NANOSCALE HEAT TRANSFER FOR THERMOELECTRIC ENERGY CONVERSION

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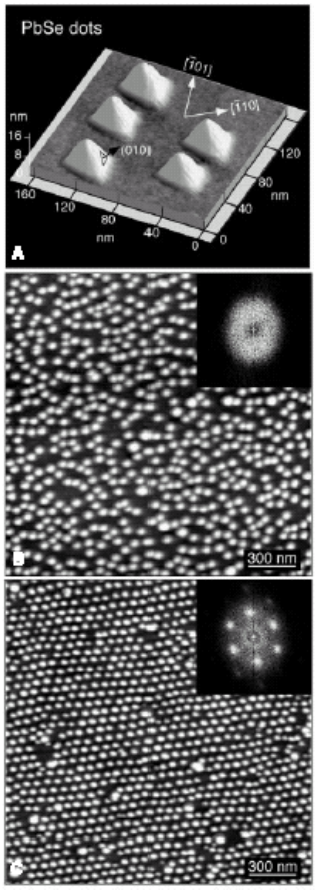
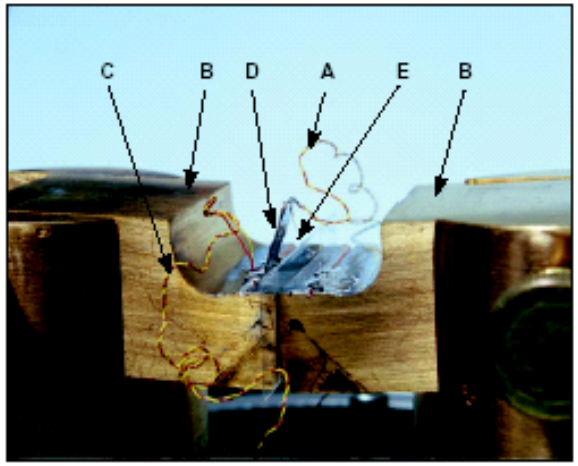
DOE/EPRI High Efficiency Thermoelectrics Workshop
February 17-20, San Diego, CA

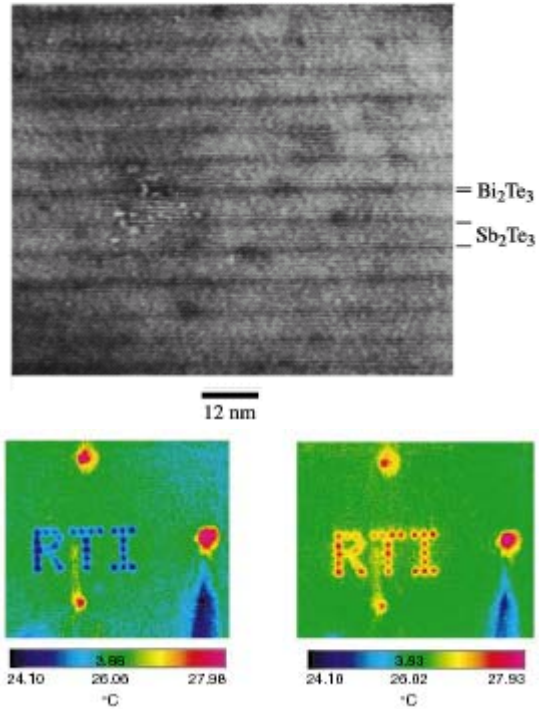
STRUCTURES WITH ENHANCED ZT





PbTe/PbTeSe Quantum Dot Superlattices

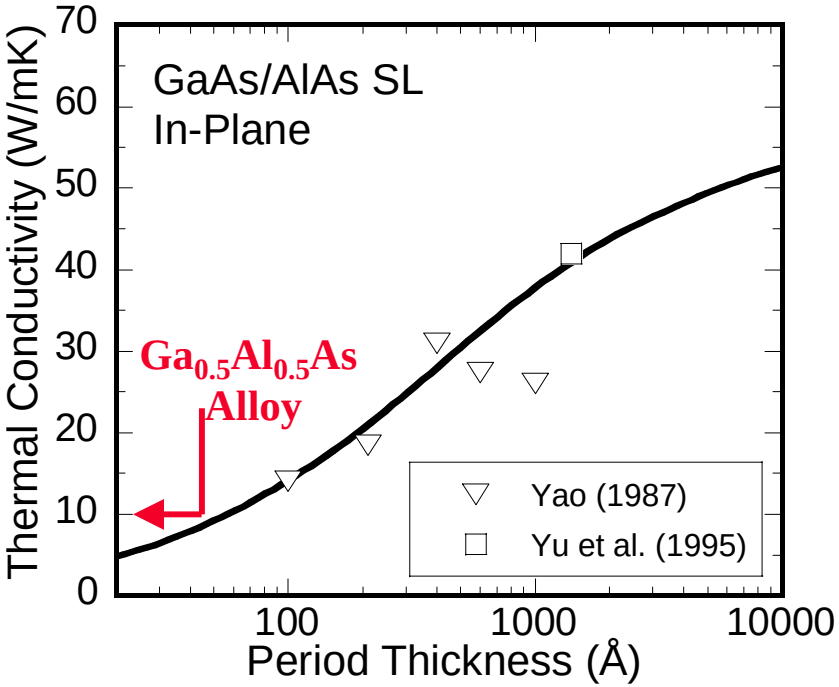
Ternary: ZT=1.3-1.6
Quaternary: ZT=2
ΔT=43.7 K, Bulk ΔT=30.8 K
T.C. Harman, Science, 2002

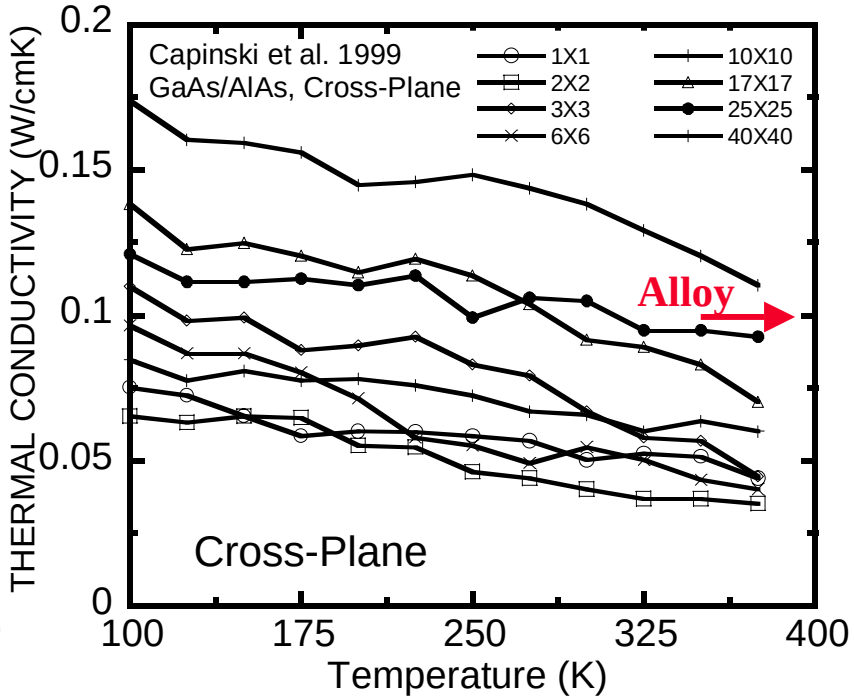


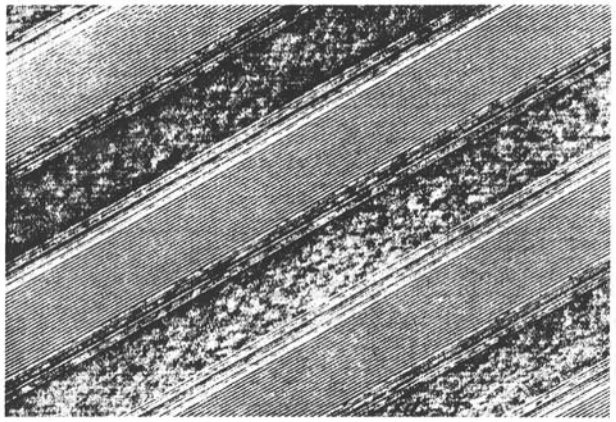
ΔT=32.2 K, ZT ~2-2.4
R. Venkatasubramanian, Nature, 2001

PbTe/PbSeTe	Nanostructure	Bulk	Bi_2Te_3/Sb_2Te_3	Superlattice	Bulk
Power Factor (μW/cmK^2)	32	28		40	50.9
Conductivity (W/mK)	0.6	2.5		0.5	1.26

Thermal Conductivity of Superlattices





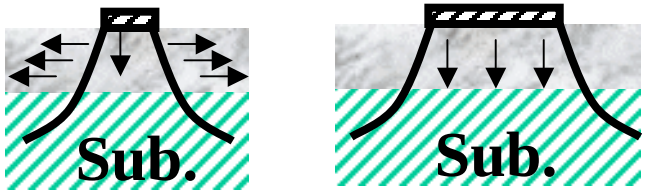


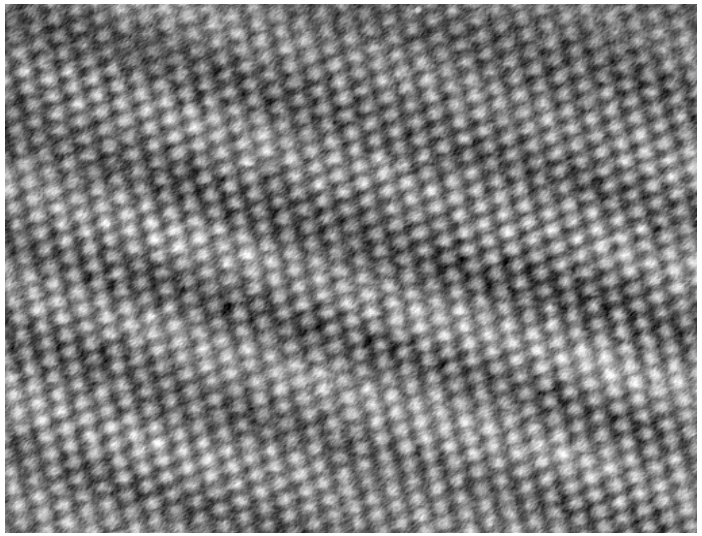
Thermal Diffusivity of GaAs/GaAlAs Thin Film ($x10^{-4}m^2/s$)

In-Plane		Cross-Plane	
Bulk	Exp.	Bulk	Exp.
0.330	0.062	0.126	0.026

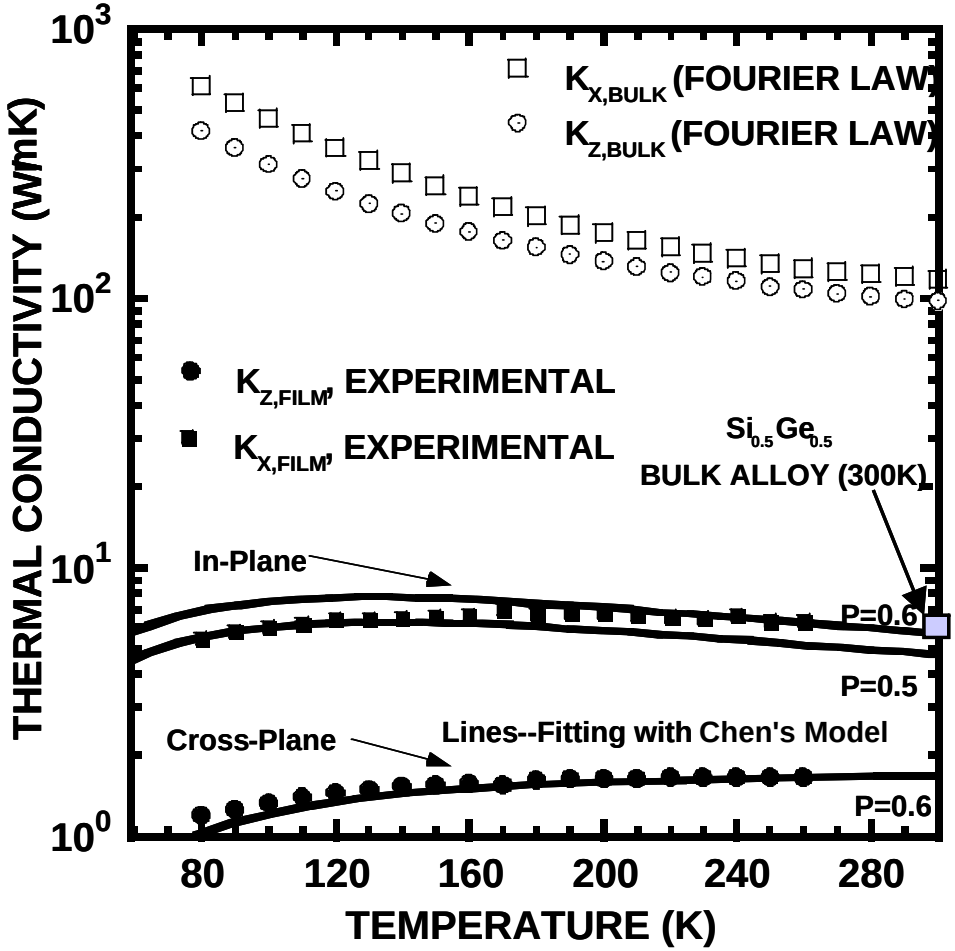
Chen et al. (1994)

THERMAL CONDUCTIVITY OF SUPERLATTICE

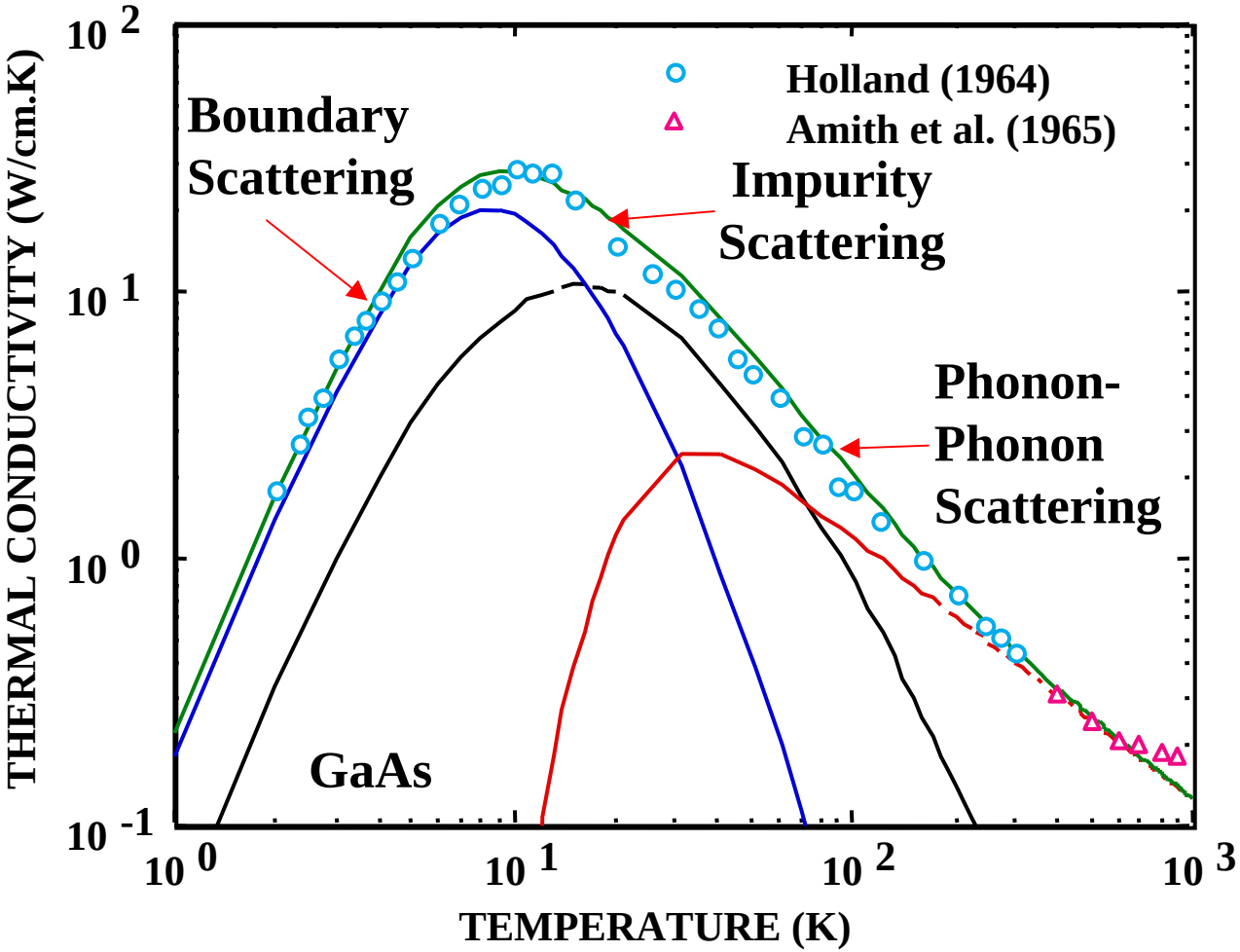




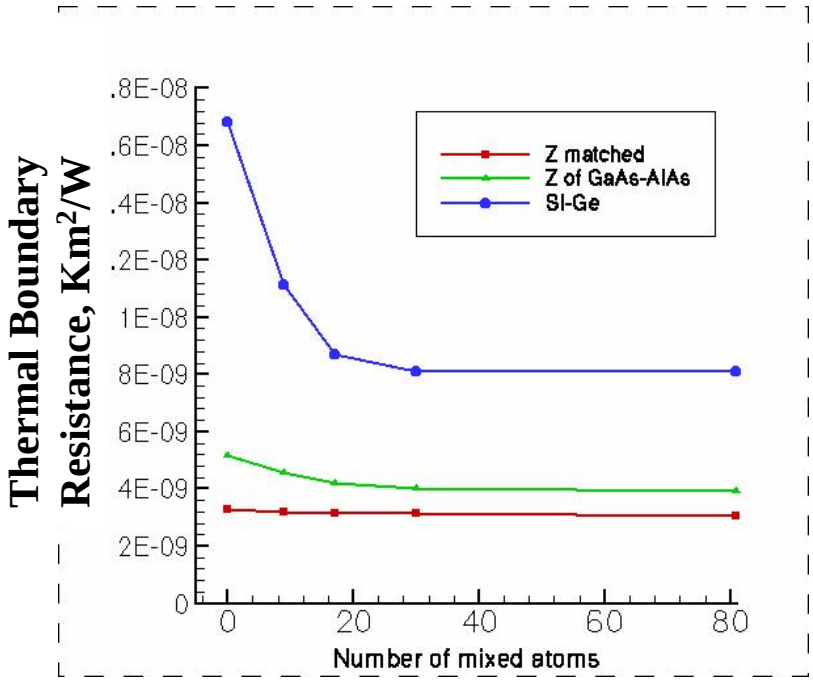
Si/Ge

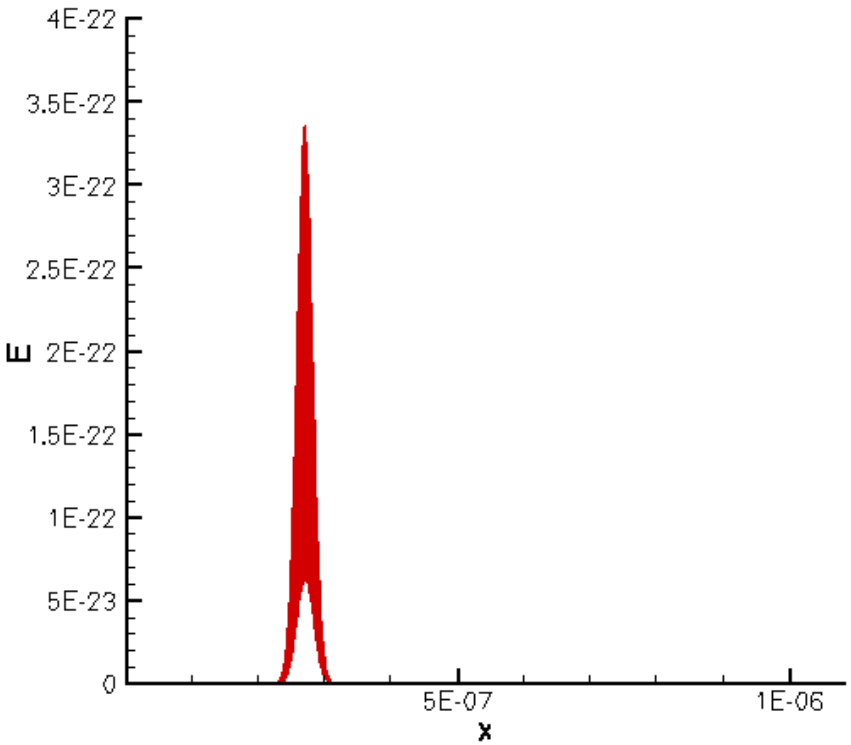


Bulk Crystal Thermal Conductivity



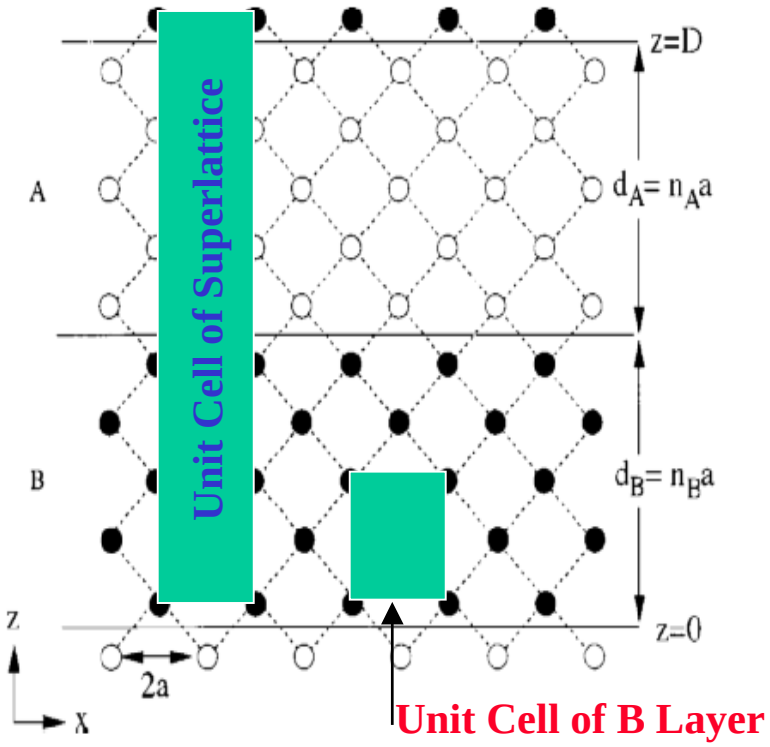
Phonon Reflection at A Single Interface



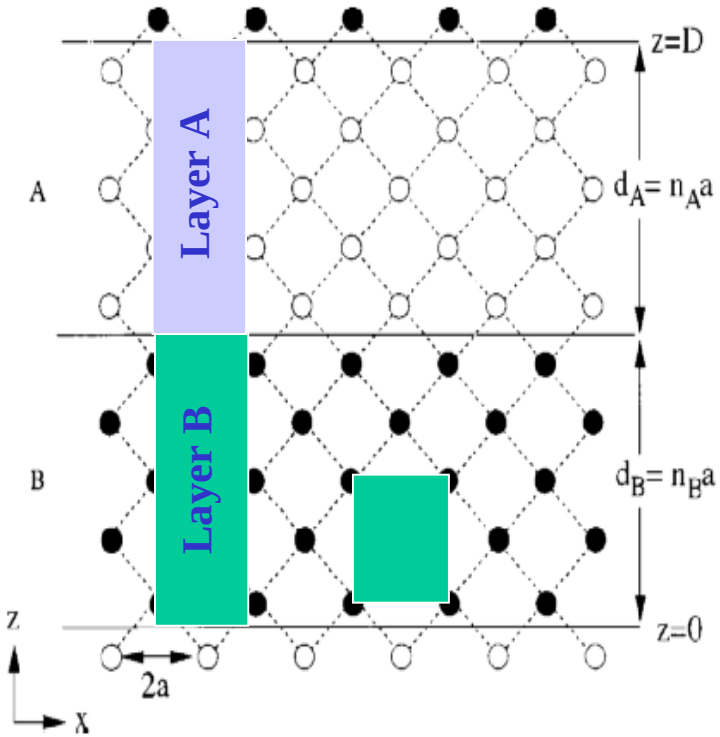


MD Simulation by J.B. Freund, UIUC

Homogeneous or Inhomogeneous?

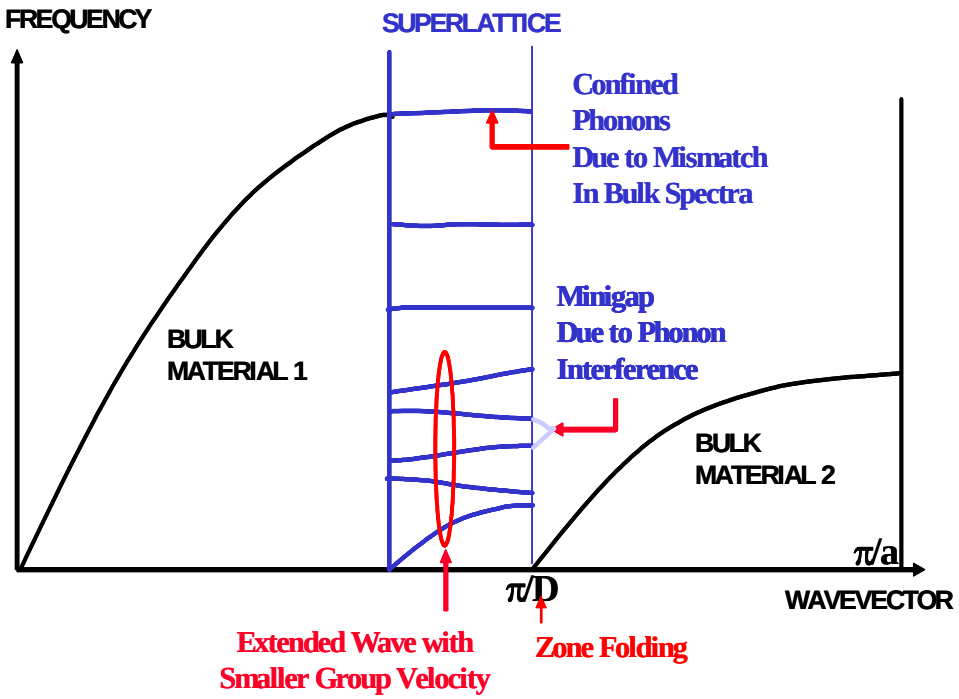


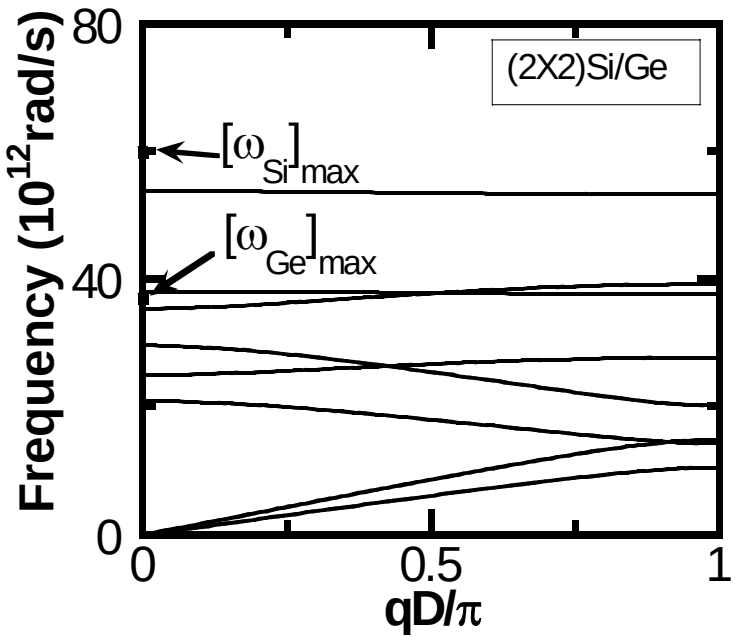
A New Crystal?



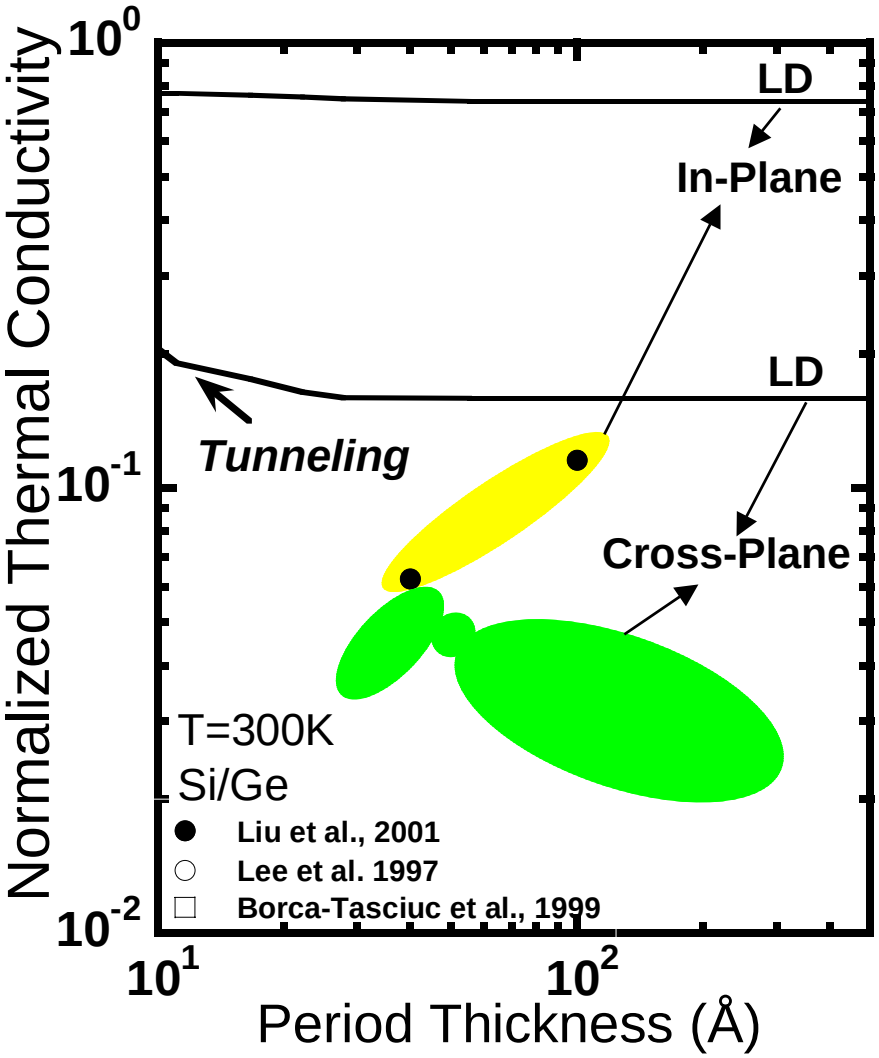
Inhomogeneous Multilayers?

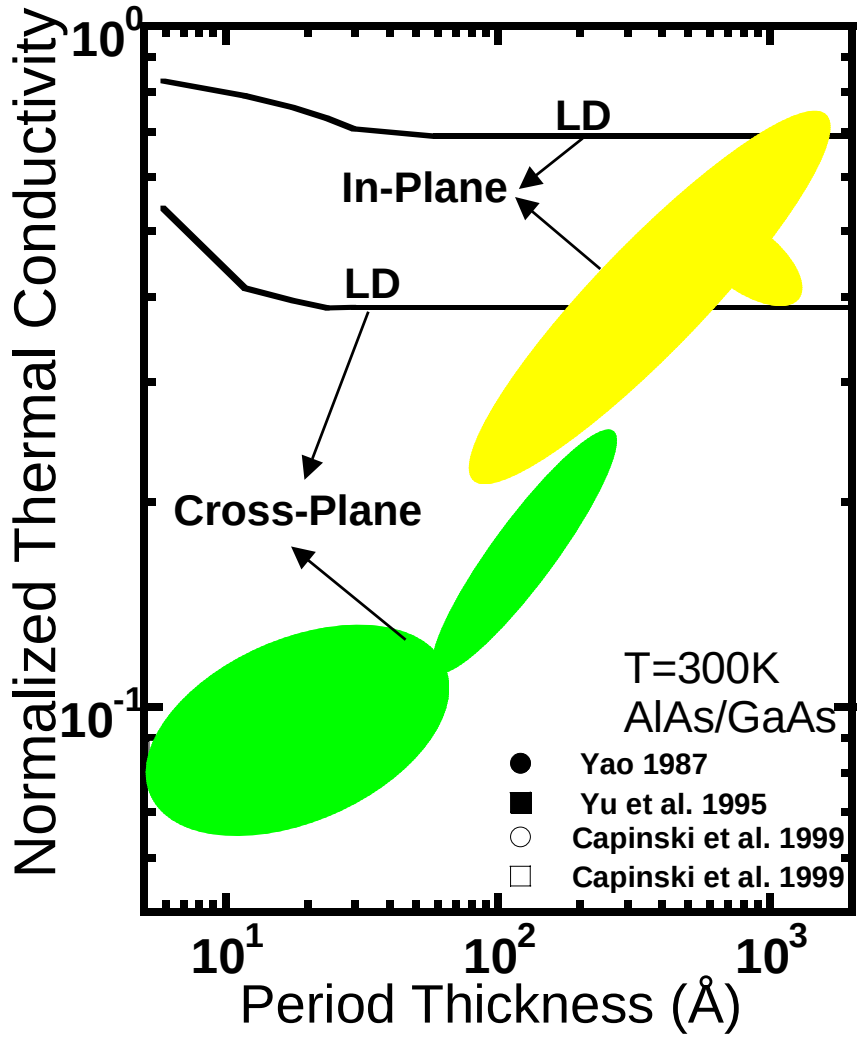
Phonons in Homogeneous Superlattice



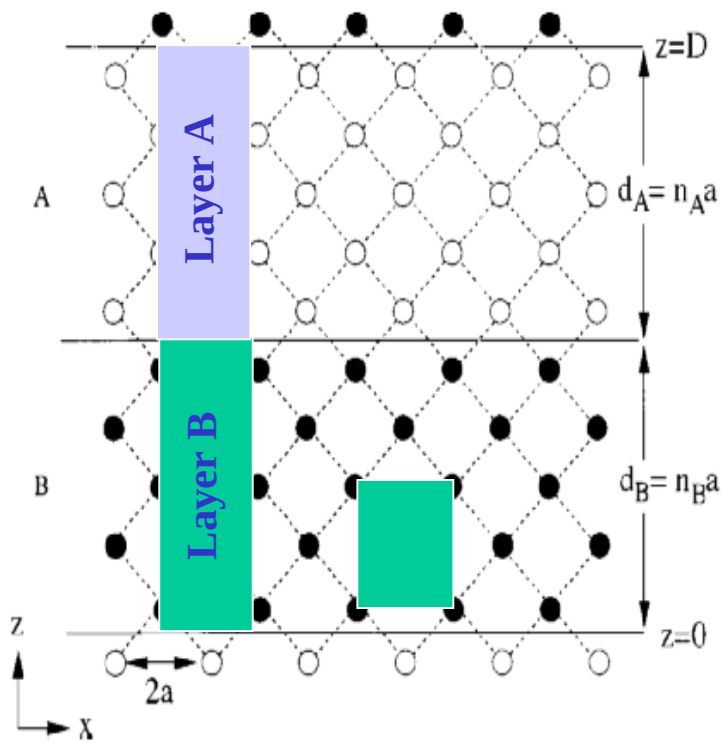


COMPARISON WITH EXPERIMENTS





Composites: Sequential Interface Scattering



Each layer has bulk phonon dispersion

- **Boltzmann Equation**

$$\cos\theta_i \frac{\partial i_i}{\partial z_i} + \frac{i_i}{\Lambda_i} = -\sin\theta_i \frac{dI_{oi}}{dx}$$

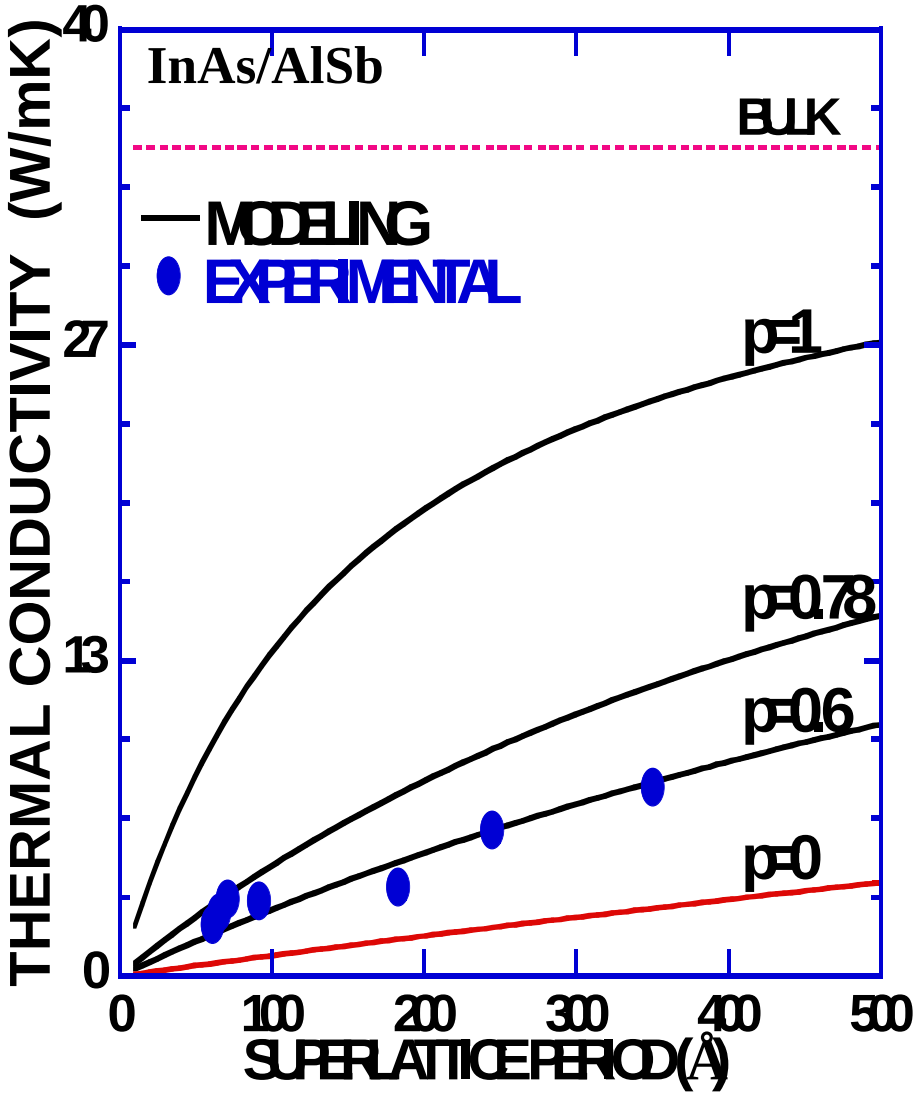
I_{oi} --- Equilibrium Intensity
i_i --- Intensity Deviation
Λ_i --- Mean Free Path

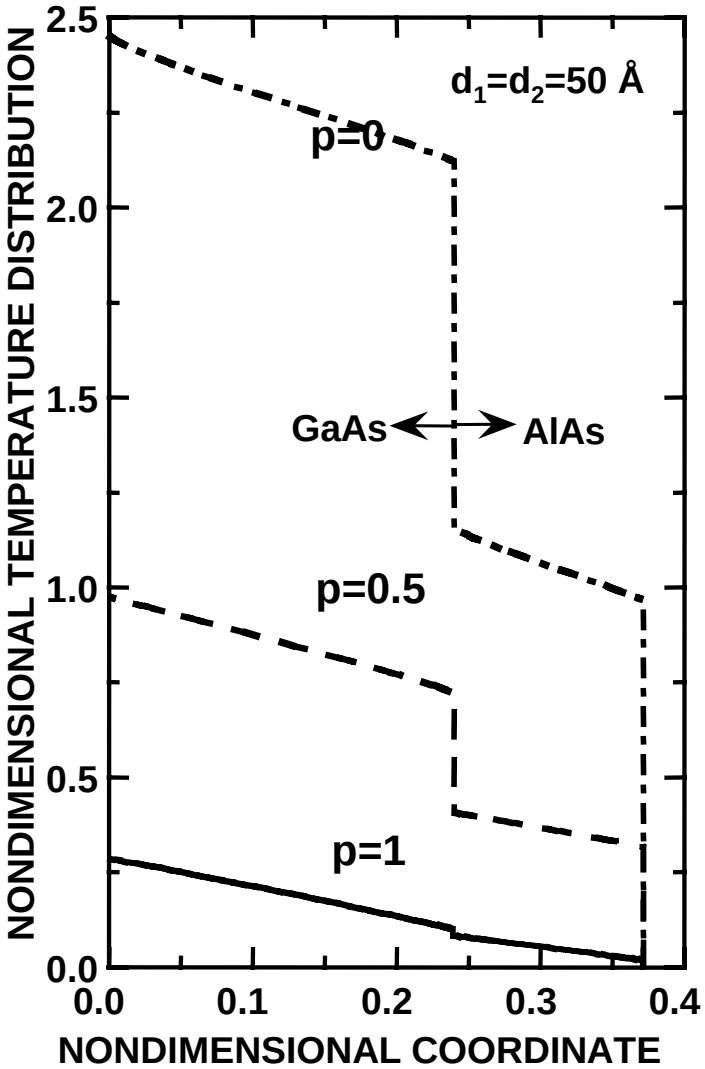
- **Interface Reflection**

Mismatch in acoustic properties
Mismatch in phonon spectrum
Interface roughness and anharmonicity

- **Interlayer Coupling**

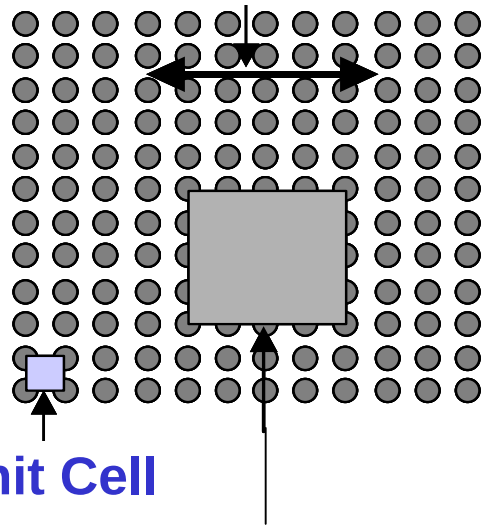
CROSS-PLANE HEAT CONDUCTION



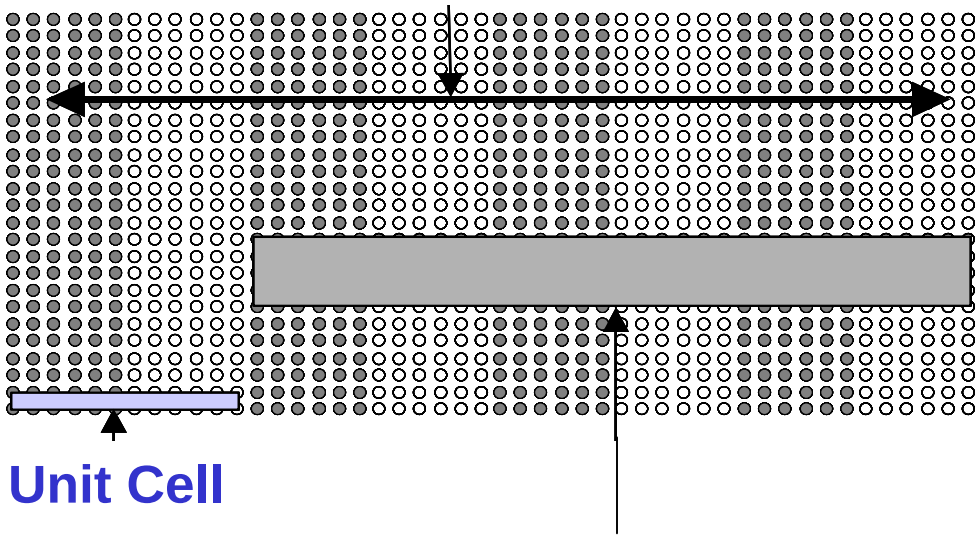


Superlattice Modes vs. Bulk Modes

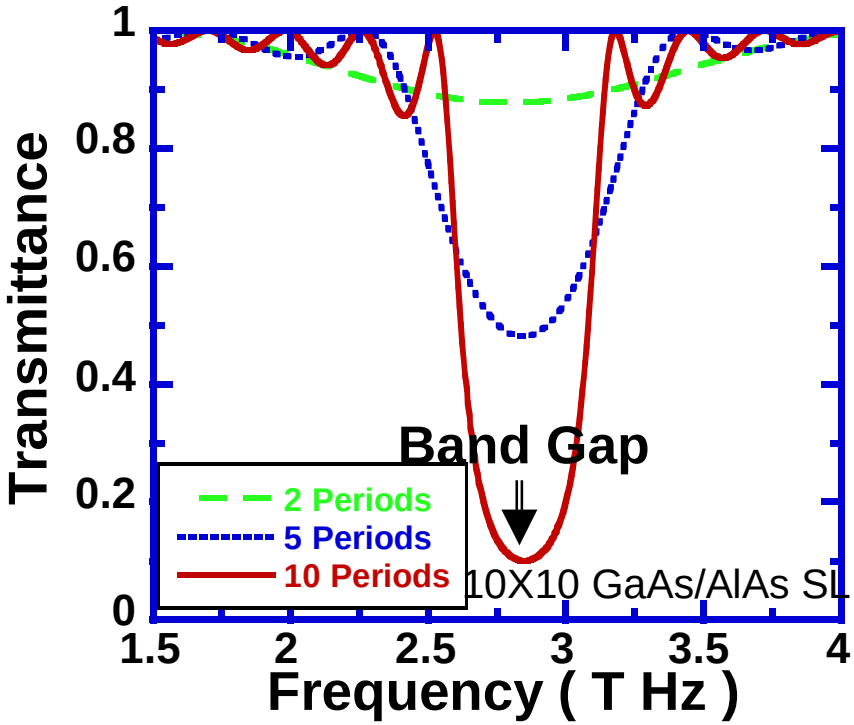
Mean Free Path in Bulk, l_{bulk}

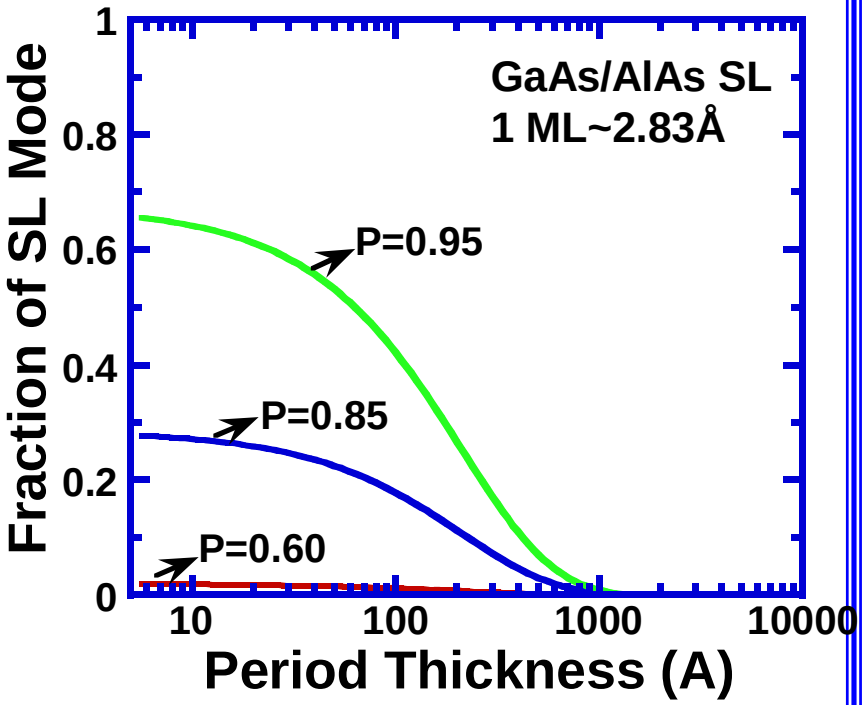


Mean Free Path in SL, l_{SL}

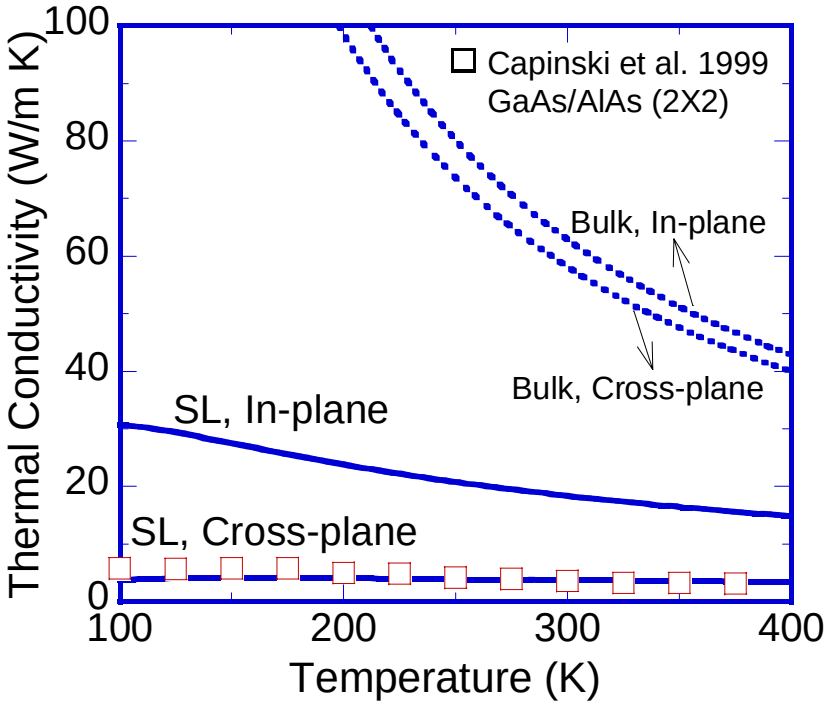


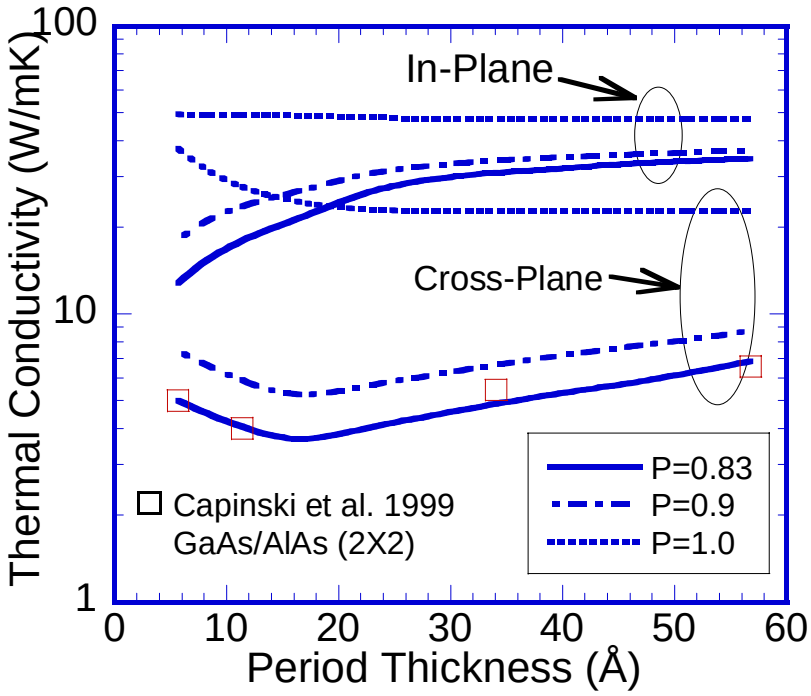
Fraction of SL Modes





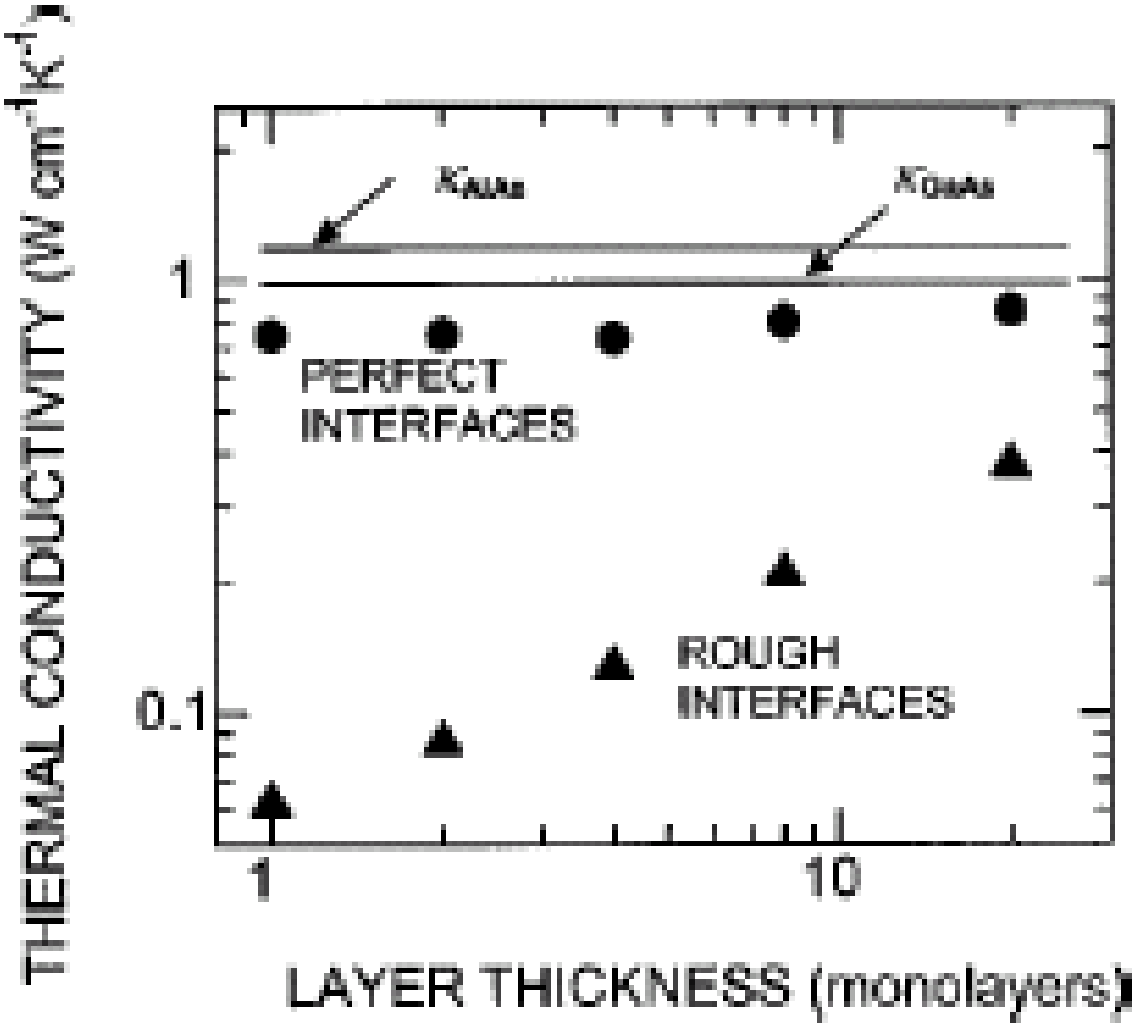
Results from Unified Lattice Dynamics Model





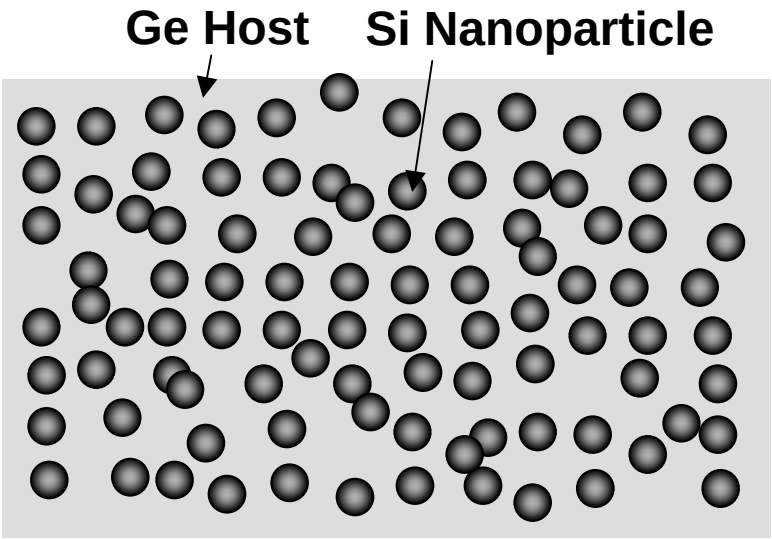
Coherence Not Important. Reduction of MFP is More Effective.

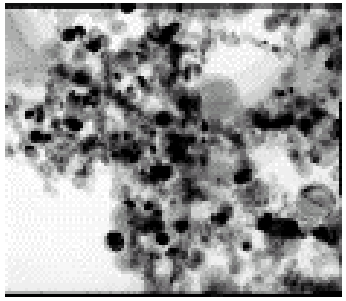
Molecular Dynamics Simulation

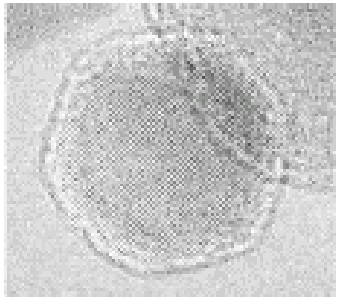


Daly et al., PRB, 2003.

Nanocomposite Approach







Preliminary
Hot Pressed Si-Ge
Nanocomposite

Phonons:

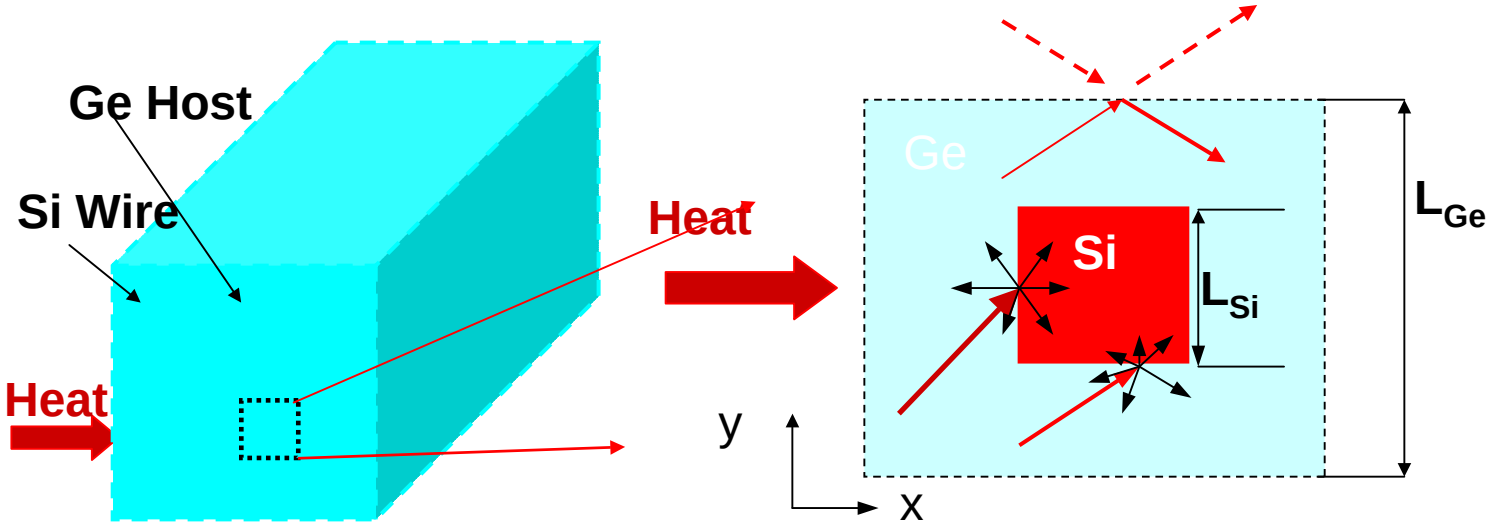
- **Reduced thermal conductivity by Interface Scattering**

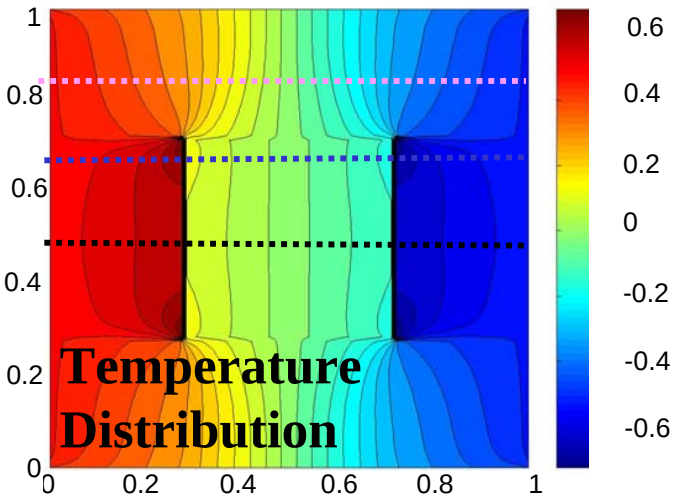
Electrons:

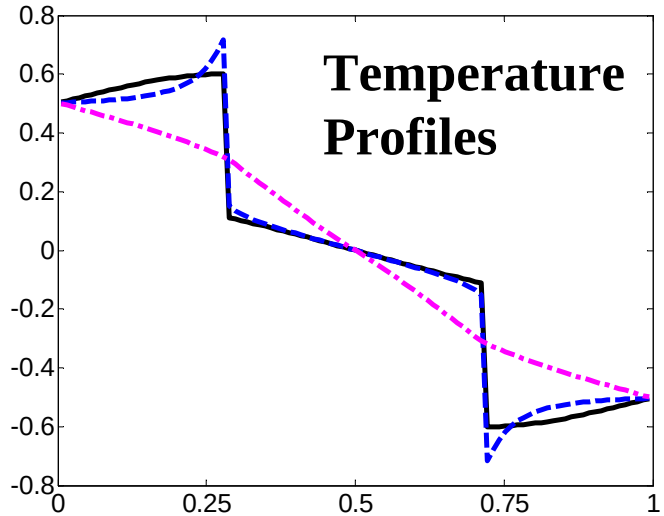
- **Control interface potential to maintain power factor**

MIT/BC/JPL

HEAT CONDUCTION IN NANOCOMPOSITE







Future Needs

- Predicative tools for interface processes
- Concurrent electron/phonon transport
- Explore different materials combinations
- Synthesize/characterize nanocomposites

Acknowledgments

Collaborators

M.S. Dresselhaus (MIT)
J.B. Freund (UIUC)
P. Gogna (JPL)
Jean-Pierre Fleurial (JPL)
Z. F. Ren (Boston College)

Graduate Students

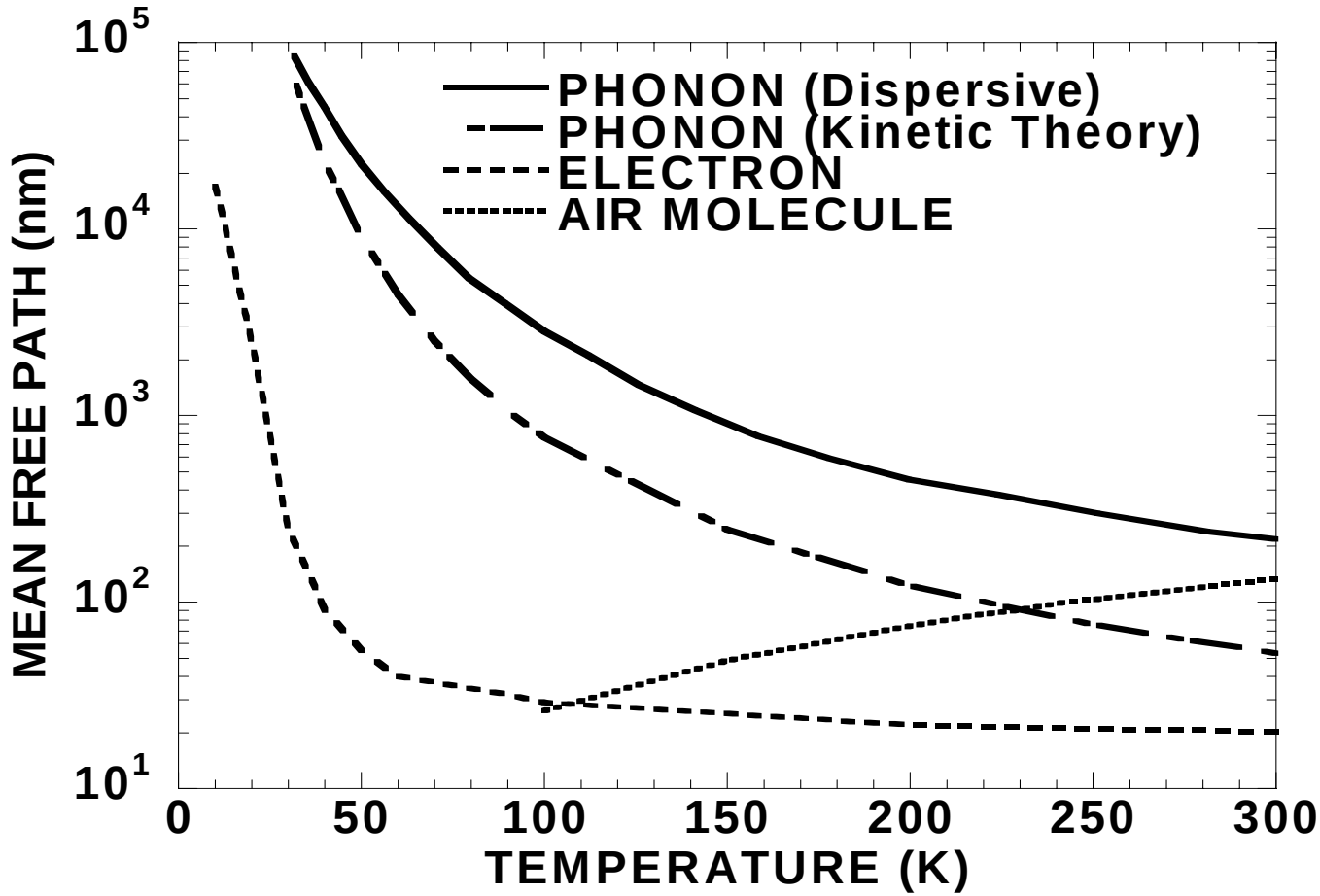
T. Borca-Tasciuc (RPI)
C. Dames
T. Harris
R.G. Yang
H. Lee
B. Yang (U. Maryland)

Past/Current Support: ONR MURI/NASA/DOE BES/NSF

MEAN FREE PATH OF HEAT CARRIERS

- **KINETIC THEORY**

$$k \approx Cv\Lambda / 3$$

- **BULK THERMAL CONDUCTIVITY**

$$k = \int C(\omega)v(\omega)\Lambda(\omega)d\omega / 3$$