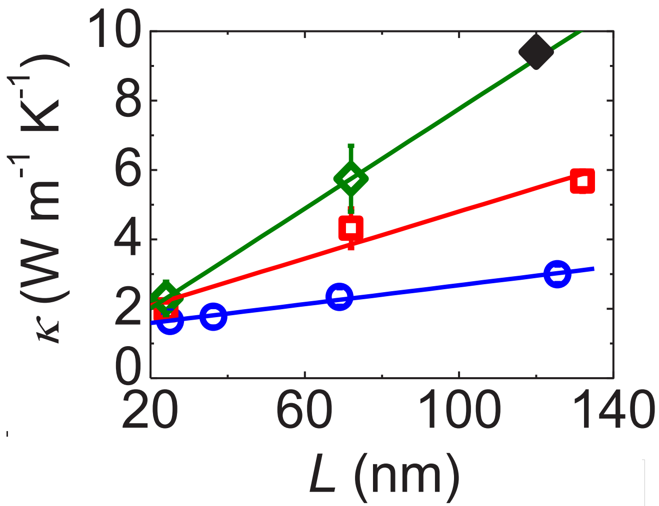
Total resistance (related to temperature rise in device) can be controlled based on selection of L and d_{SL}



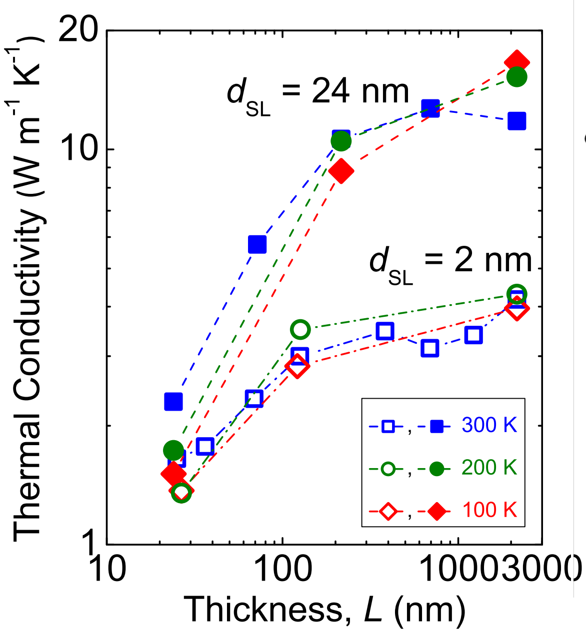


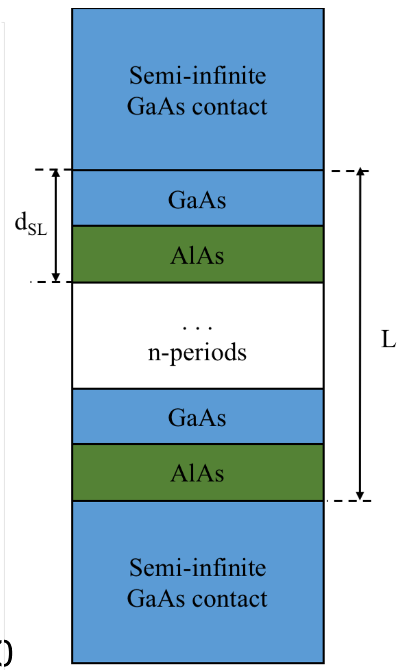
Cheaito et al, *PRB* **97**, 085306 (2018)

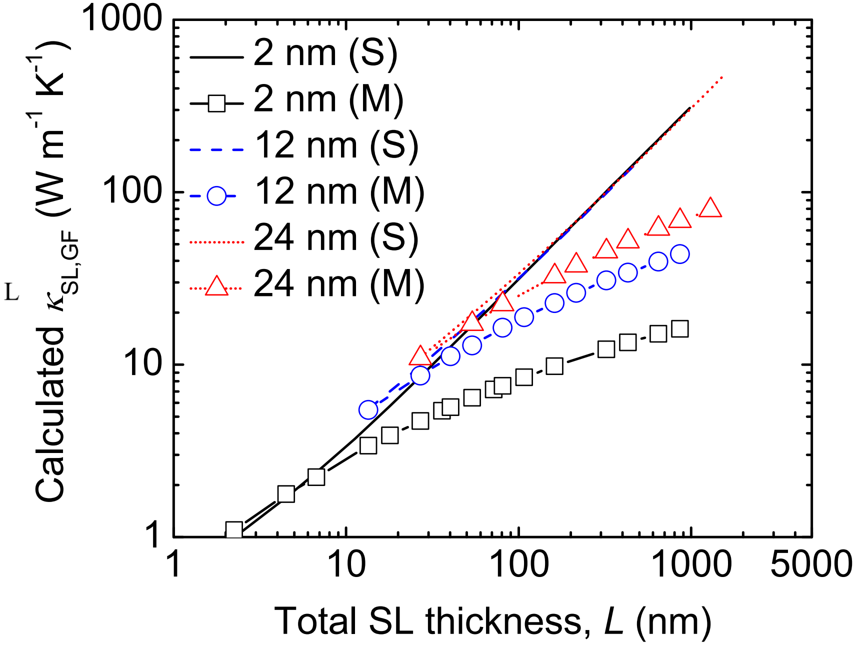
Predicted: Can not conclude coherent transport from $\kappa \sim L$



- **The linear relationship between κ vs. L does not imply coherence in SLs?**
- **Can predict linear κ vs. L in AGF simulations with and w/o phase destroying mixing at interfaces**





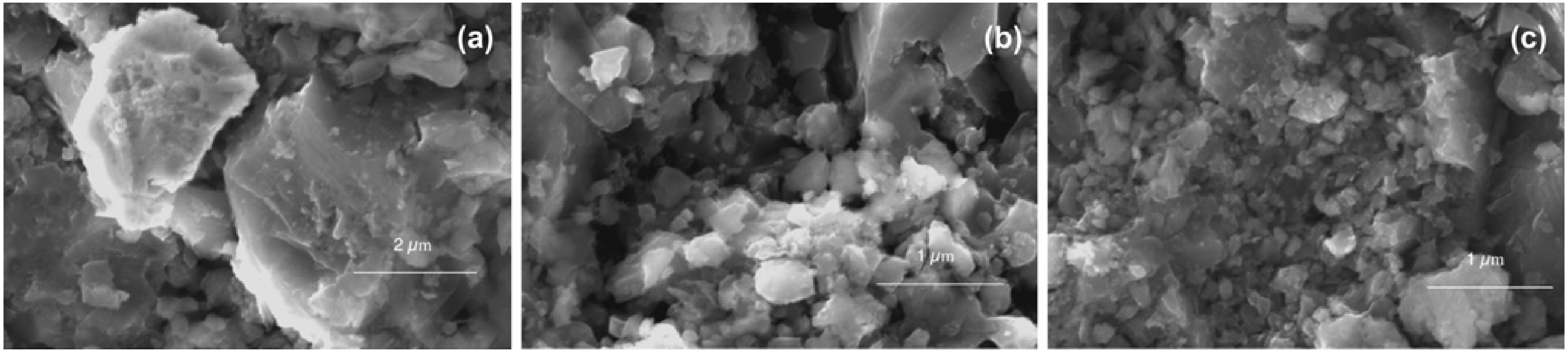


Cheaito et al, *PRB* **97**, 085306 (2018)

Can this be extended to nanograined systems?

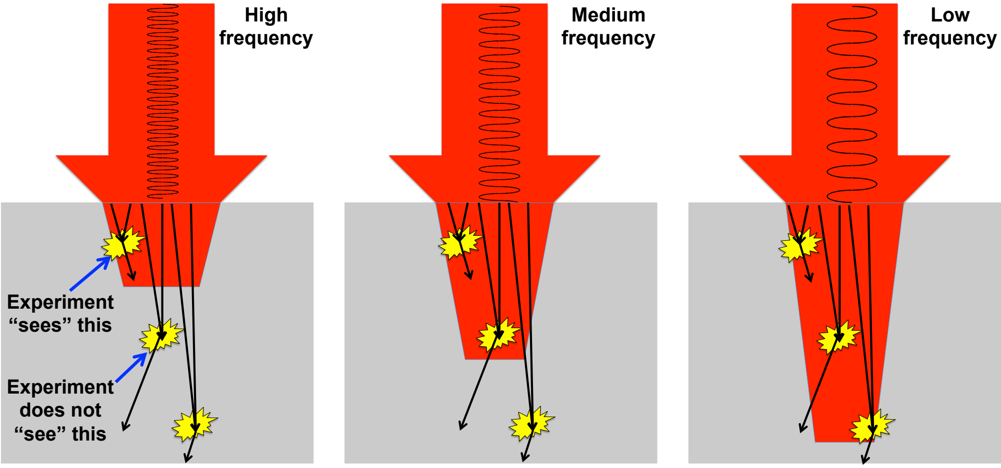
- **Known: Long wavelength phonons may not "see" interfaces if interface density is high enough**
- **Predicted: Even at incoherent interfaces, long wavelength phonons can ballistic traverse interfaces**

- **Investigate at nanograined silicon germanium alloys**
- **Do long wavelength phonons see boundaries if Λ>>grain size?**

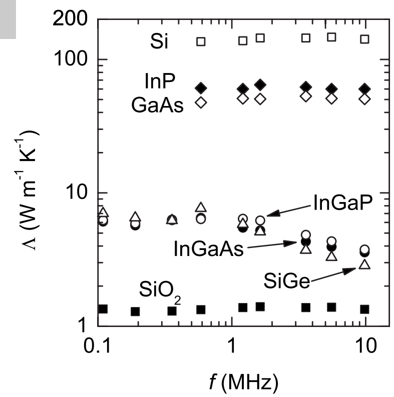


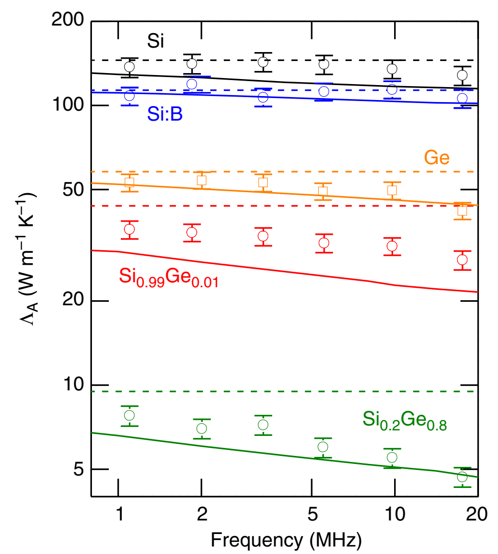
Chen et al, *APL* **111**, 131902 (2017)

Why Si-Ge nanograined alloys?

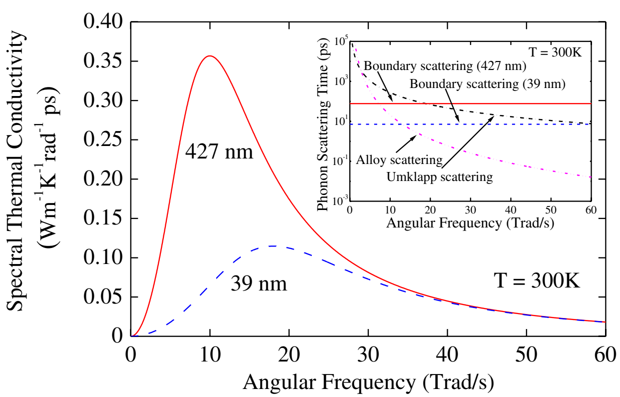


Frequency dependent TDTR can be used for MFP spectroscopy



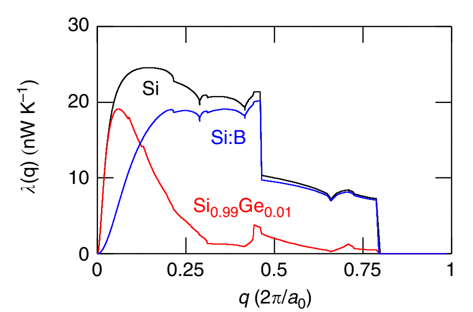


Long wavelength phonons carry most of the heat

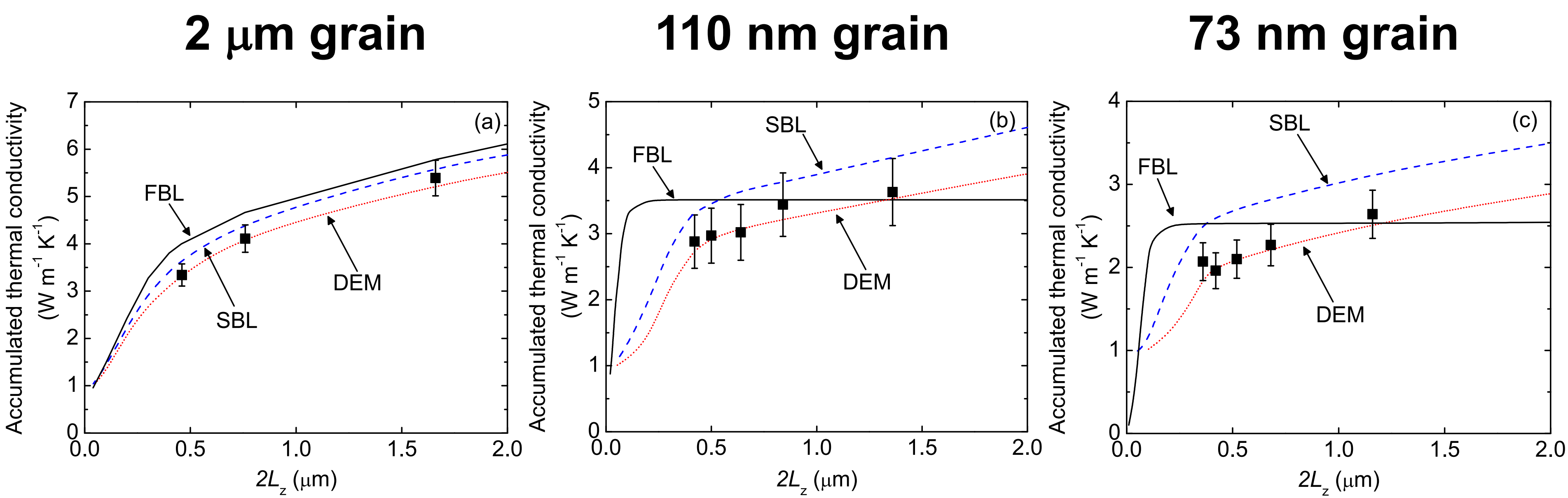


Cheaito et al, *PRL* **109**, 195901 (2012)

From
PRB **76**, 075207 (2007)
Nat. Comm. **5**, 5075 (2014)



Phonons don't "see" grain boundaries if Λ is long enough

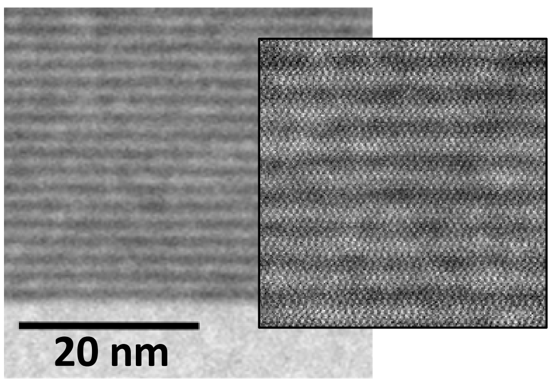


Models

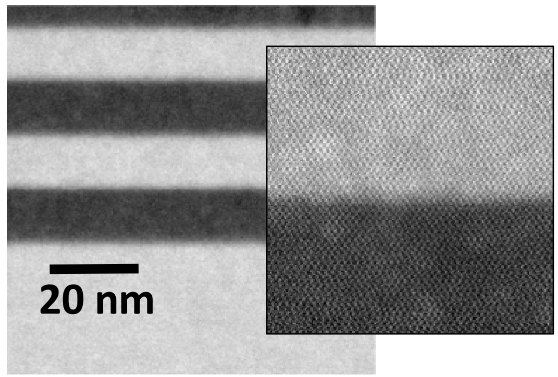
- FBL: all phonons scatter at boundary
- SBL: phonons with wavelengths >> grain size do not scatter at boundary (consider scattering cross sections)
- DEM: SBL + differential effective medium

Chen et al, *APL* **111**, 131902 (2017)

Summary/outlook – boundaries for selective phonon filters



d_{SL} = 2 nm



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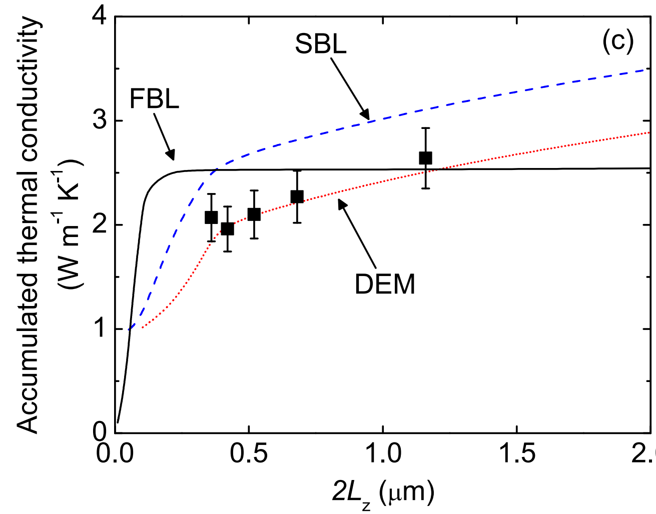

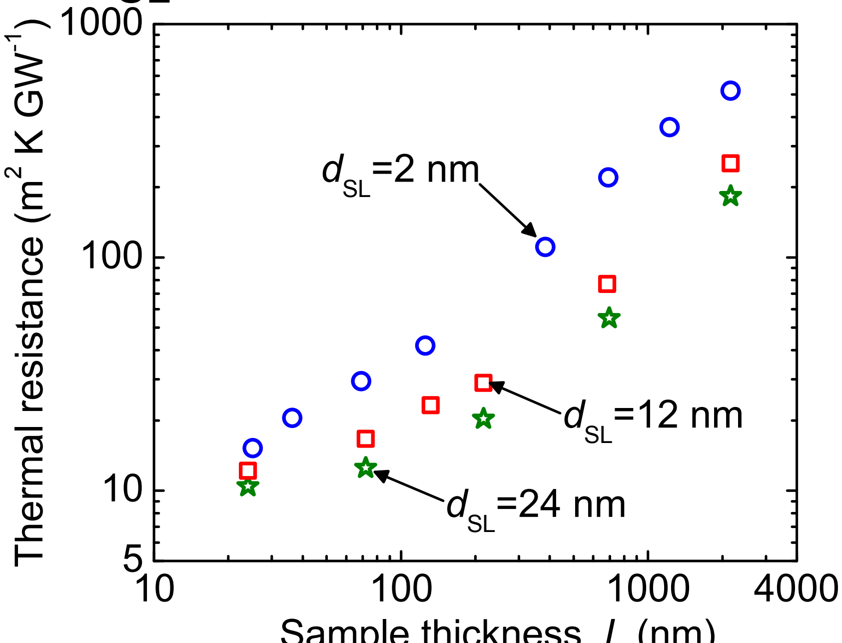

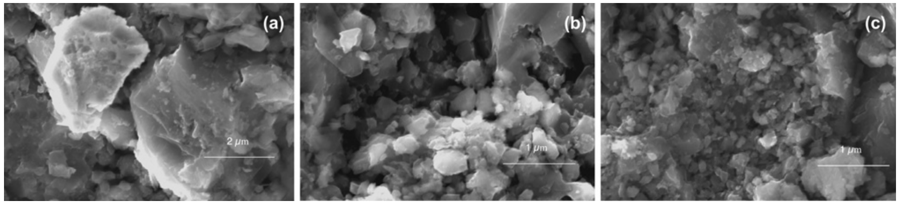

Summary/outlook – boundaries for selective phonon filters

PHYSICAL REVIEW B **97**, 085306 (2018)

Interplay between total thickness and period thickness in the phonon thermal conductivity of superlattices from the nanoscale to the microscale: Coherent versus incoherent phonon transport

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Ballistic transport of long wavelength phonons and thermal conductivity accumulation in nanograined silicon-germanium alloys

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