

Heat Conduction by Molecular Dynamics Technique

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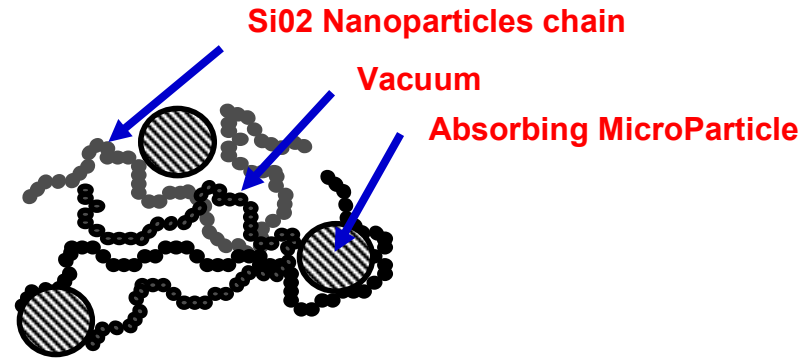
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UNDERSTANDING AND MONITORING MATERIALS PROPERTIES

NEW MATERIALS contain nano-micro architected structures

o NANOFIBERS:

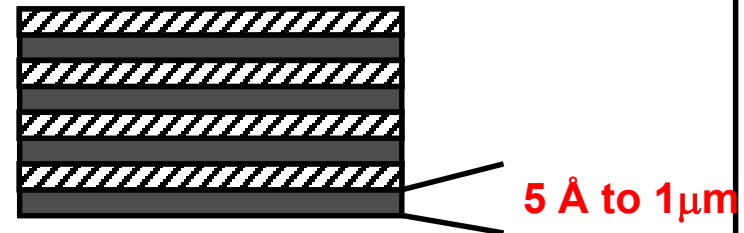
*multiscale complex materials
ultra insulating (0.007 W/mK)*



o SUPERLATTICES

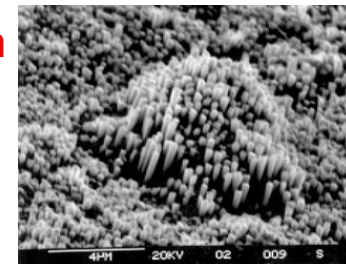
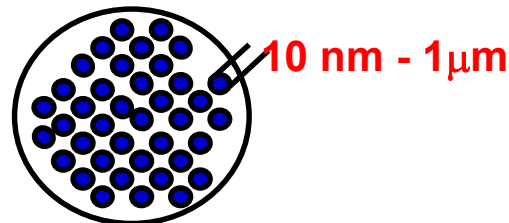
monitoring thermal conductivity

$$\lambda_{Bulk}/10 < \lambda < \lambda_{Bulk}$$



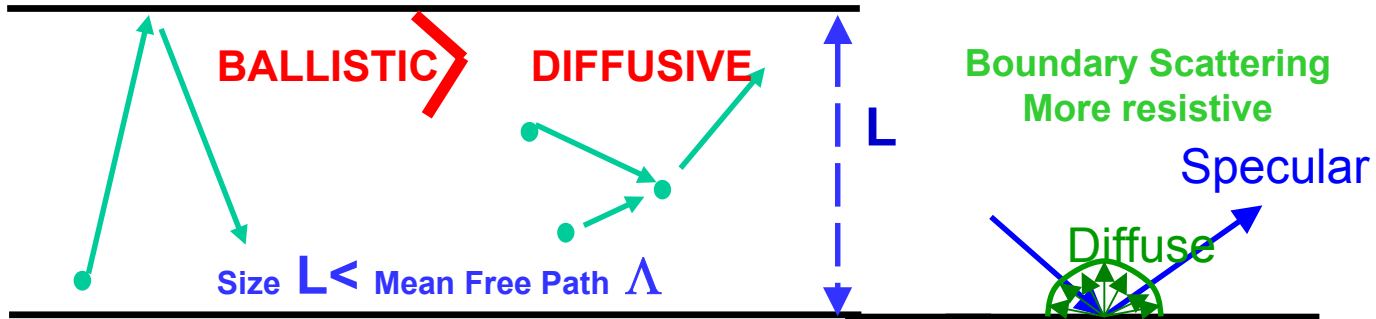
o NANOWIRES templates:

monitoring anisotropy



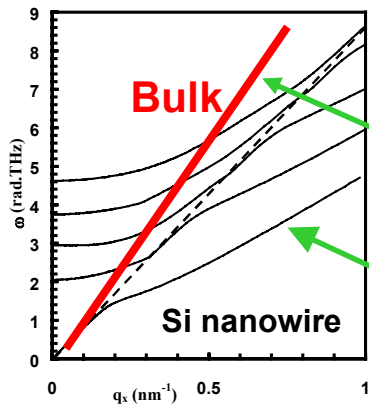
LOW-DIMENSIONAL PHYSICS FOR HEAT CONDUCTION

o Ballistic Transport of Phonons



o Phonon Confinement

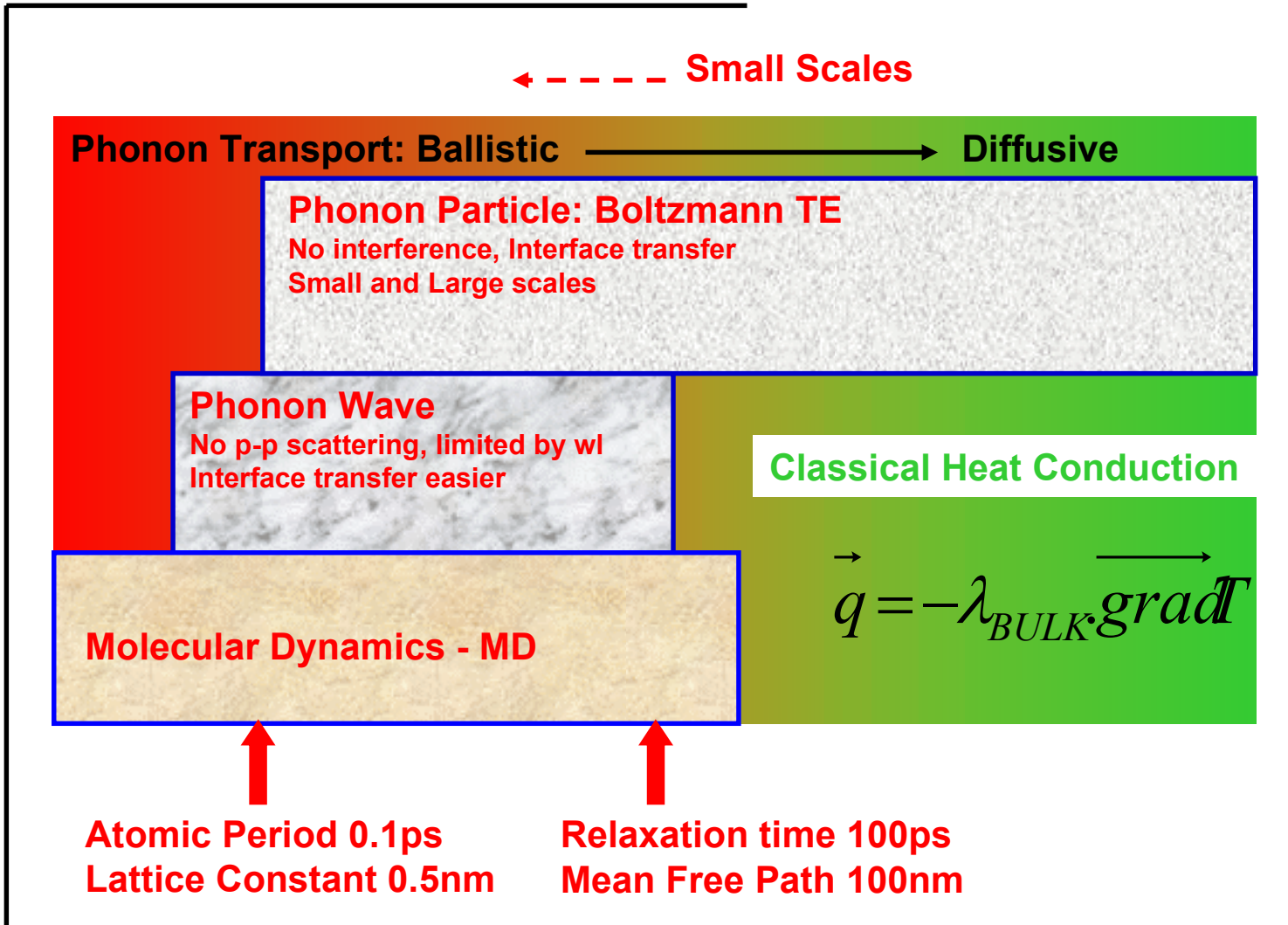
v_G and Λ Reduction



$$\vec{q} = -\lambda_{BULK} \cdot \text{grad } T$$

$$\lambda_{\text{eff}}(\text{size}) < \lambda_{BULK}$$

SITUATION of MD



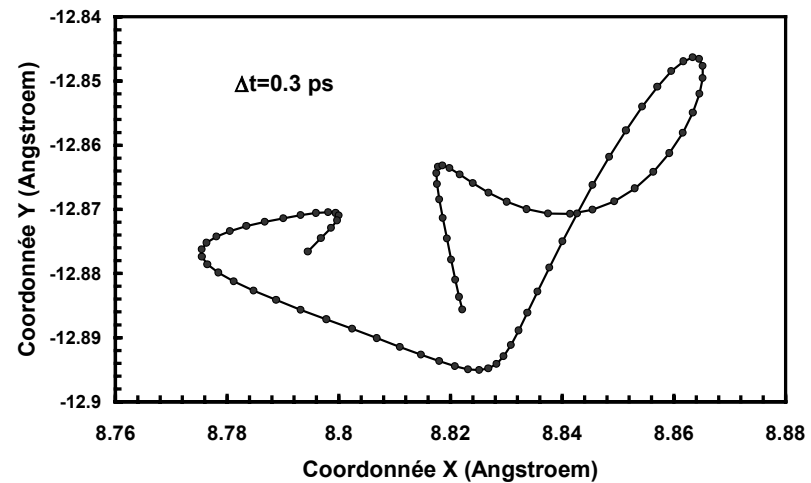
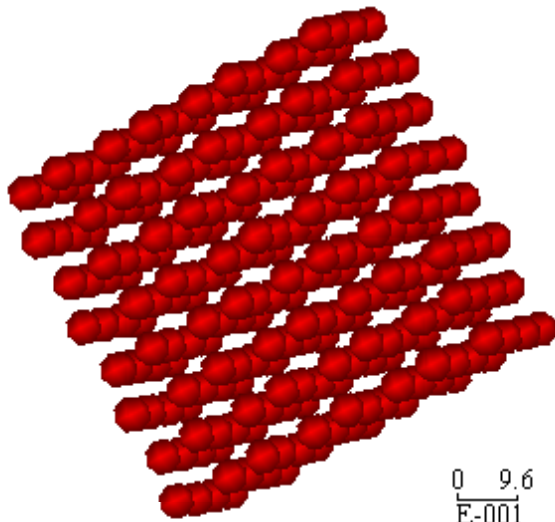
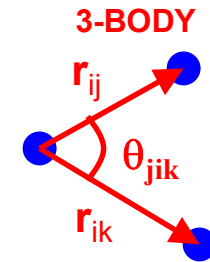
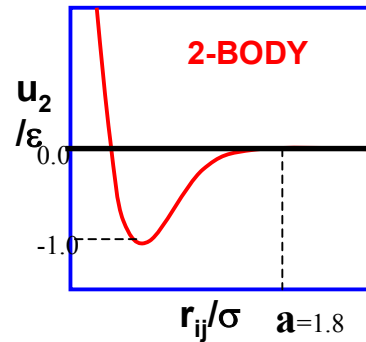
MOLECULAR DYNAMICS TECHNIQUE

COMPUTE ALL ATOMIC TRAJECTORIES

• 2nd NEWTON LAW

$$M \frac{d^2 \mathbf{r}_i}{dt^2} = \sum_{\substack{j=1 \\ j \neq i}}^N \mathbf{F}_{ij}$$

• STILLINGER-WEBER POTENTIAL

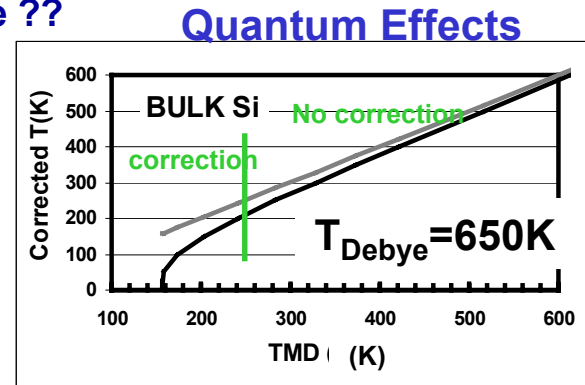


ADVANTAGES OF MD TECHNIQUE

- o Phonon Scattering is Difficult to Model:
Phonon Particle Approach: Relaxation Time ??
Phonon Wave Approach: No scattering.

MD PROVIDES A COMPLETE DESCRIPTION OF PHONON SCATTERING

EXAMPLE: NANOWIRE



- o Phonon Transport Approach Assumes Fully Periodic Lattices

MD ALLOWS TO INCLUDE ATOMIC DEFAULTS and STRAINS

EXAMPLE: SUPERLATTICE

- o Non-Equilibrium Short Time Heat Conduction

MD DESCRIBE HT BEHAVIOUR AT GigaHTz FREQUENCIES

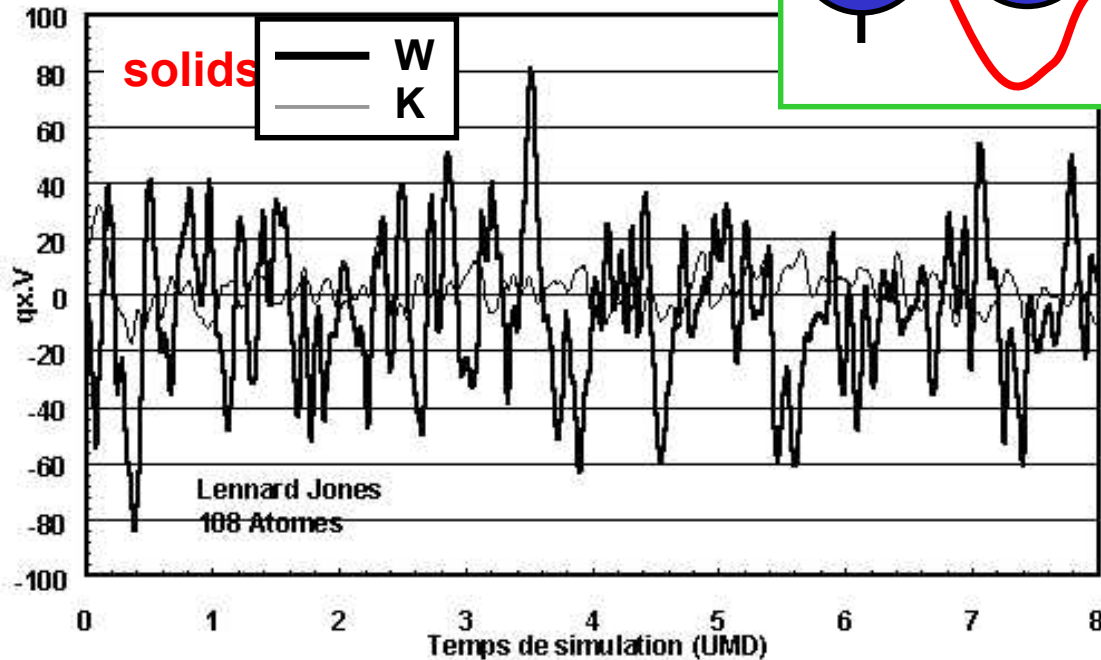
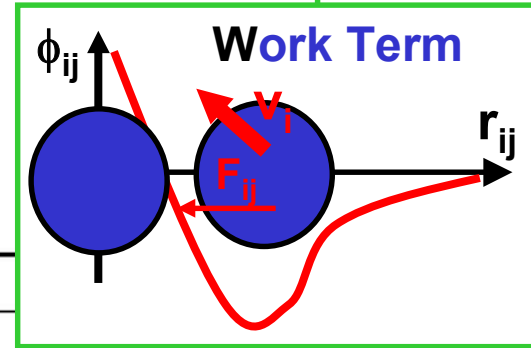
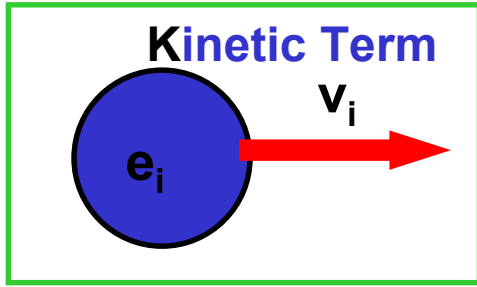
EXAMPLE: IN BULK SI

HEAT FLUX by MD

o Kinetic and Work terms

$$\mathbf{q}_0(t) = \frac{1}{V} \left[\sum_{i=1}^N e_i \mathbf{v}_i - \frac{1}{2} \sum_{\substack{j=1 \\ j \neq i}}^N \left(\mathbf{v}_i \cdot \left(\overrightarrow{\mathbf{F}}_{ij} \cdot \mathbf{r}_{ij} \right) \right) \right]$$

(Note: The first term is crossed out with a red 'X' and labeled 'solids' in red text above it.)



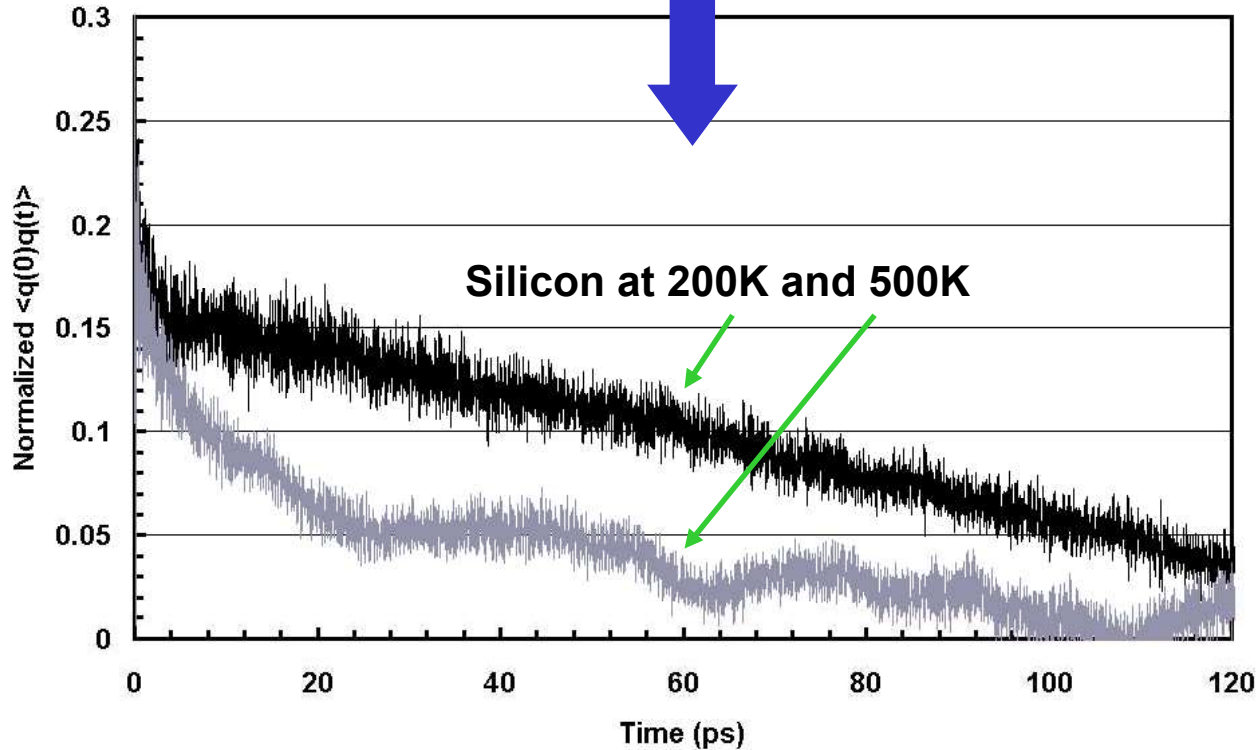
THERMAL CONDUCTIVITY by MD

o Fluctuation-Dissipation Theorem

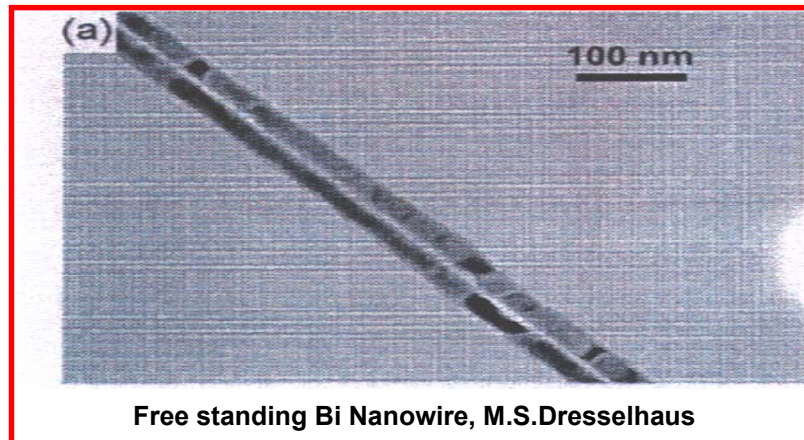
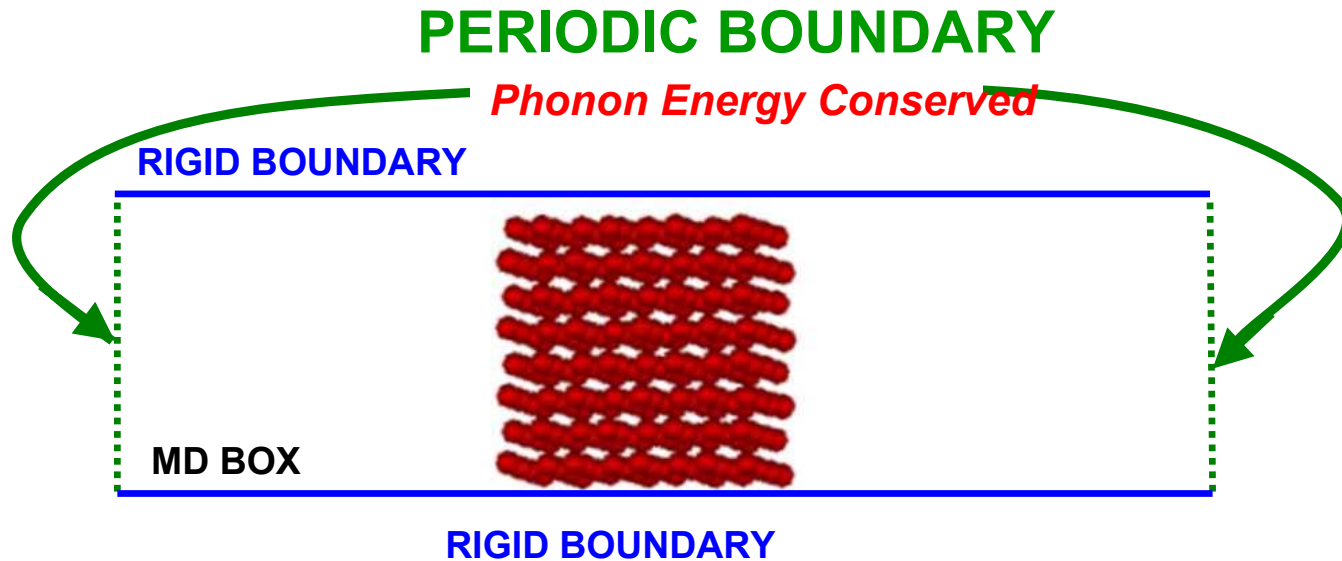
$$\text{gradT} \times \underbrace{\lambda(\omega) = \frac{V}{3k_B T_0^2} \int_0^\infty \langle \mathbf{q}_0(0) \mathbf{q}_0(\tau) \rangle e^{i\omega\tau} d\tau}_{\text{Autocorrelation}} \times \text{gradT}$$

The Flux The Force

$\omega=0$, Thermal Conductivity



SILICON NANOWIRE MD MODEL



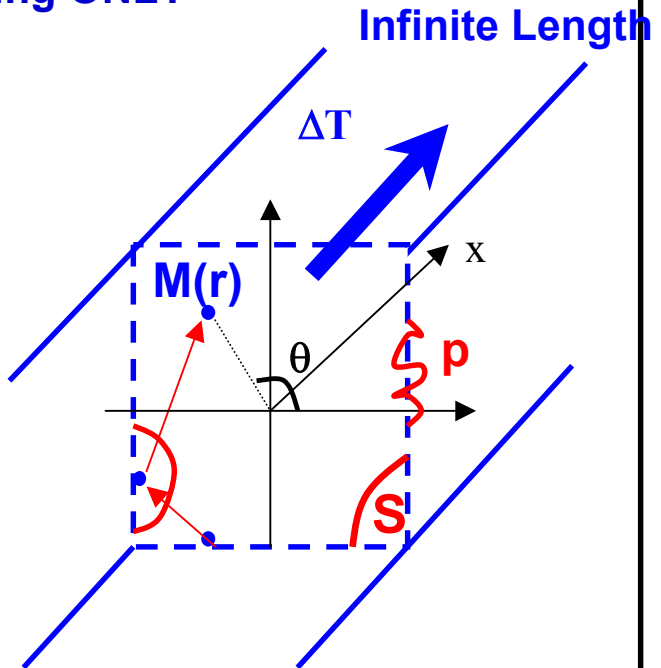
BOLTZMANN TRANSPORT EQUATION

o 1D solution to BTE: Boundary Scattering ONLY

$$\frac{\partial g(\nu)}{\partial t} + \mathbf{v} \cdot \text{grad} g(\nu) = -\frac{g(\nu)}{\tau_{Bulk}}$$

$$g(\mathbf{r}) = \Lambda_{Bulk} \cdot \cos\theta \cdot \frac{\partial T}{\partial x} \cdot \frac{\partial g_0}{\partial T} \cdot [1 - G(\mathbf{r}, \mathbf{p})]$$

(Ziman -Electrons and Phonons)



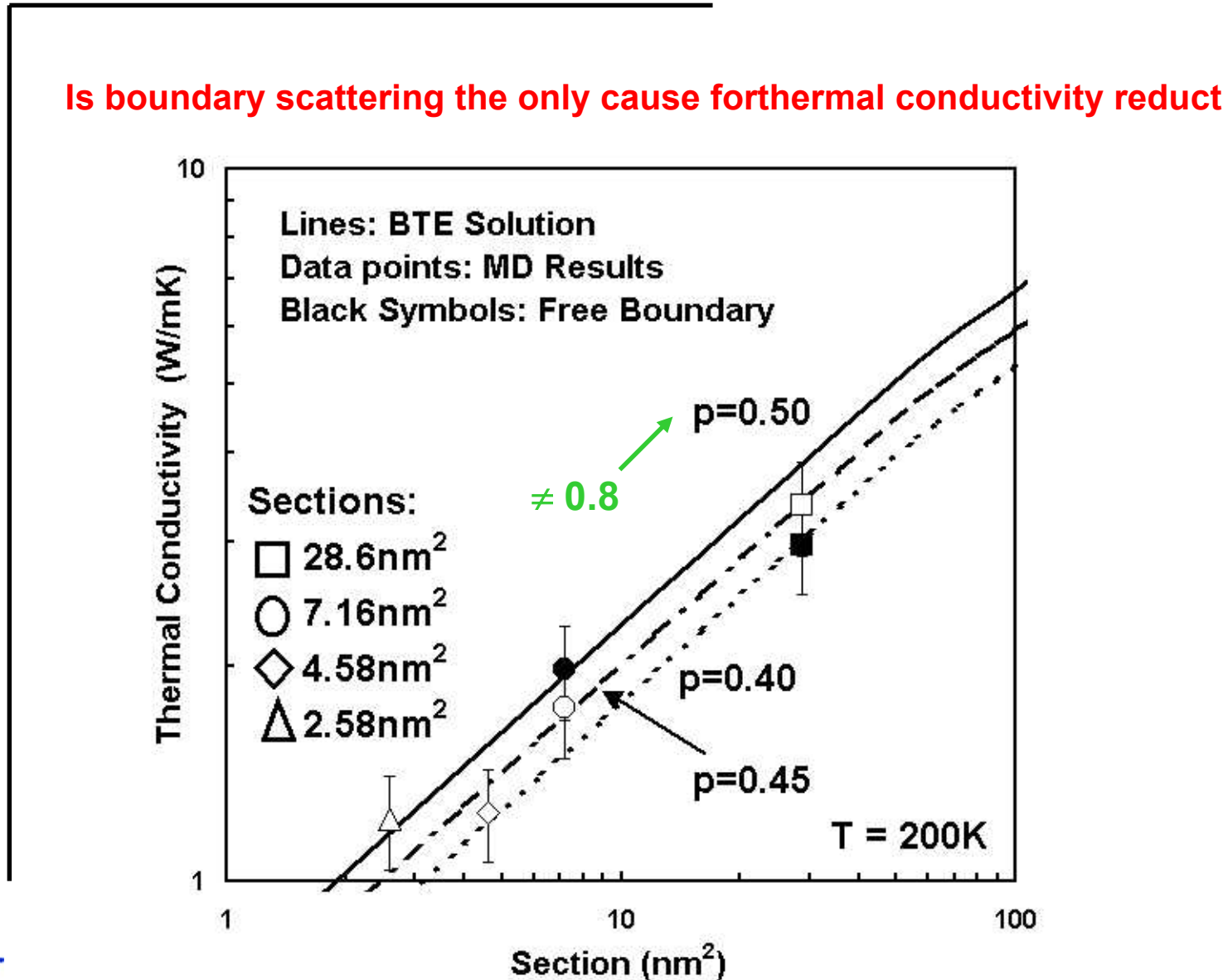
$$q(\mathbf{r})S = \frac{1}{4\pi} \int_{4\pi} \int_{\nu=0}^{\nu_D} v(\mu) \cdot \hbar v \cdot g(\mathbf{r}) \cdot D(\nu) \cdot d\nu \cdot d\Omega$$

$$\frac{\lambda_{nw}}{\lambda_{Bulk}} = \left(1 - \frac{\Lambda_{Size}}{\Lambda_{Bulk}} \right)$$

Function of G only

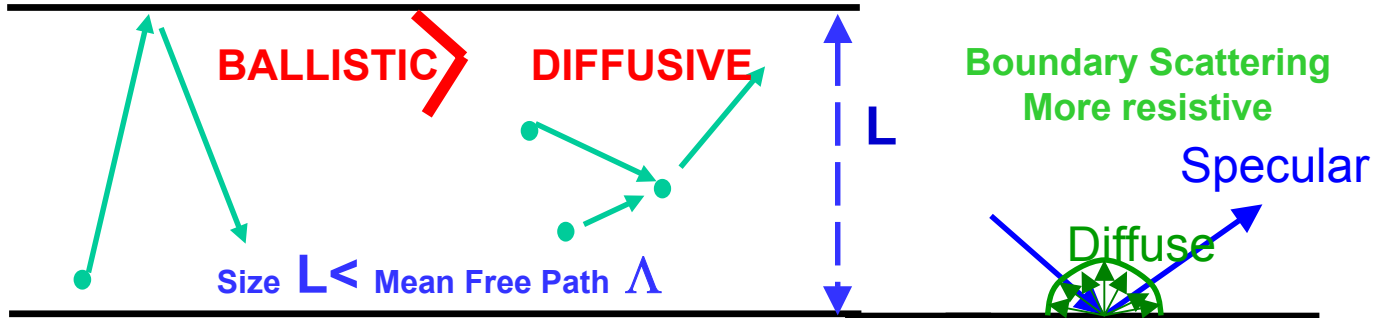
COMPARISON BETWEEN MD&BTE RESULTS

Is boundary scattering the only cause for thermal conductivity reduction?



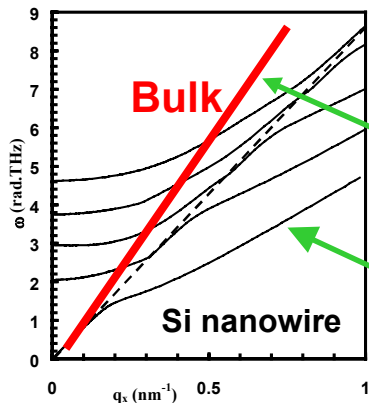
PHONON CONFINEMENT EFFECT ON HEAT CONDUCTION

o Ballistic Transport of Phonons



o Phonon Confinement

v_G and Λ Reduction



~~$$\vec{q} = -\lambda_{BULK} \cdot \text{grad } T$$~~

$$\lambda_{\text{effective}} < \lambda_{BULK}$$

$$\frac{\partial^2 u}{\partial t^2} = v_t^2 \cdot \nabla^2 u + (v_l^2 - v_t^2) \nabla(\nabla \cdot u)$$

RPTE - THE DISCRETE ORDINATE METHOD

$$\Omega \text{grad} L_\omega = \kappa_\omega (L_\omega^0 - L_\omega)$$

o S_8 , discretizing in 48 directions (Ω , w_m) for finite length wire

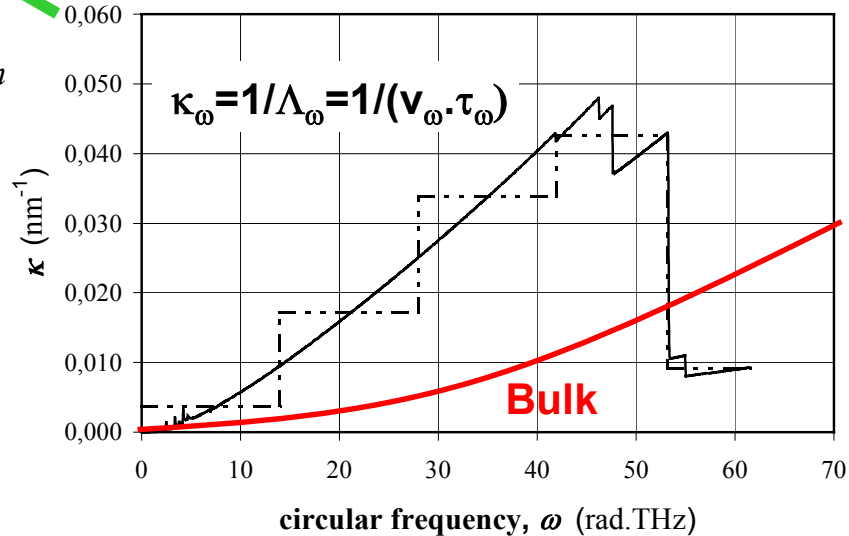
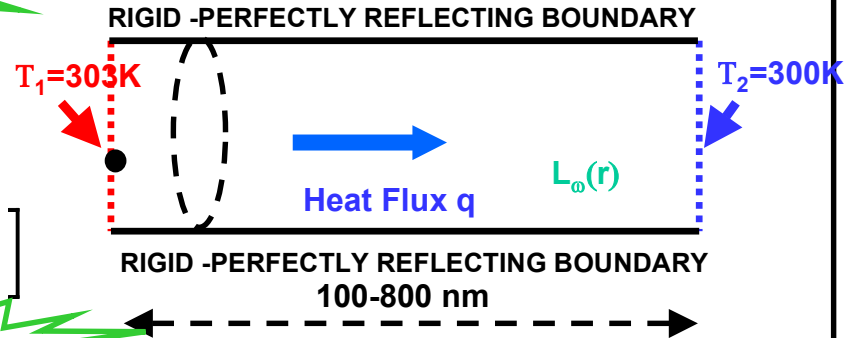
$$L_\omega = \sum_p \hbar \omega \cdot g_\omega^p(r) \cdot v_\omega^p(\Omega)$$

$$\Omega_m \cdot \nabla L_{k,m} = \kappa_k [L_{k,m}^0 - L_{k,m}]$$

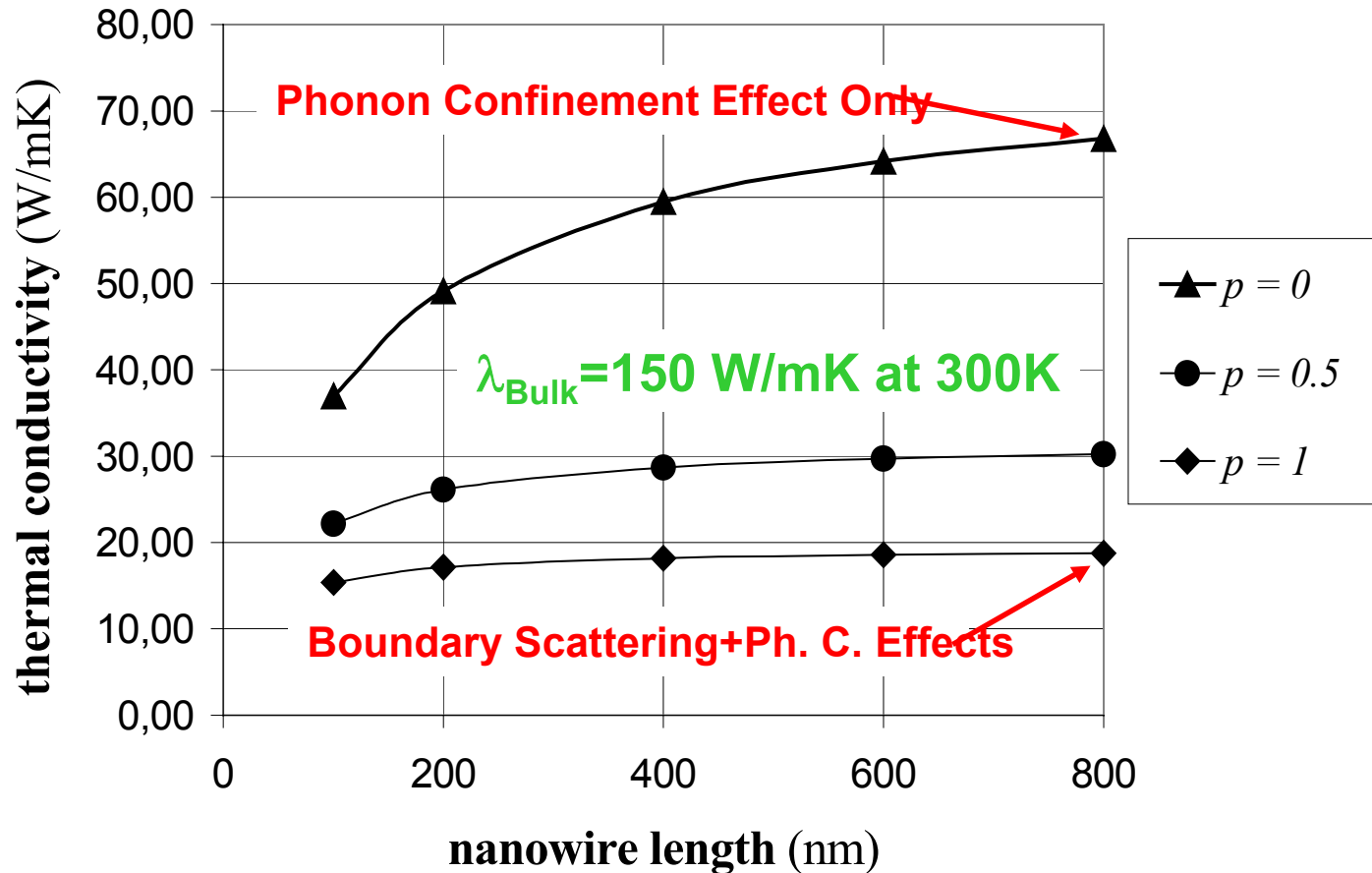
$$q_{i,j} = \sum_{k=1,5} \sum_{m=1,48} w_m \cdot L_{k,m,i,j} \Omega_m$$

$$\lambda = \frac{q \cdot L}{T_1 - T_2}$$

$T_{ij} ?$

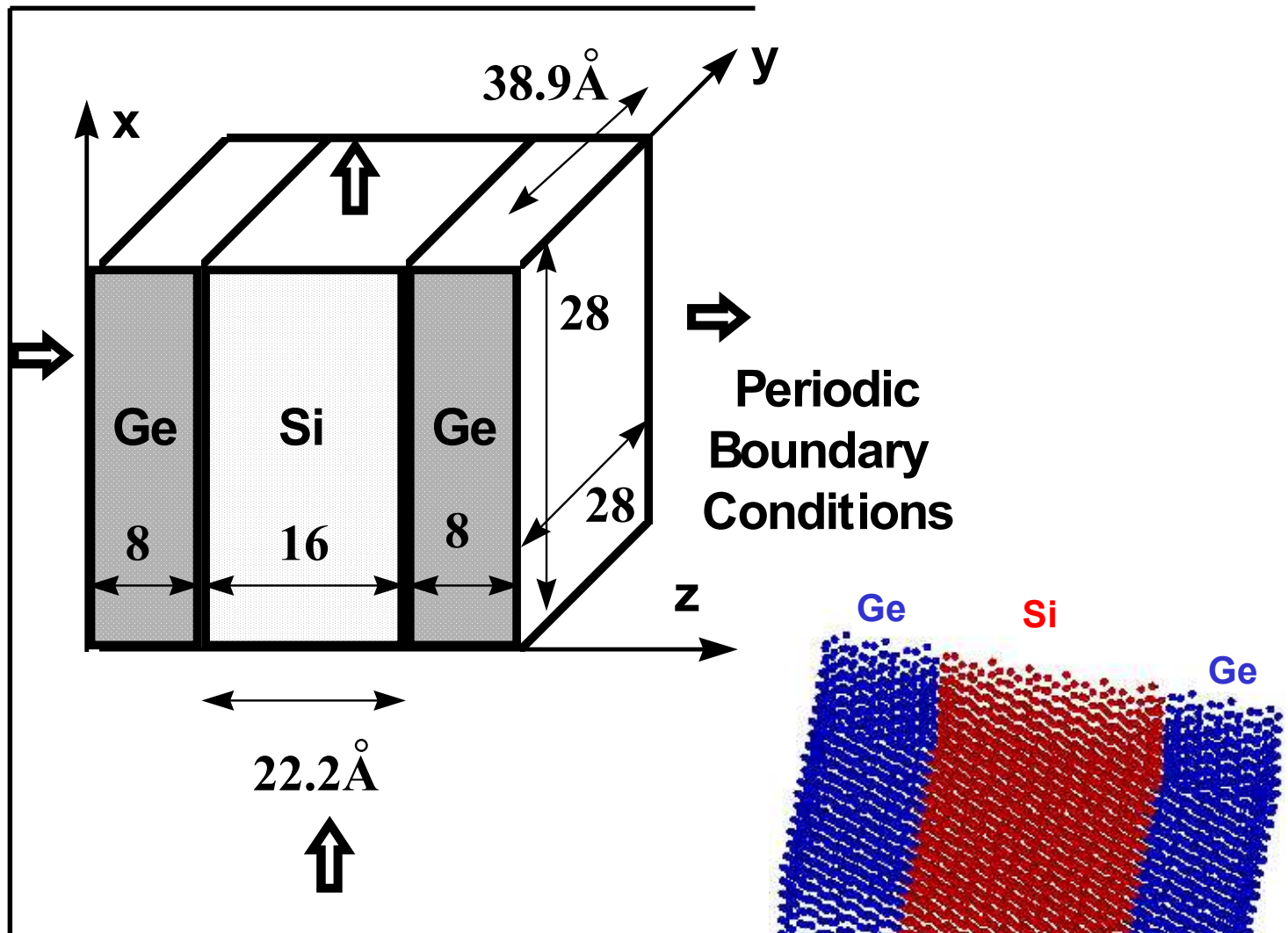


PHONON CONFINEMENT vs BOUNDARY SCATTERING



PHONON CONFINEMENT: 50% REDUCTION
BOUNDARY SCATTERING: 70% REDUCTION

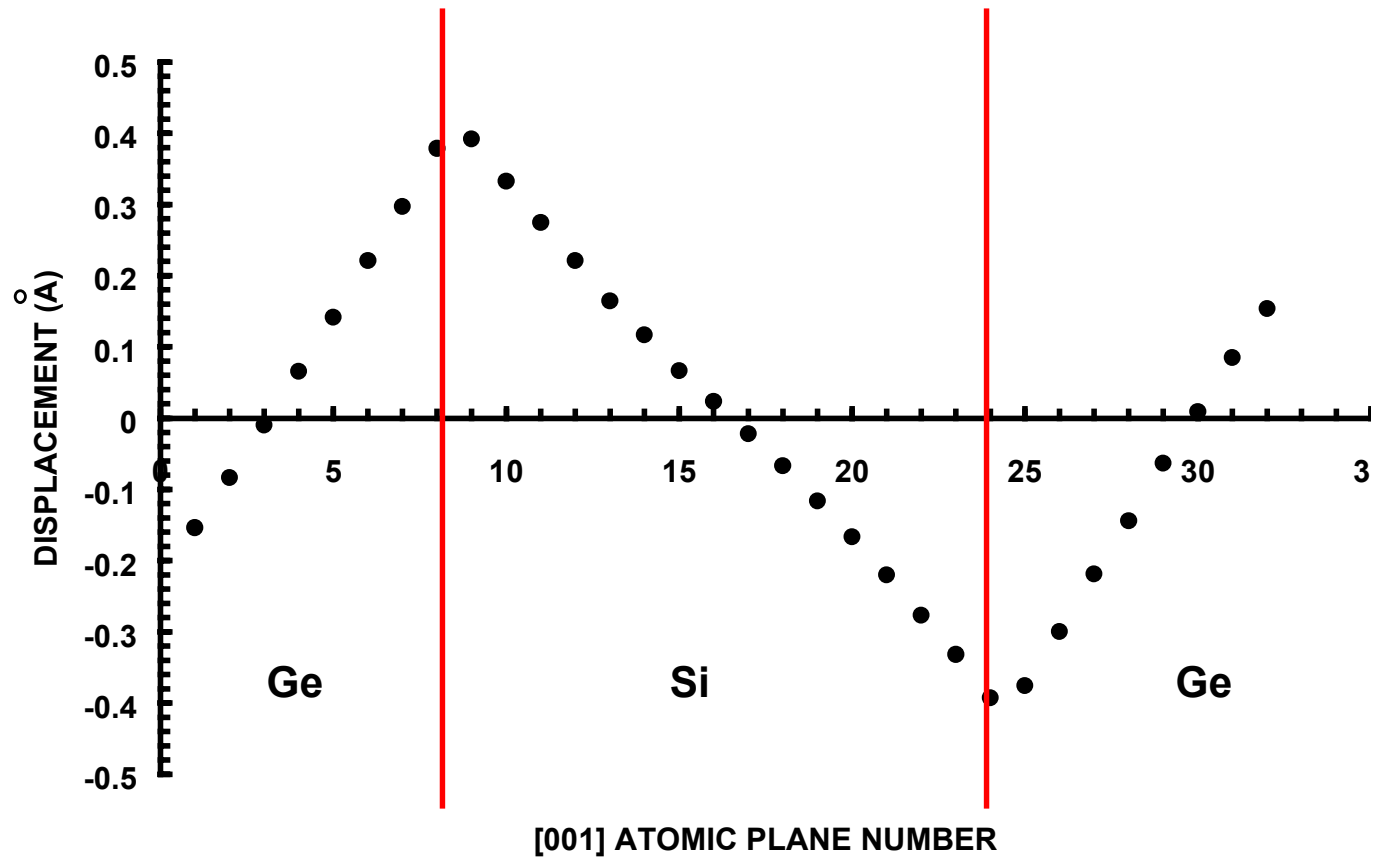
Si/Ge SUPERLATTICE MD MODELING



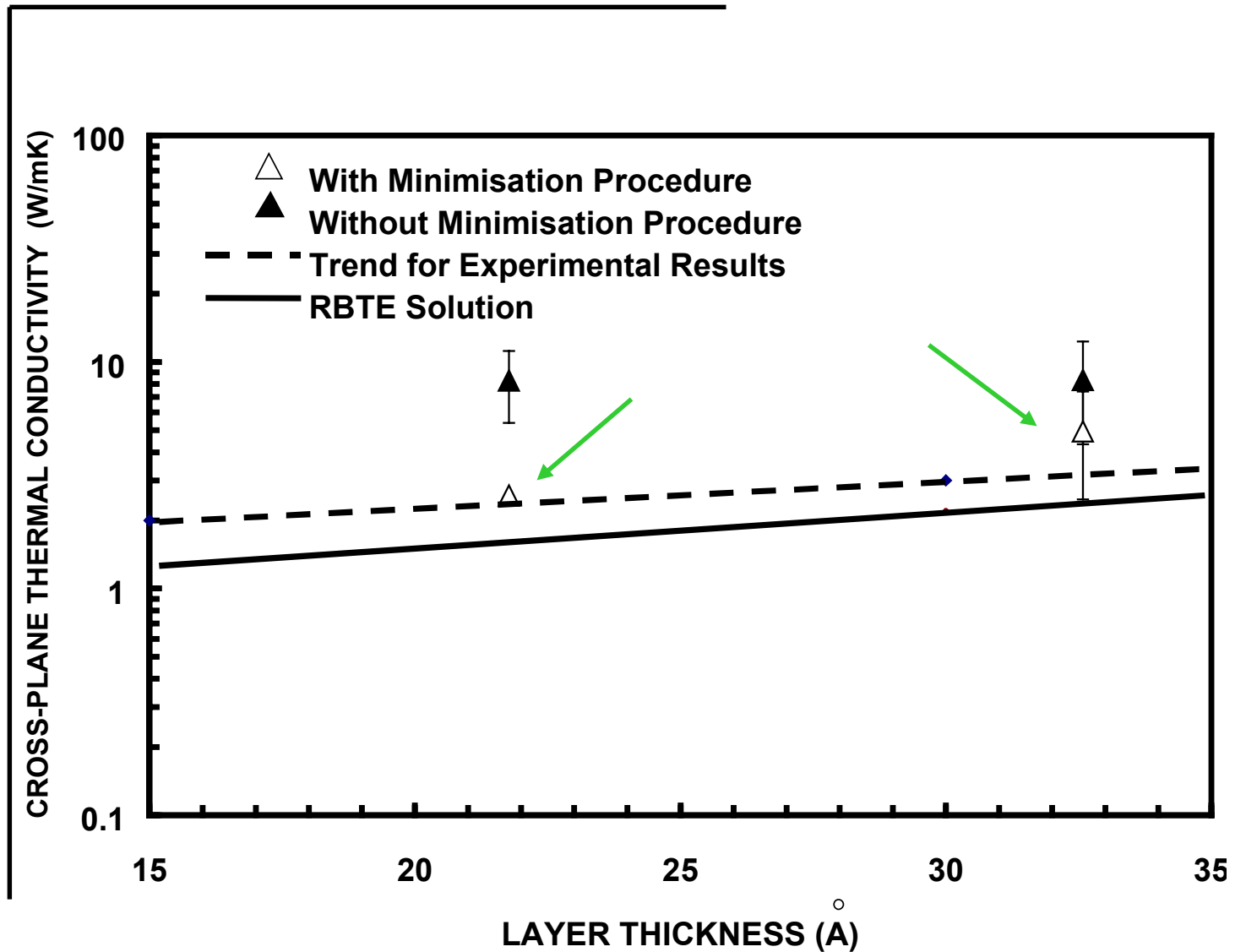
STRAIN EFFECT ON SUPERLATTICE STRUCTURE

- o Starting with mean lattice constant

- o Implementing Conjugate Gradient Method



SUPERLATTICE THERMAL CONDUCTIVITY



EFFECTIVE THERMAL CONDUCTIVITY AT GIGAHERTZ FREQUENCIES

o Fluctuation Dissipation Theorem

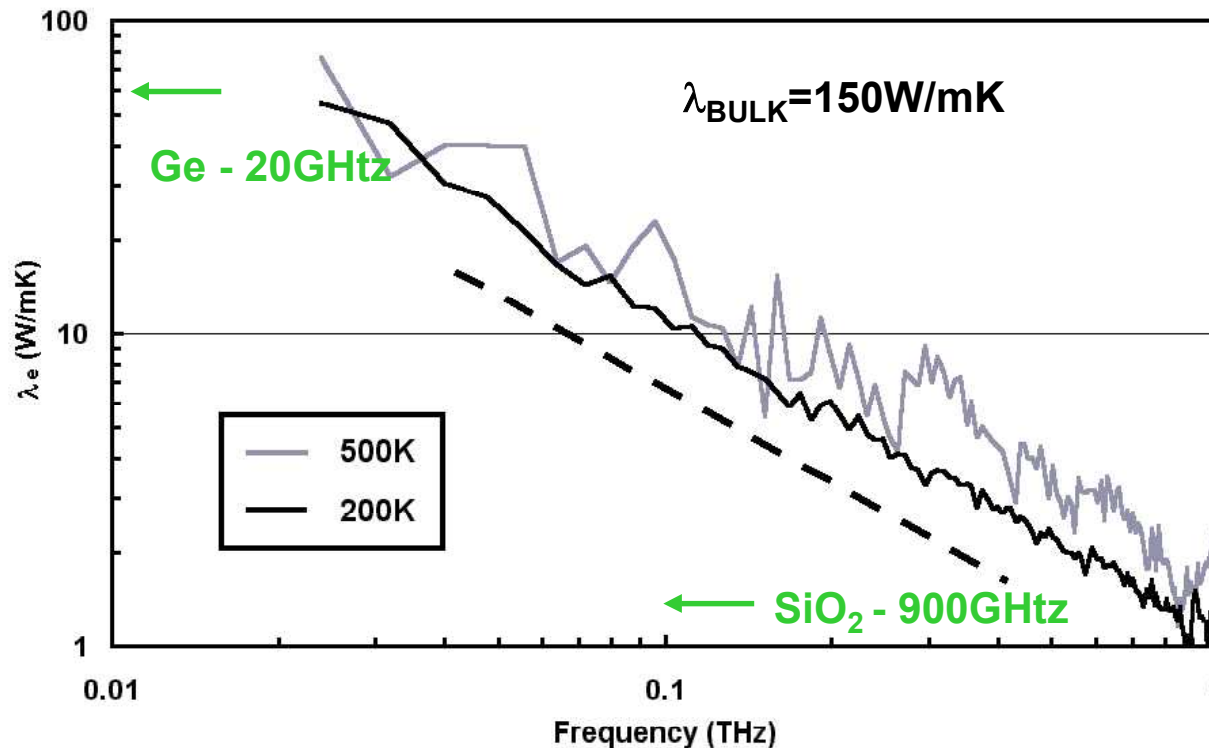
$$\lambda_e = \frac{V}{3 \cdot k_B \cdot T^2} \int_0^{\infty} \langle q_0(0) q_0(t) \rangle e^{i\omega t} dt \cdot \|\vec{\text{grad}}T\|$$

$$\langle q_0(0) q_0(t) \rangle = \langle q_0(0)^2 \rangle e^{-\frac{t}{\tau}}$$



$$\lambda_e = \frac{V}{3 \cdot k_B \cdot T^2} \cdot \frac{\langle q_0(0)^2 \rangle}{\sqrt{1/\tau^2 + \omega^2}}$$

o ω^{-1} dependence at Giga frequencies



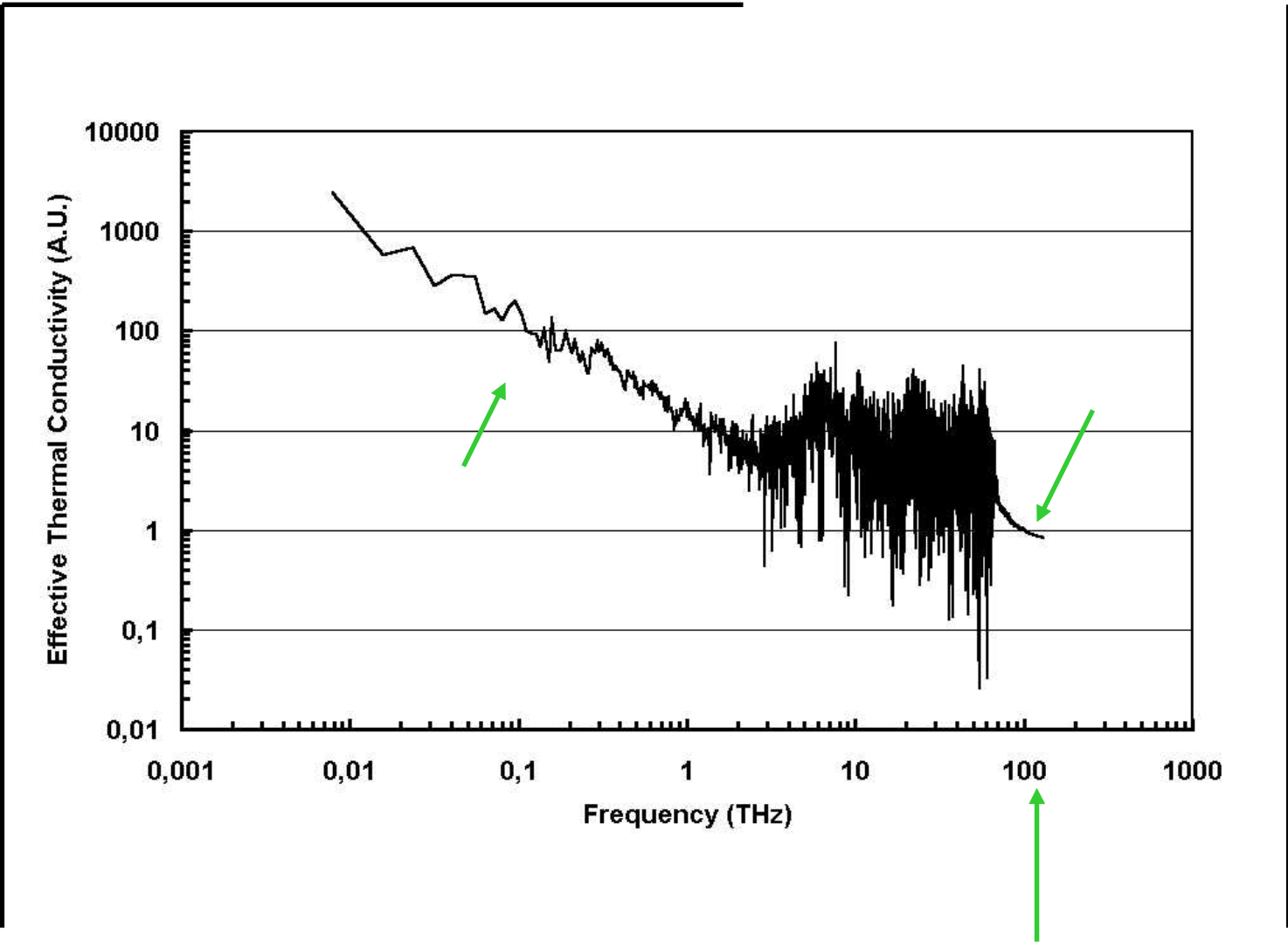
CONCLUSION

MOLECULAR DYNAMICS TECHNIQUE:

- o COMPLETELY DESCRIBES PHONON SCATTERING
- o ALLOWS THE SIMULATION OF DEFAULTS/STRAINS
- o GIVES ACCESS TO NON-EQUILIBRIUM REGIMES

- IS VERY HEAVY IN TERMS OF COMPUTATION TIME
- RELIES ON THE INTERACTION POTENTIAL VALIDITY
- DOES NOT INCLUDE QUANTUM EFFECTS

ULTRA SHORT TIME HEAT CONDUCTION



ω^{-1} LAW FOR Si THERMAL CONDUCTIVITY AT GIGAHERTZ FREQUENCIES

