# New thermal mechanisms in sub-10nm structures

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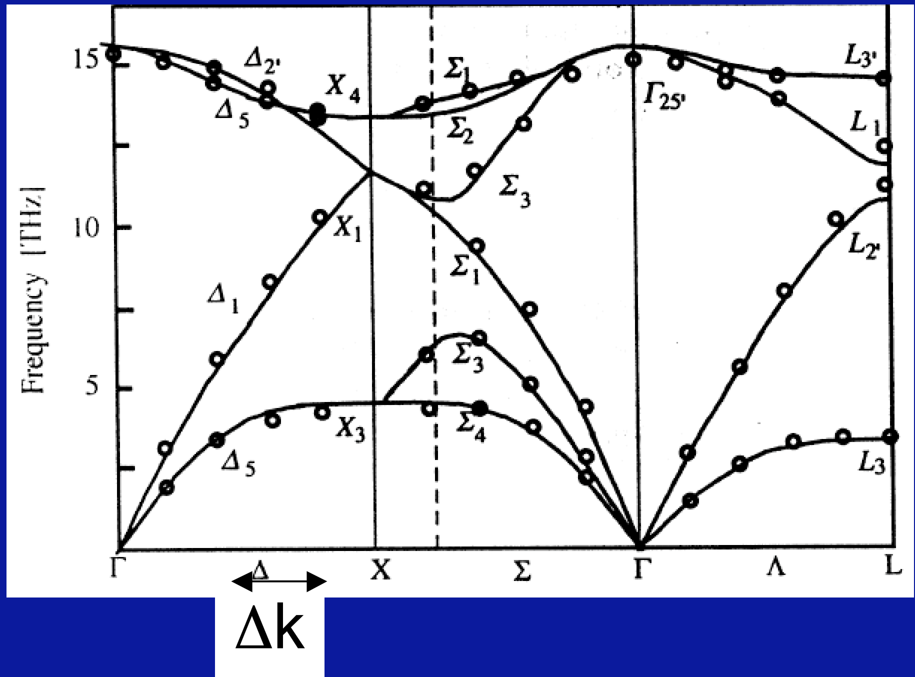
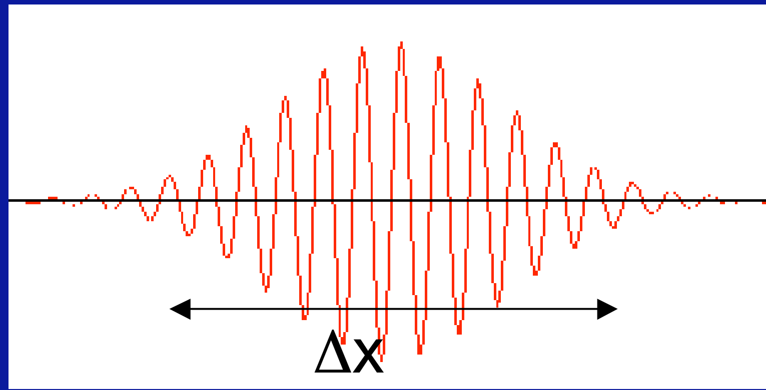
## PHONON PARTICLE/PHONON WAVE

$$\Delta k . \Delta x > 2\pi$$

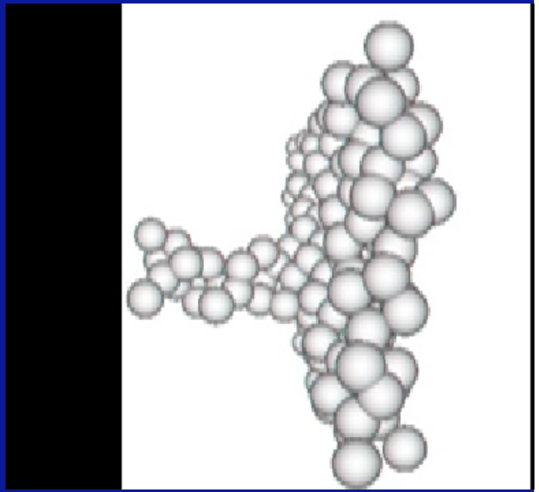


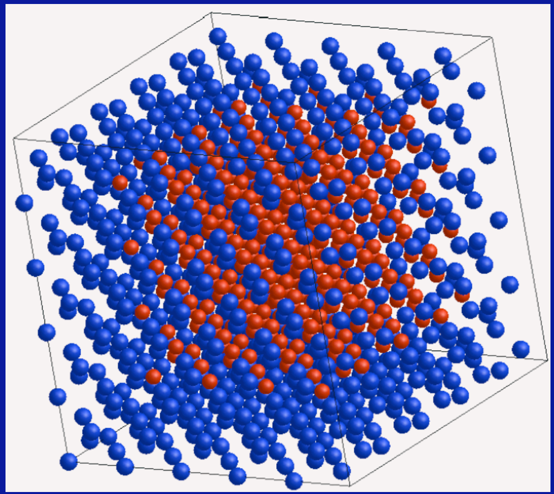




$$\Delta k < p/a \Rightarrow \Delta x > 10a = 5nm$$

## New thermal mechanisms in sub-10nm structures

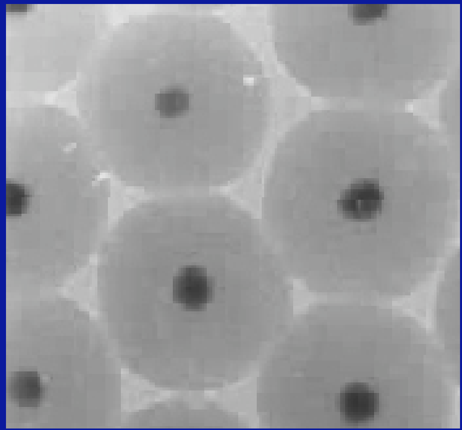
1. Heat Conduction in Nanowires



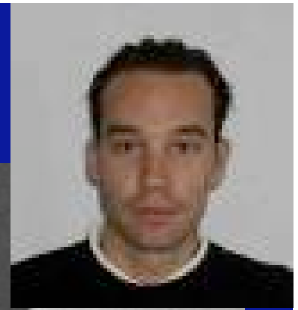


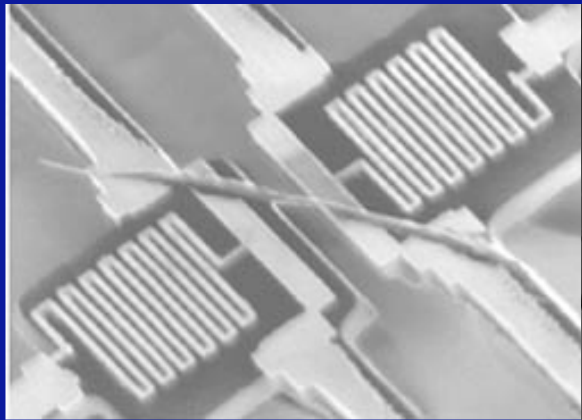
2. 3D atomic scale phononic crystals

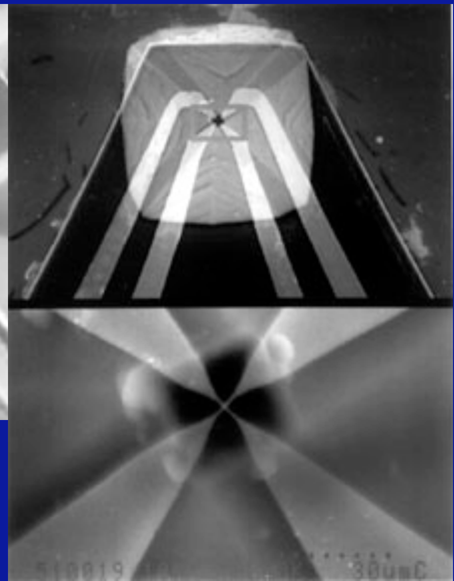
3. Transient Non Fourier Heat Conduction



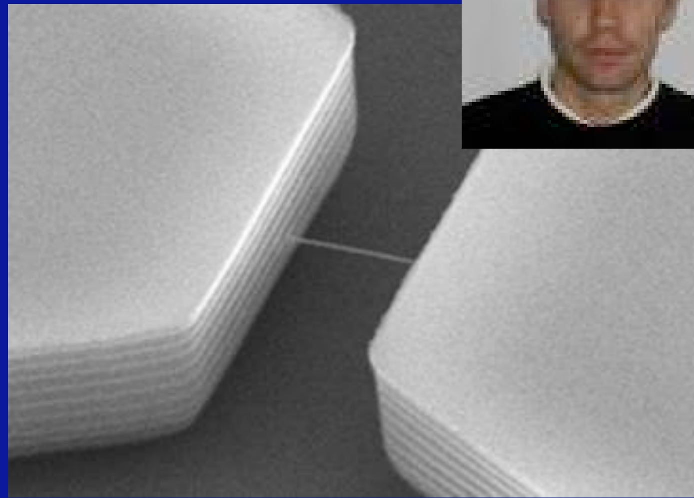
# 1-Nanowires and Thermal Contact Resistances



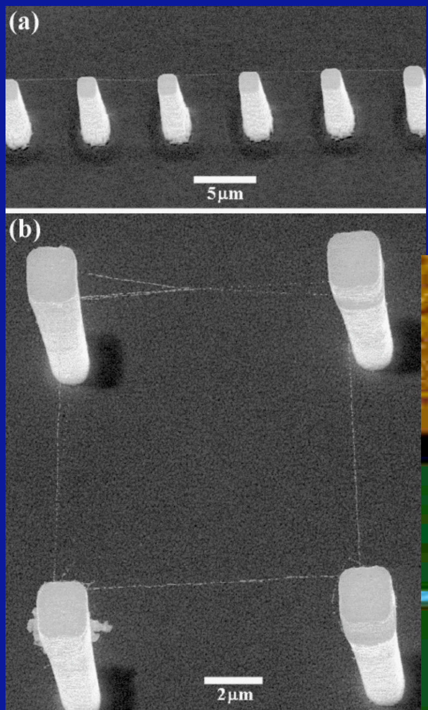




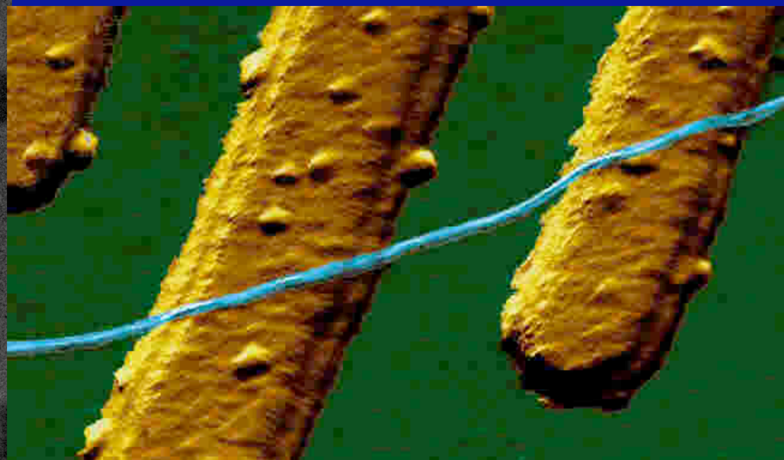
Metrology



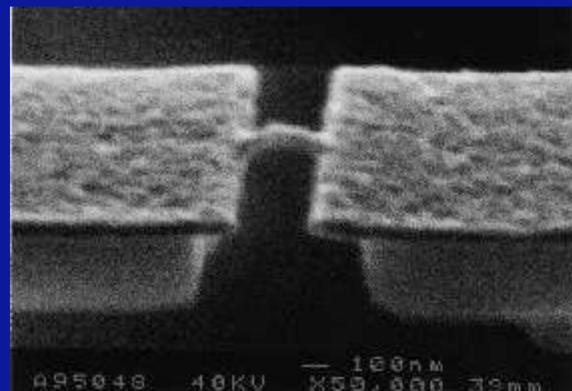
Spectrometry

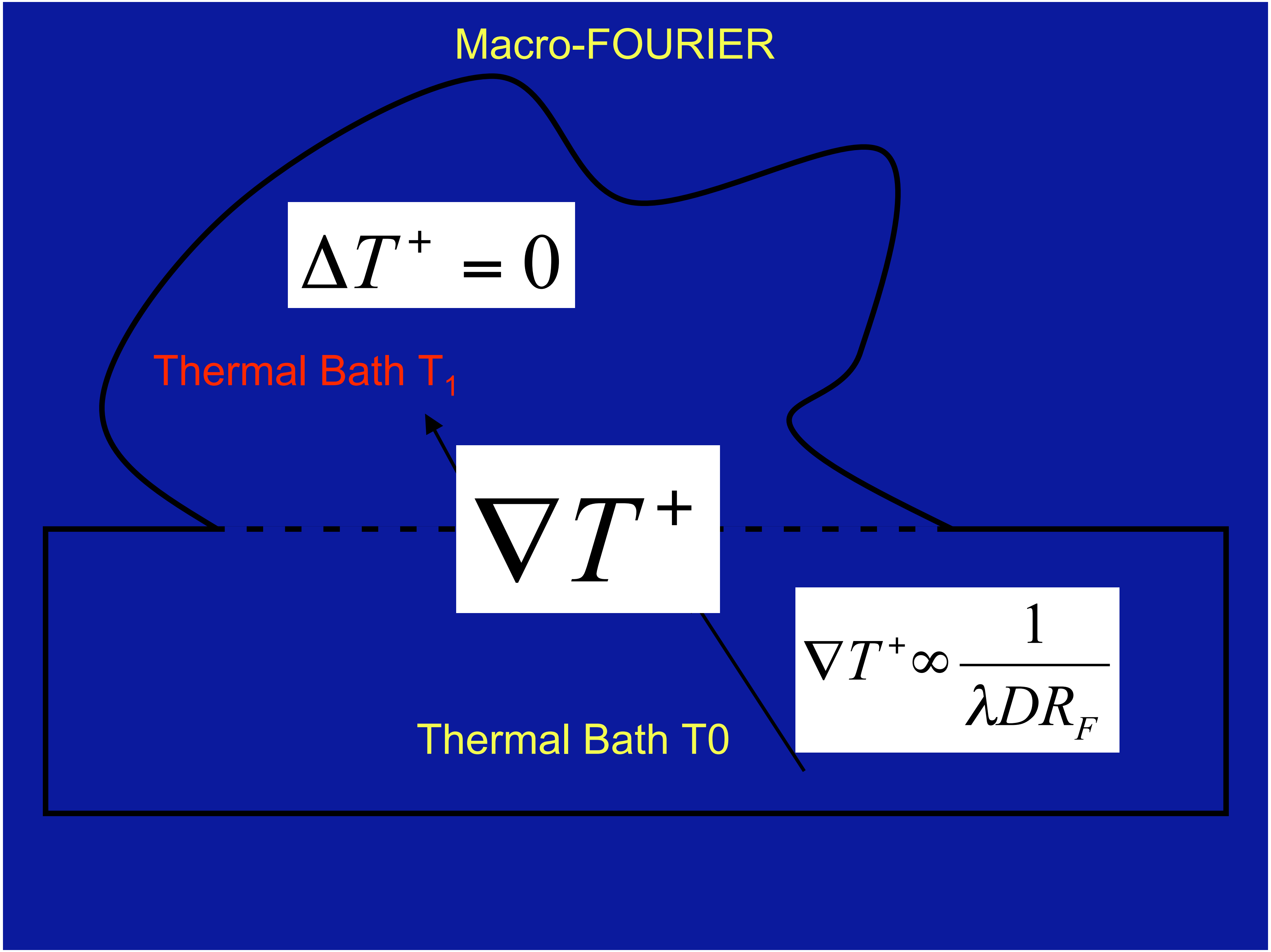



NanoElectronics

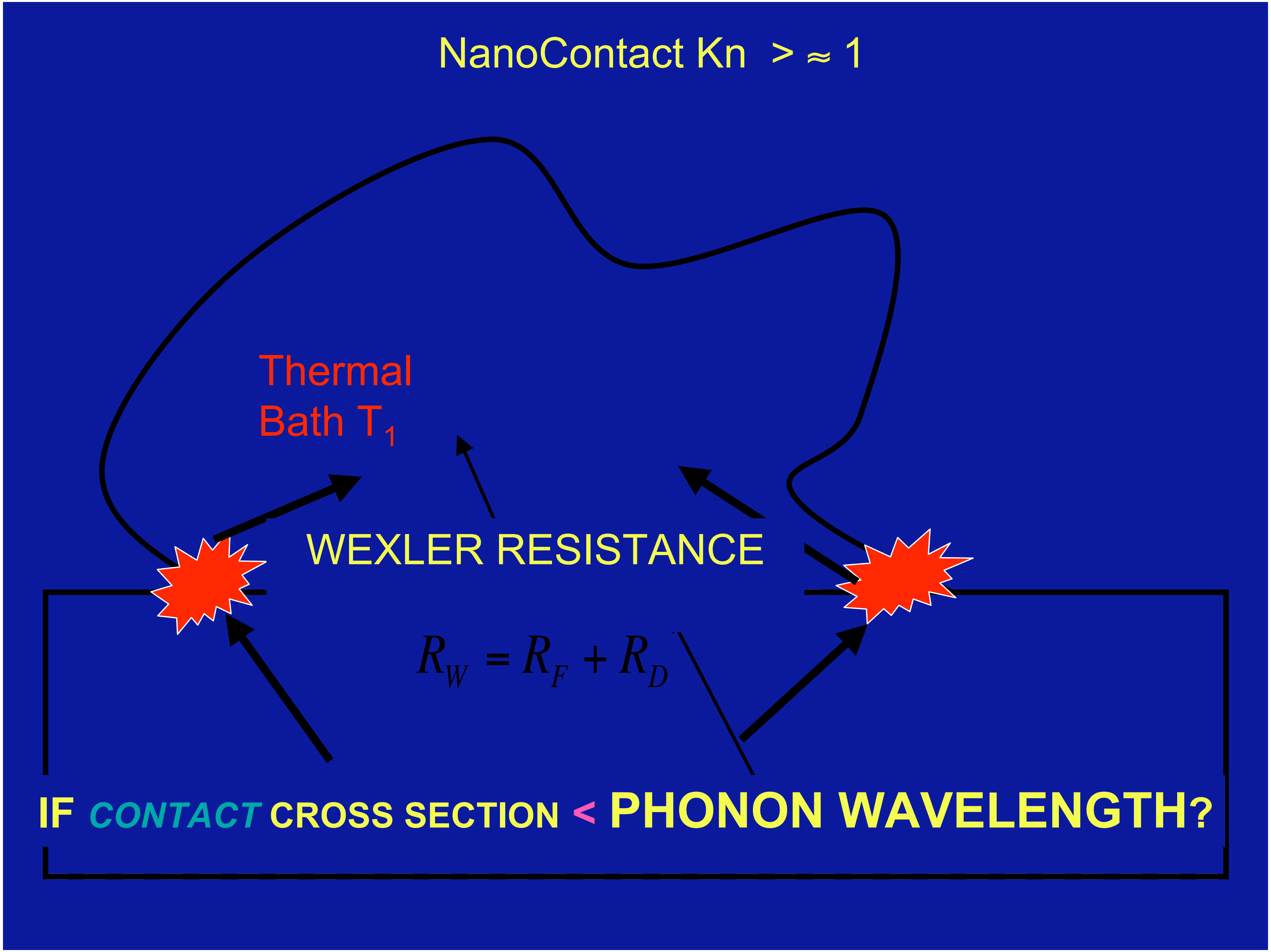


Molecular Junction

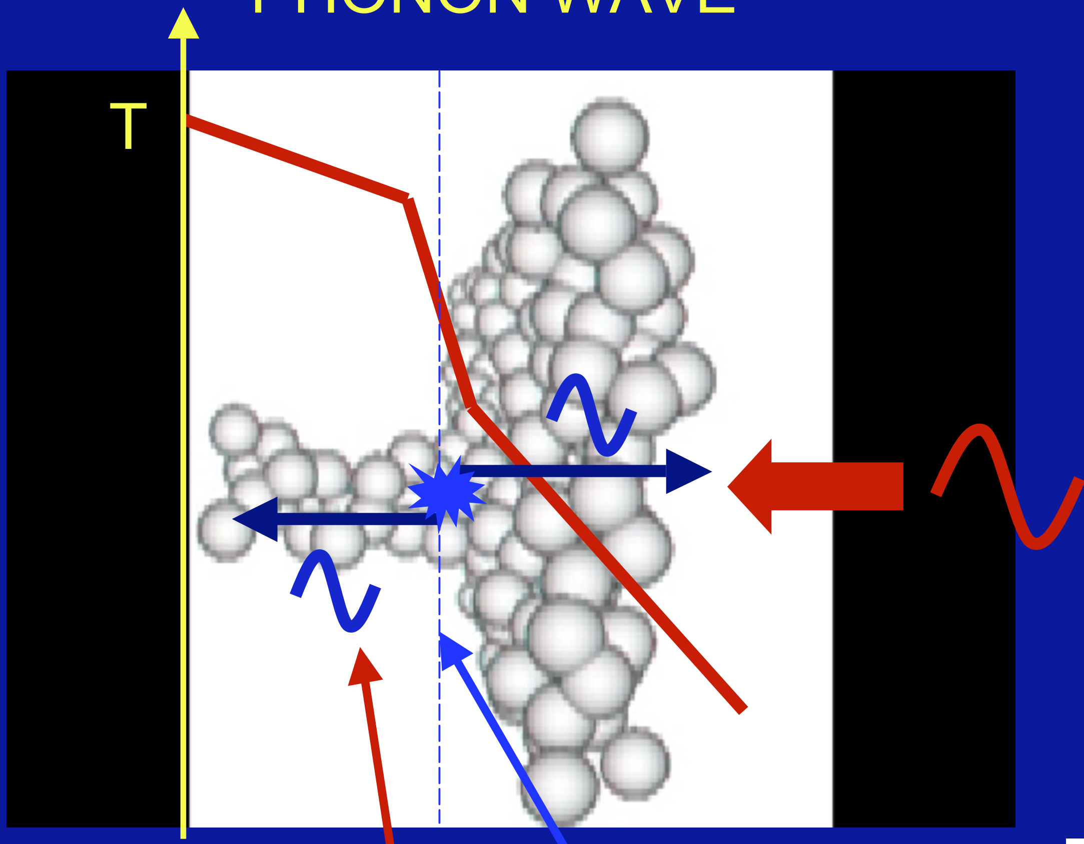




Macro-FOURIER
$\Delta T^{+} = 0$
Thermal Bath $T_1$
$\nabla T^{+}$
$\nabla T^{+} \infty \frac{1}{\lambda D R_F}$
Thermal Bath T0

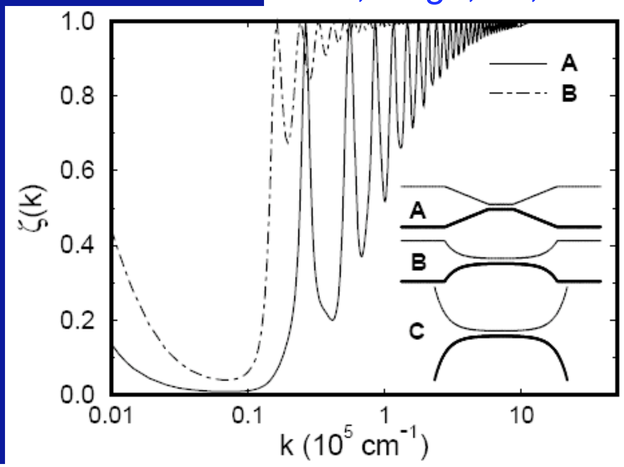

NanoContact Kn > ≈ 1
Thermal
Bath T1
WEXLER RESISTANCE
$R_W = R_F + R_D$
IF CONTACT CROSS SECTION < PHONON WAVELENGTH?

# PHONON WAVE

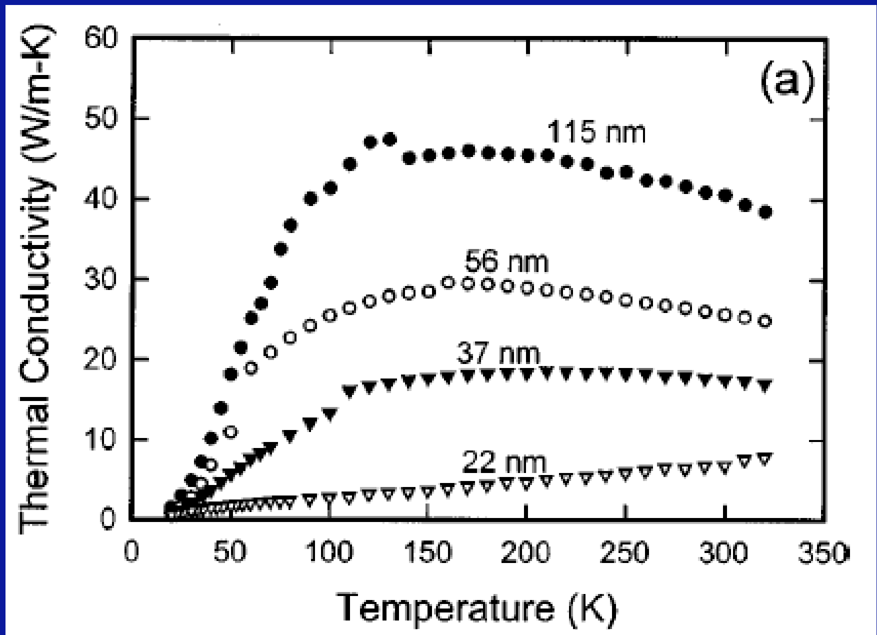



$$\dot{Q} = \sum_{\alpha} \int_0^{\infty} \frac{dk}{2\pi} \hbar\omega_\alpha(k) v_\alpha(k) (\eta_R - \eta_L)\zeta_\alpha(k)$$

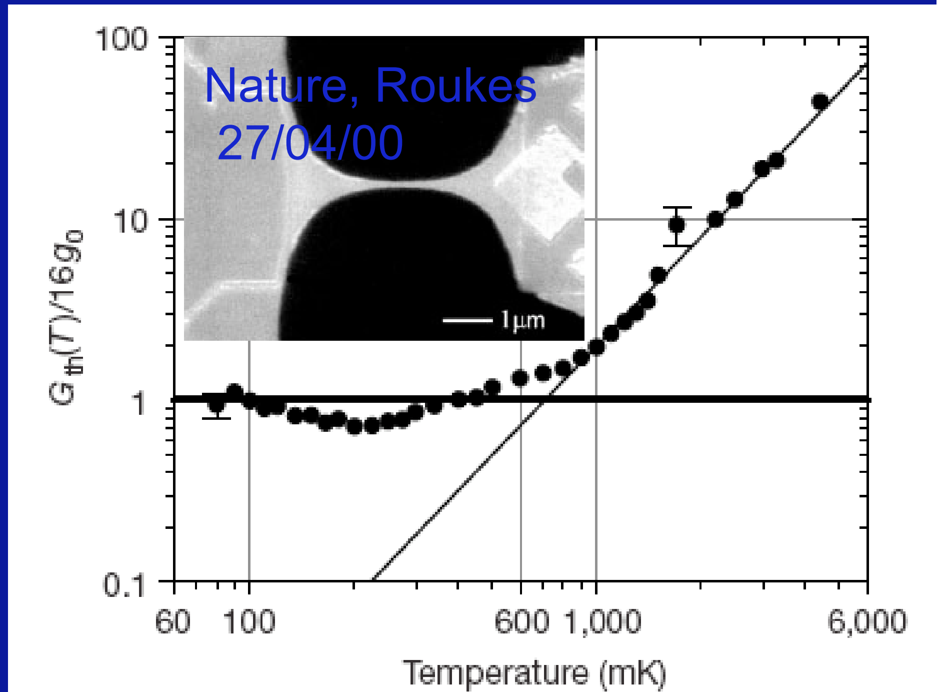
PRL, Rego, 81, 232

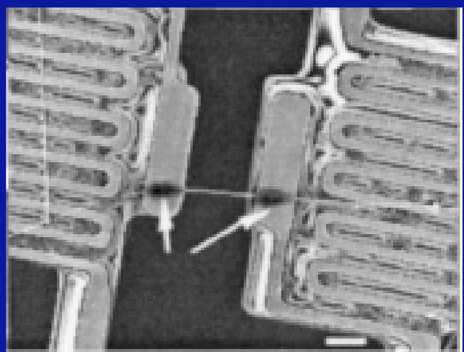


# *The Mysterious Story of Nanowires Thermal Conductivity*




APL Li&Majumdar, 83, 2934, 2003



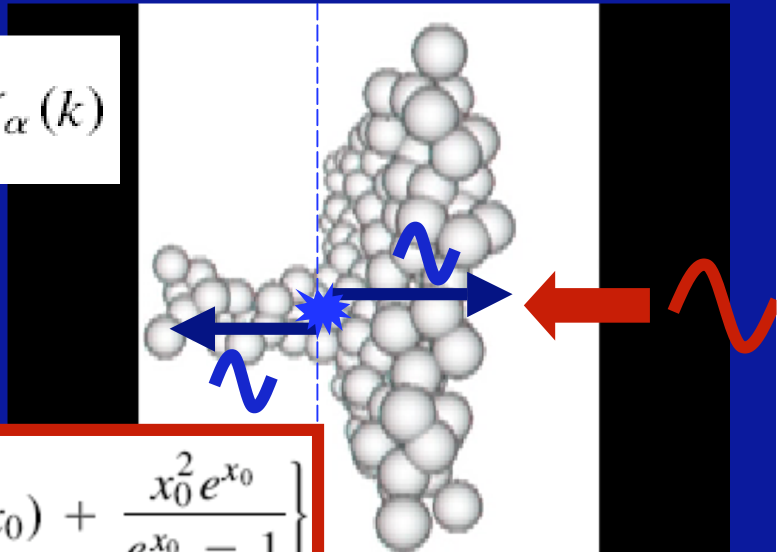
M.R. says:

*not obtained* for long wires

# Wire Thermal Conductance

$$\dot{Q} = \sum_{\alpha} \int_0^{\infty} \frac{dk}{2\pi} \hbar\omega_{\alpha}(k) v_{\alpha}(k) (\eta_R - \eta_L) \zeta_{\alpha}(k)$$

1D in k-space



$$\kappa = \frac{k_B^2 \pi^2}{3h} T N_{\alpha} + \frac{k_B^2}{h} T \sum_{\alpha'}^{N_{\alpha'}} \left\{ \frac{\pi^2}{3} + f(x_0) + \frac{x_0^2 e^{x_0}}{e^{x_0} - 1} \right\}$$

Quantum of Conductance

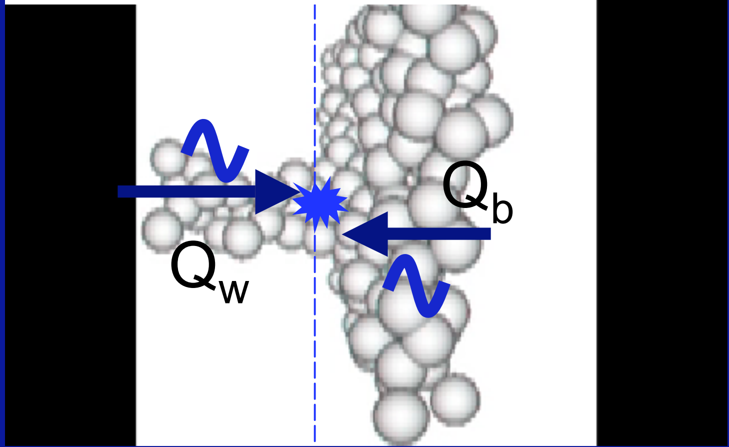
-Conductance of **1 phonon** BRANCH /NOT/ 1 Quantum

-Temperature Dependent

-Predominant CONDUCTANCE?

# CONTACT CONDUCTANCE

$$Q = t_b Q_b - t_w Q_w$$




$$Q = G \cdot (T_w - T_b)$$

$$G = \frac{1}{2} \{ t_b C_b v_b + t_w C_w v_w \}$$

$$t_w = \frac{C_b v_b}{C_b v_b + C_w v_w}$$

Diffuse Transmission: Phonons loose memory at interface

=> MAXIMUM FLUX

$$\frac{1}{G} = \frac{1}{C_w v_w} + \frac{1}{C_b v_b}$$

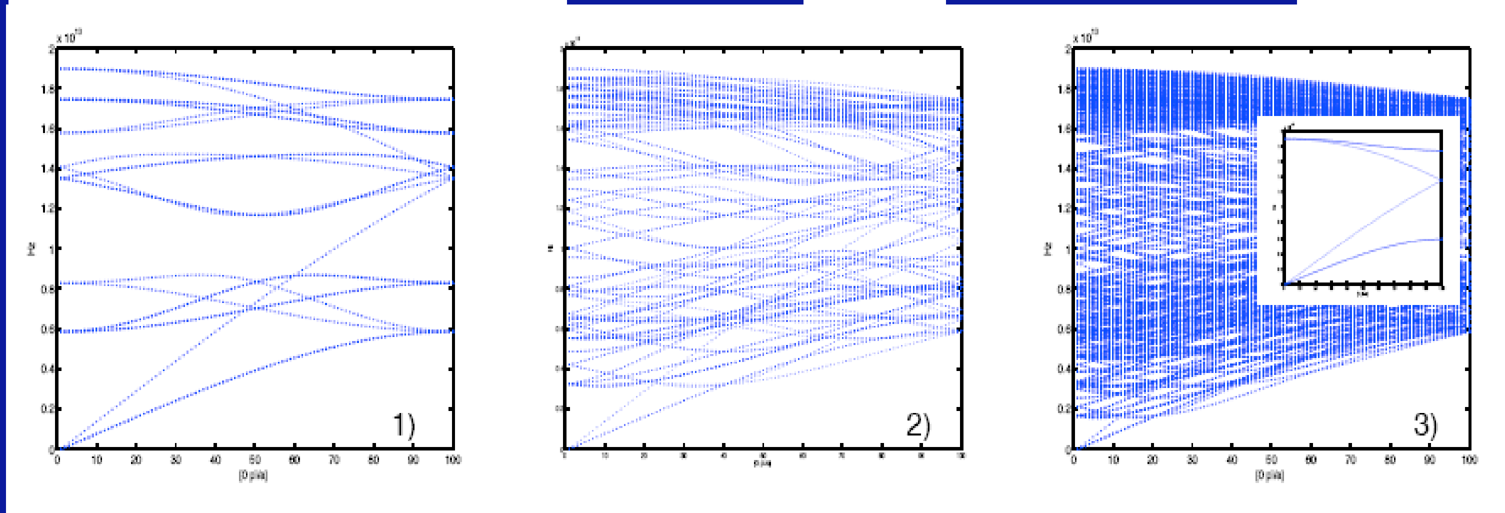
$$C_b v_b = \frac{\partial Q_b}{\partial T} = \pi g_{3D} \sum_m \int_{||\mathbf{k}||} \hbar \omega_{m,\mathbf{k}} \frac{\partial \tilde{n}}{\partial T} v_{m,\mathbf{k}} k^2 d||\mathbf{k}||$$

$$C_w v_w = \frac{\partial Q_w}{\partial T} = g_{1D} \sum_m \int_{||\mathbf{k}||} \hbar \omega_{m,\mathbf{k}} \frac{\partial \tilde{n}}{\partial T} v_{m,\mathbf{k}} d||\mathbf{k}||$$

# DISPERSION CURVES

## Lattice dynamics

2x2cells in section | 5x5 | 10x10




Motion Equation

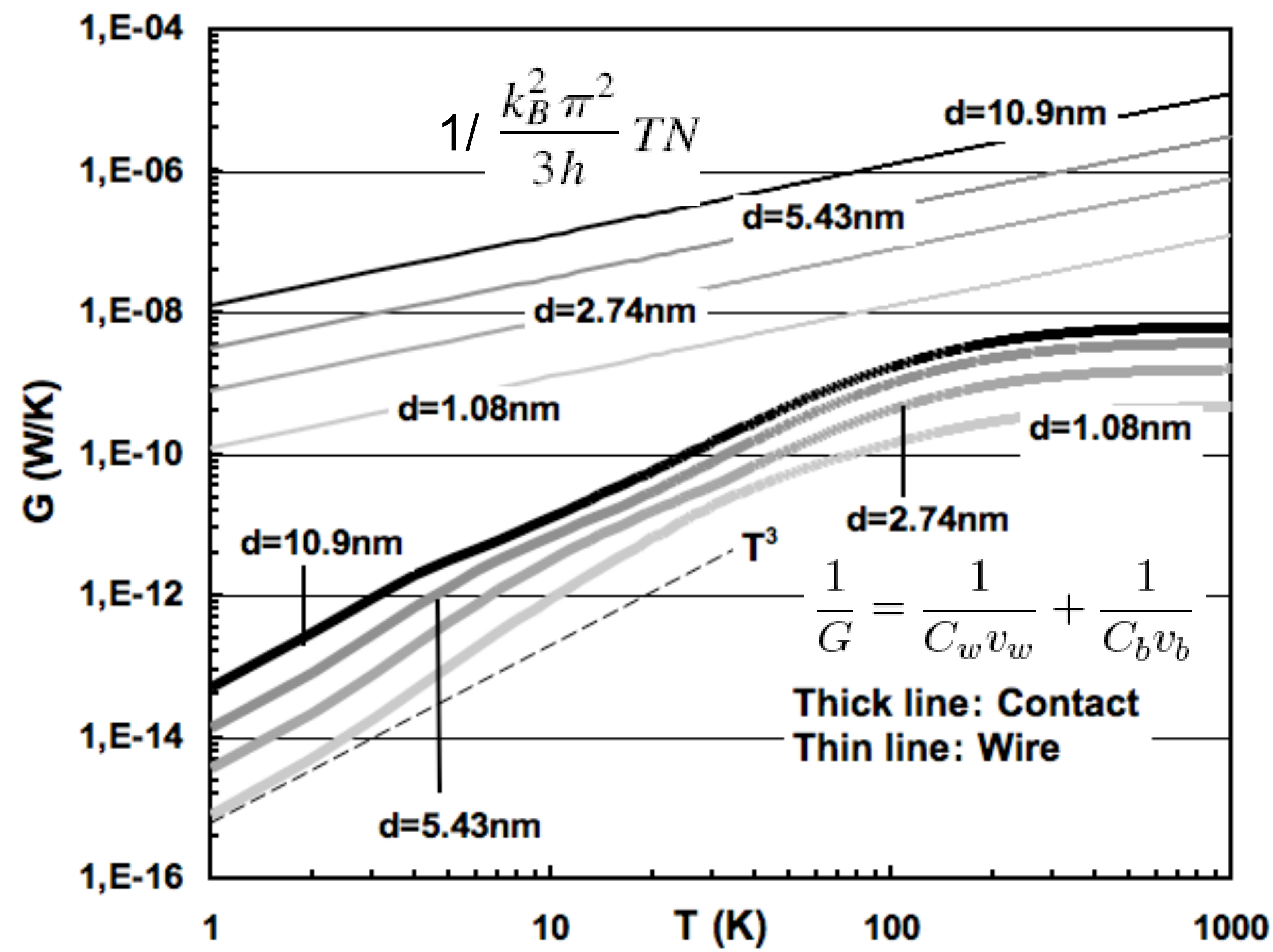
$$m_k \ddot{u}_{lk_\mu} = \sum_{l'k',\nu} \phi_{lk_\mu,l'k'_\nu} u_{l'k'_\nu}$$

Solution:

Plane Monochromatic Wave

$$\omega^2(\mathbf{q}) e_{k_\mu} = \sum_{k',\nu} D_{\mu\nu} \binom{\mathbf{q}}{kk'} e_{k_\mu}$$

# WIRE vs CONTACT

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**CONTACT RESISTANCE PREDOMINANT 2 ODM**

# CONCLUSION Nanowire and Contact

**Heat flux in of SUB-10nm NANOWIRES**
**is dominated**
**by *CONTACT RESISTANCE***

QUANTUM THERMAL CONDUCTANCE

CAN NOT BE *MEASURED* IN THOSE WIRES

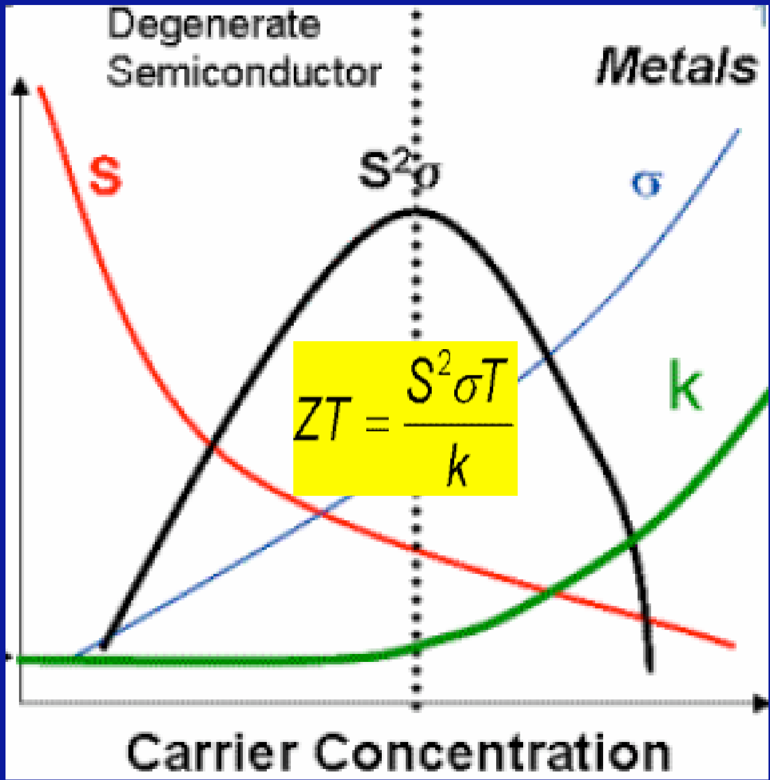
2 to 5 Orders of Magnitude Difference between Resistances

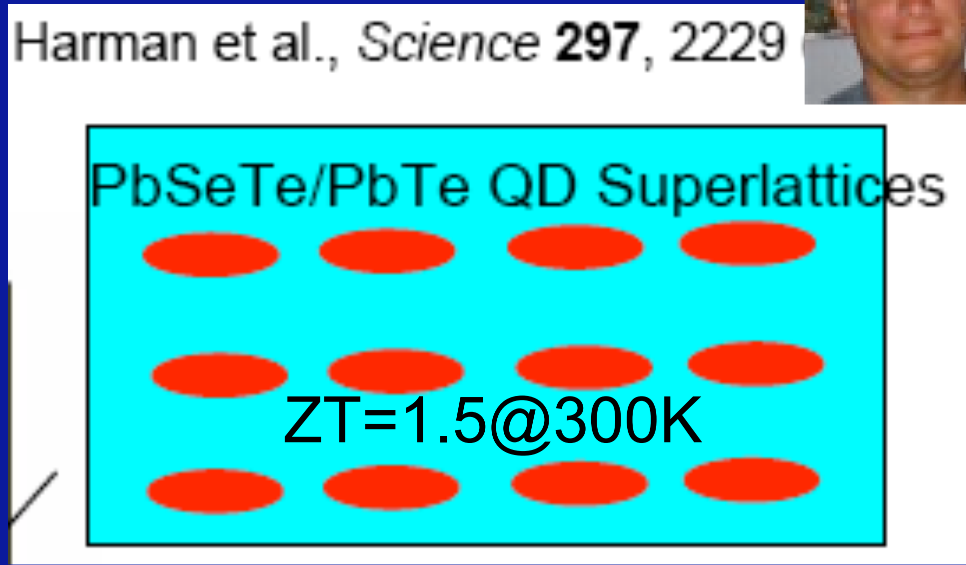
Thermal resistance of wave effects much larger
than Fourier and *Wexler* Resistances

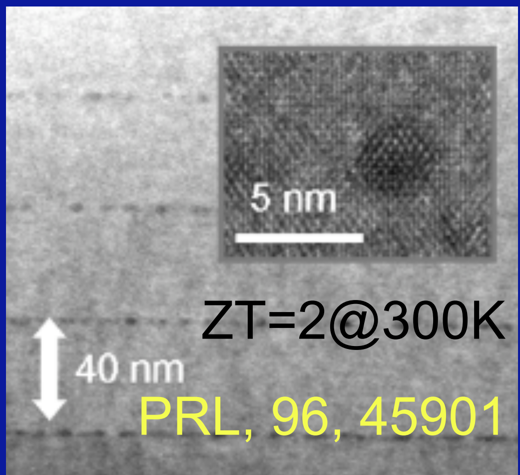
Might be interesting for thermoelectrics or insulating materials

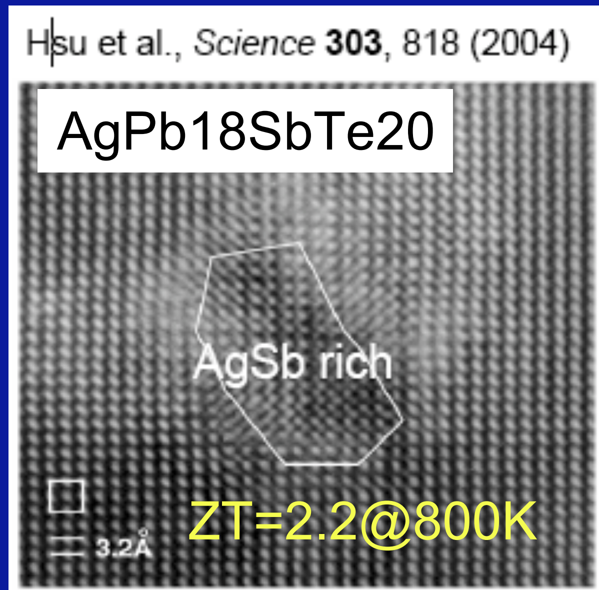
The shape of the contact has significant impact

# 2- 3D Atomic Scale Phononic Crystals



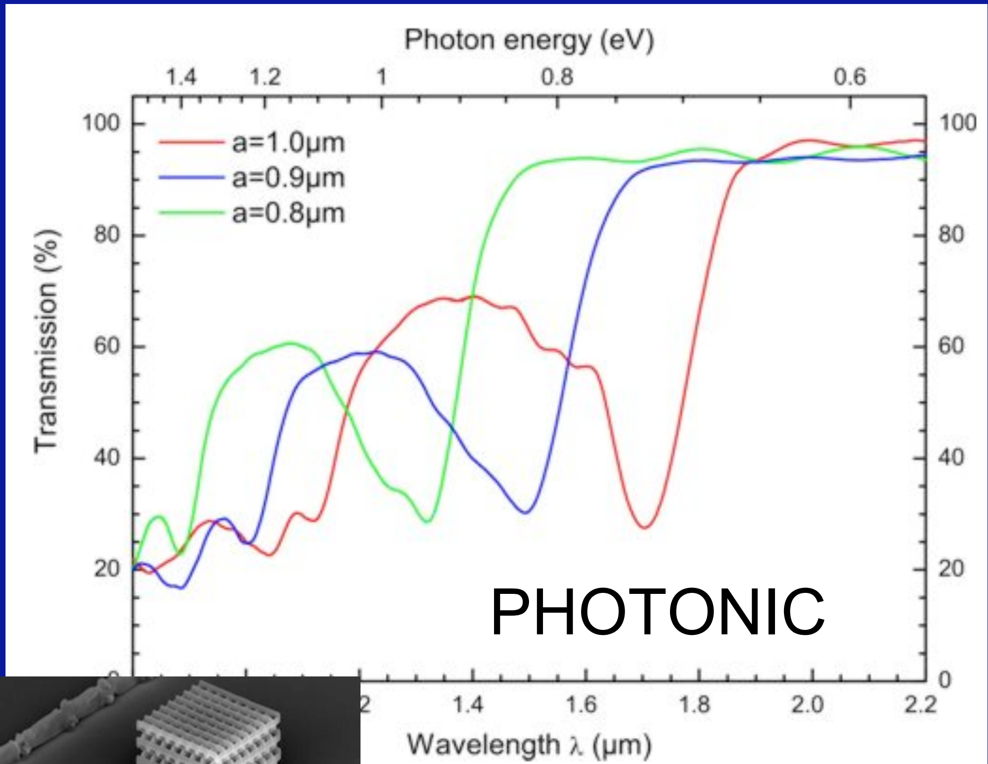



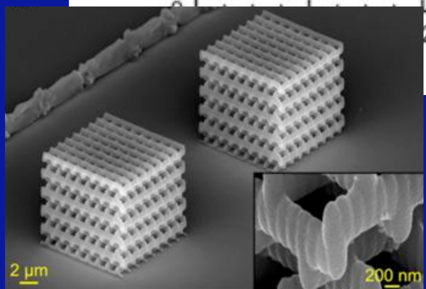



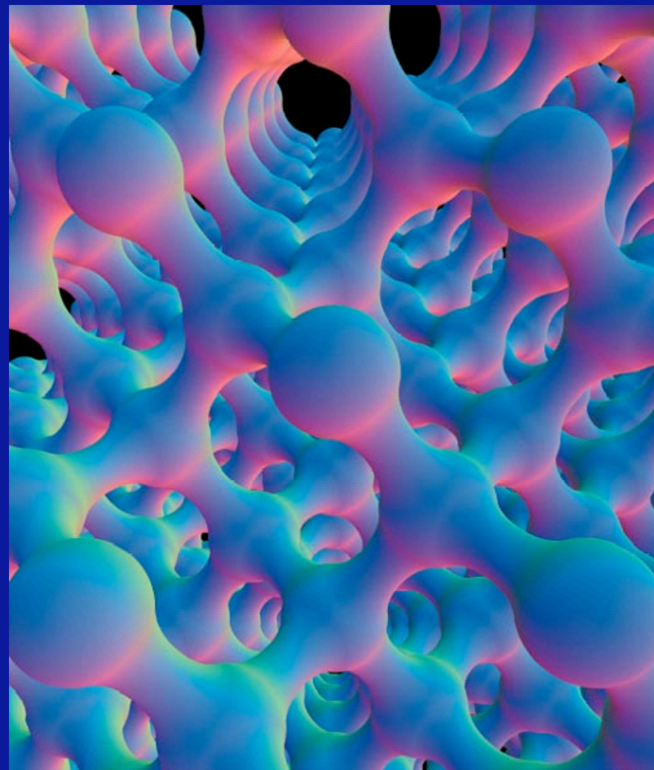




THERMAL CONDUCTIVITY

# 3D-PHONONIC CRYSTALS



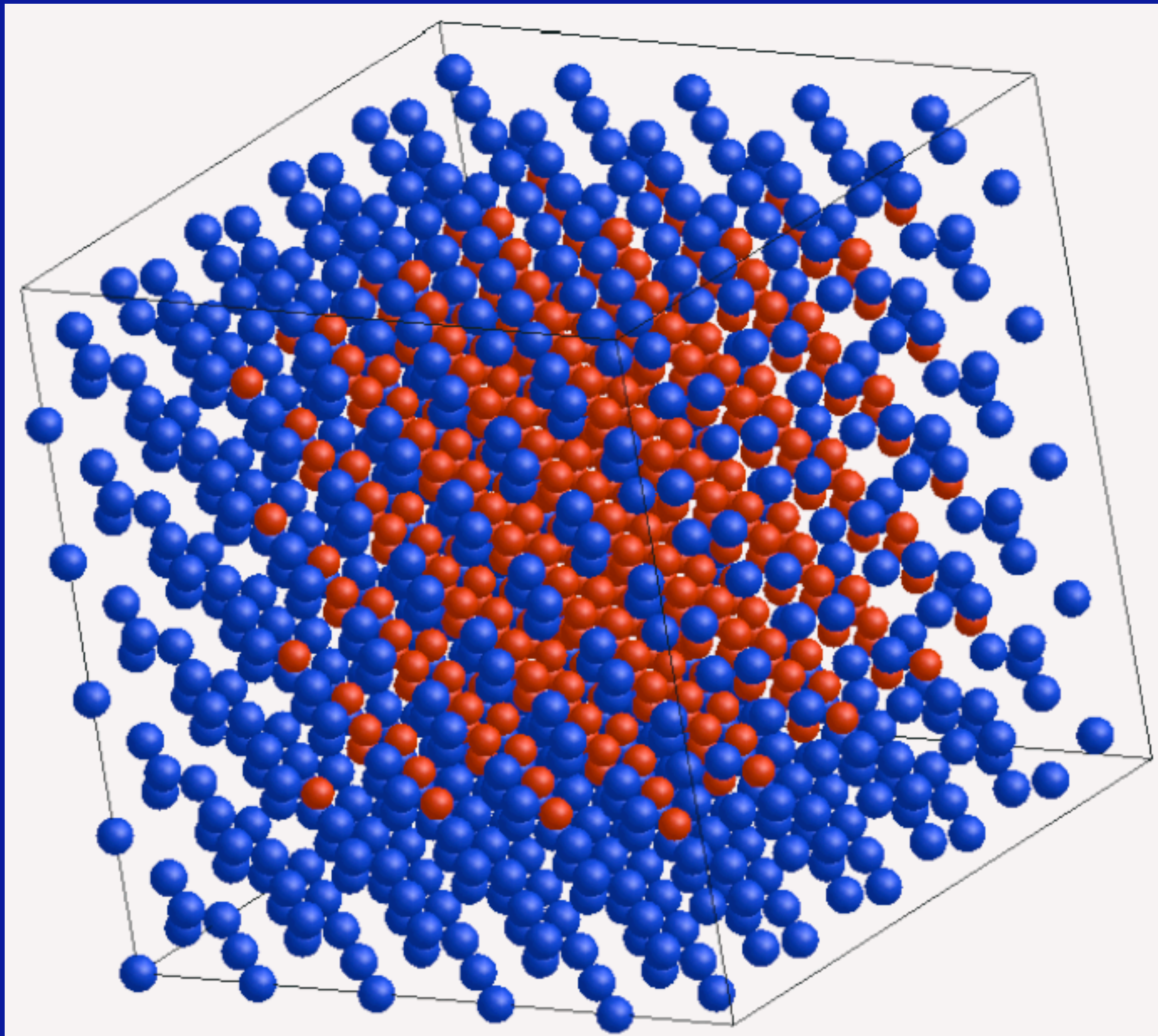



3D PHONONIC CRYSTALS
*TO GENERATE GAPS*
IN PHONON SPECTRA?

THERMAL PHONONS λ≈1nm => ***ATOMIC SCALE PERIOD***

# STRUCTURE



Ge in Si

5 Lattice Constants

*Cubic NanoParticles*

SW potential

Periodic Boundaries

Lattice Dymamics

# THERMAL CONDUCTIVITY

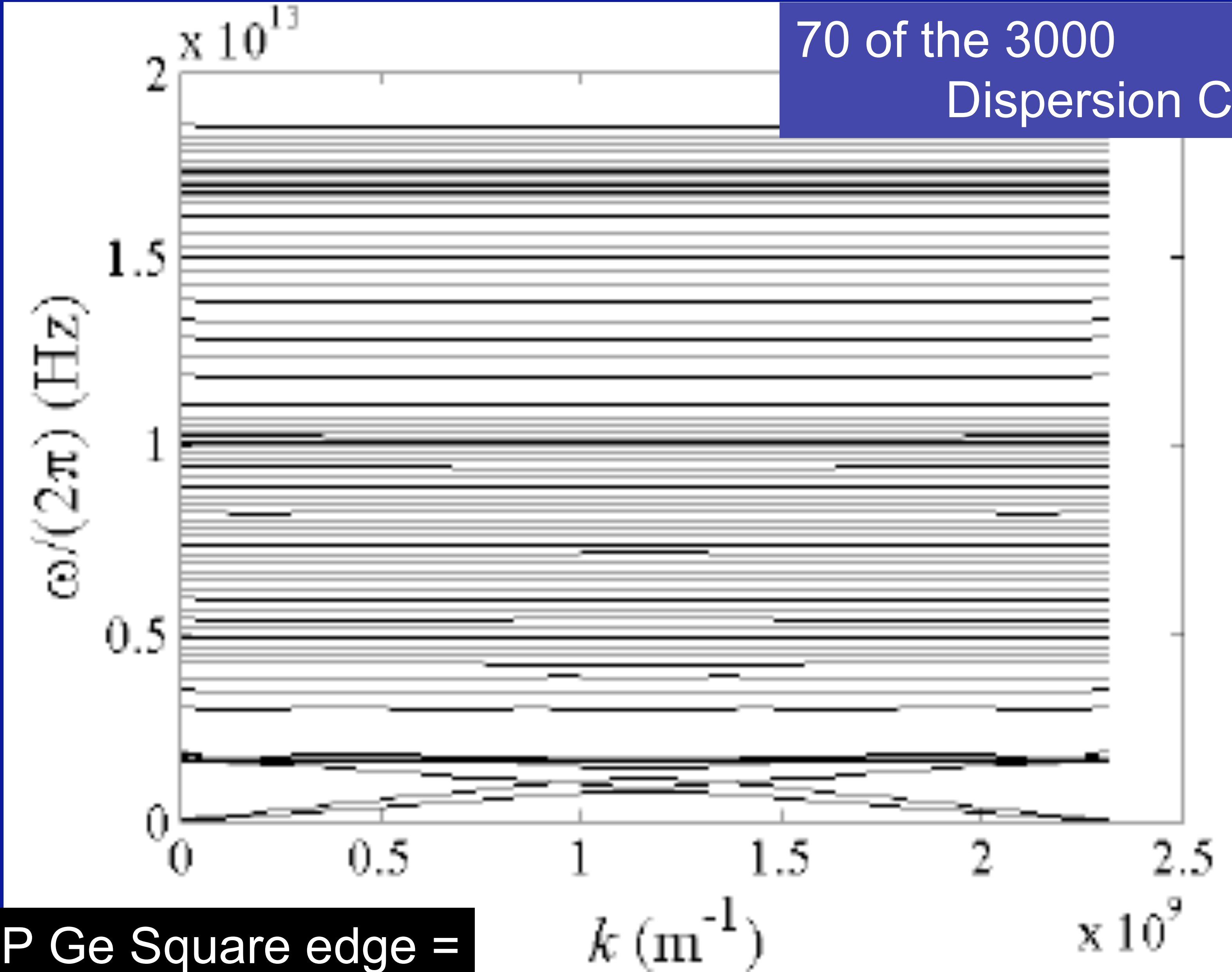
$$\lambda = \frac{1}{3}\frac{\hbar}{2\pi^2}\sum_m \int_0^{2\pi/d} \Lambda_{k,m} k^2 \omega_{k,m} \frac{\partial n_{k,m}^{(0)}}{\partial T} \left|v_{k,m}\right| dk$$

$$\lambda \approx \frac{1}{3}\langle\Lambda\rangle\langle C_p v\rangle$$

$$\langle C_p v\rangle = \frac{\hbar}{2\pi^2}\sum_{m=1}^{N_m} \int_0^{2\pi/d} k^2 \omega_{k,m} \frac{\partial n_{k,m}^{(0)}}{\partial T} \left|v_{k,m}\right| dk$$

$$\langle\Lambda\rangle = \frac{d}{2\pi N_m}\sum_{m=1}^{N_m} \int_0^{2\pi/d} \Lambda_{k,m} dk,$$

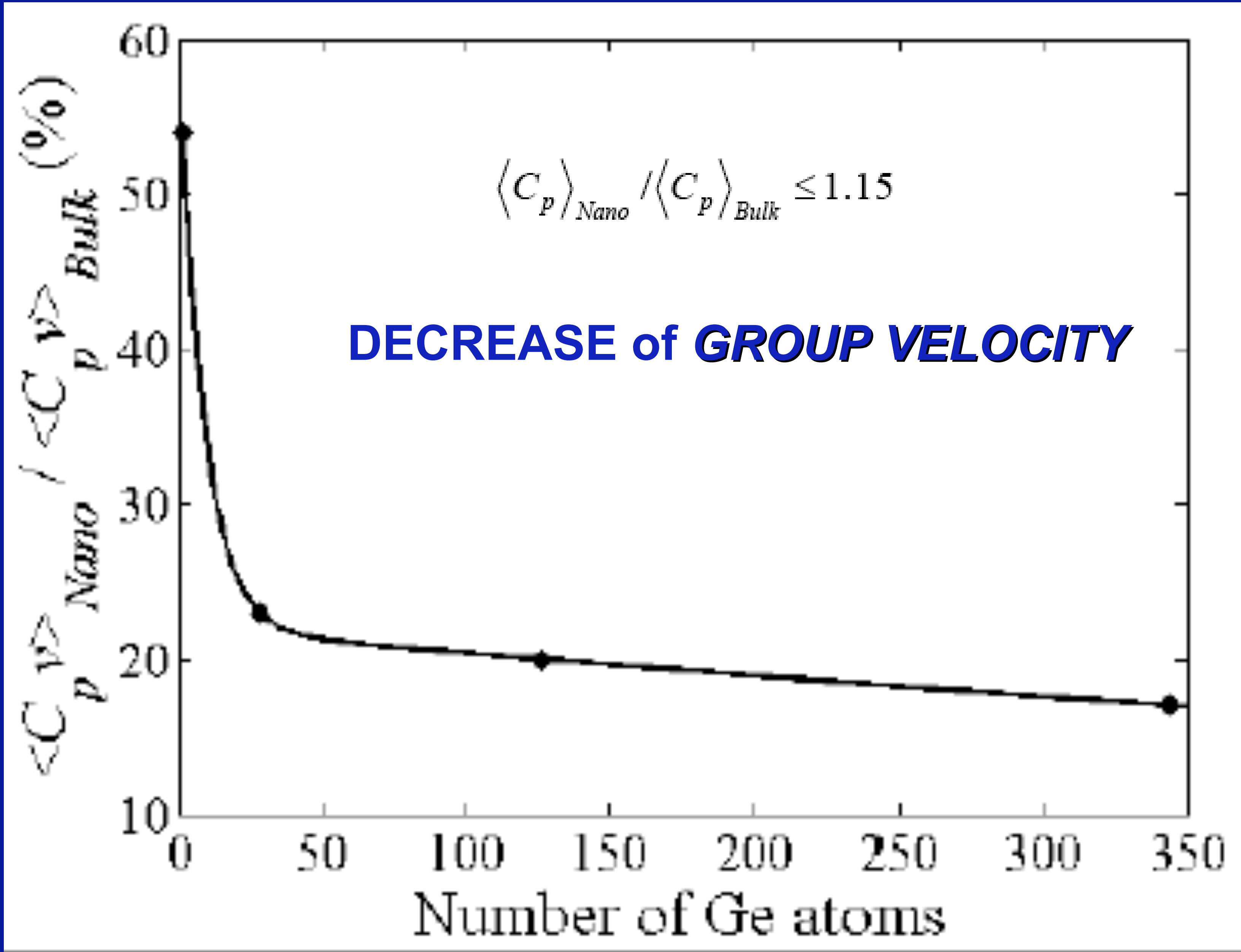
# DISPERSION CURVES




70 of the 3000 Dispersion Curves

NanoP Ge Square edge = 3 Lattice constants

<Cp.v>




Submitted PRB

# CONCLUSION 3D Phononic Crystals

NO PHONON GAP but
1 ORDER OF MAGNITUDE Decrease
*Of GROUP VELOCITY*

PRESUMPTION OF MFP DECREASE
BY 1-2 ORDER OF MAGNITUDE

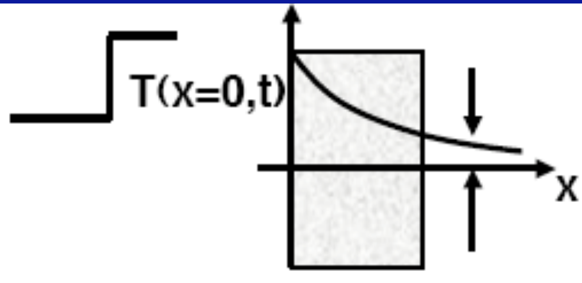
POSSIBLE CONDUCTIVITY DECREASE by FACTOR 1000 = 0.1 W/mK!

LESS THAN ALLOY, GLASS and WATER

# 3- TRANSIENT NON FOURIER CONDUCTION

Velocity of Heat ?

$$\frac{T(x,t)-T_0}{T_{Bound}-T_0} = erfc\left(\frac{x}{\sqrt{4\alpha t}}\right)$$

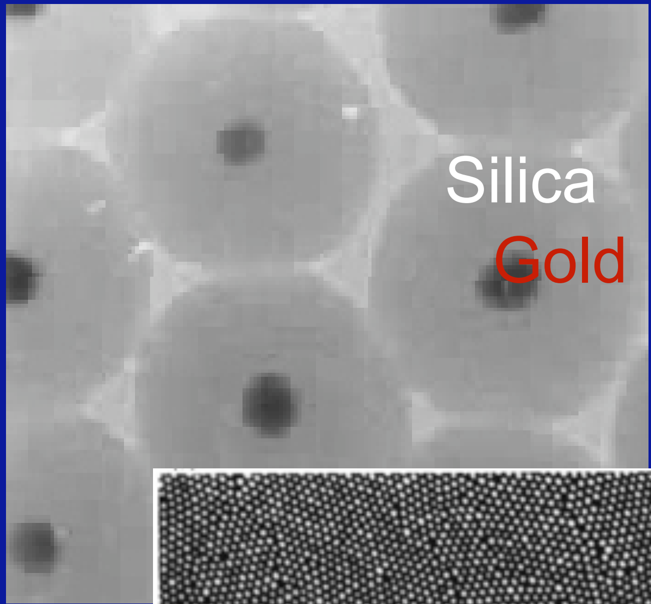


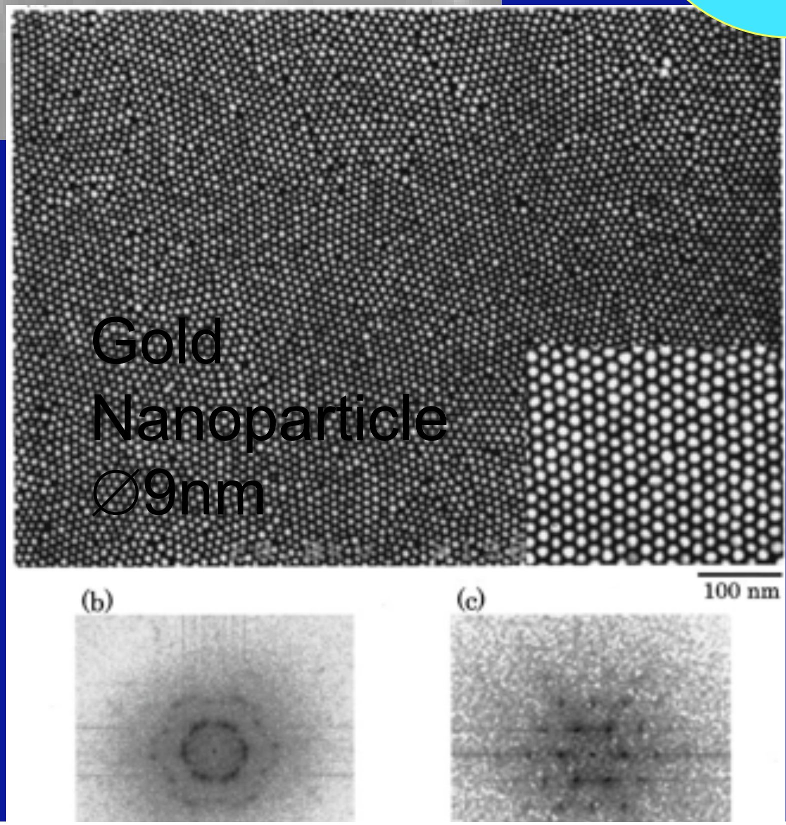

Cattaneo-Vernotte Model: Inertia

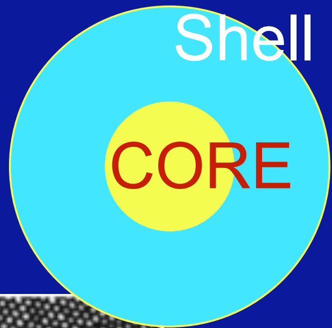
$$\tau . dq/dt + q = -\lambda .\ gradT$$

NEVER PROVED EXPERIMENTALLY

# EXPERIMENT




Pump-Probe Femtolaser

Core Electron absorbing

*Relaxing on Core Phonons*

Conduction to Shell

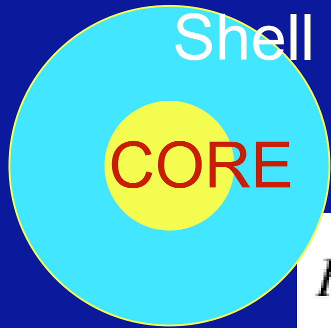
Shell Heat conduction:

Fourier or Non-Fourier

# 2-STEP+BALLISTIC-DIFFUSIVE MODELS

$$C_e \frac{\partial T_e}{\partial t} = -G(T_e - T_l) + P_{vol}(t)$$

$$V_p C_l \frac{\partial T_l}{\partial t} = V_p G(T_e - T_l) - H(t)$$



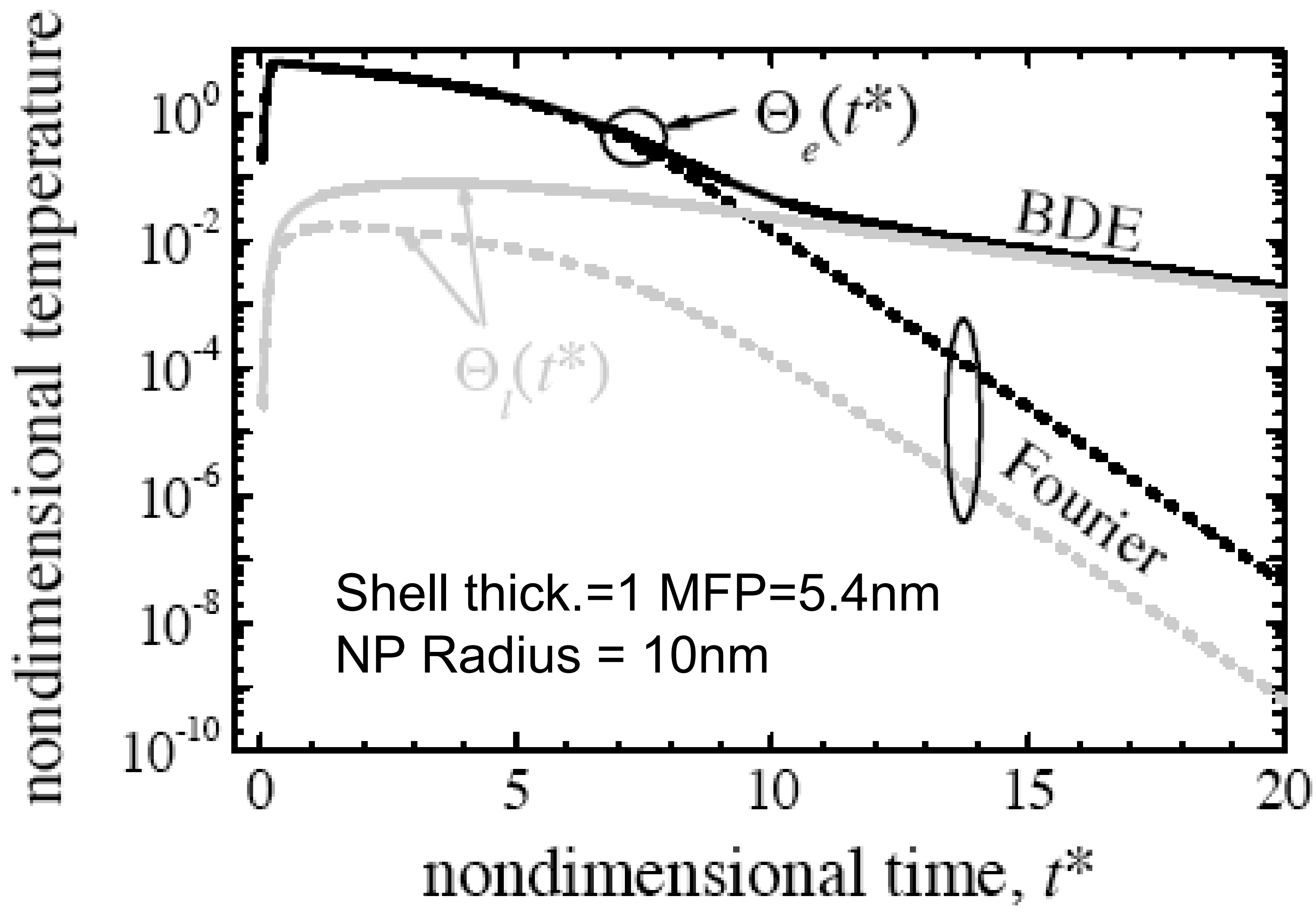

$$H(t) = \int_{S_p} \mathbf{q}(\mathbf{r}, t) \cdot \mathbf{n}\, ds$$

BALLISTIC-DIFFUSIVE EQUATION

$$C\left(\tau \frac{\partial^2 T_m}{\partial t^2} + \frac{\partial T_m}{\partial t}\right) = \nabla(k \nabla T_m) - \nabla \cdot \mathbf{q}_b + \left(\dot{q}_e + \tau \frac{\partial \dot{q}_e}{\partial t}\right),$$

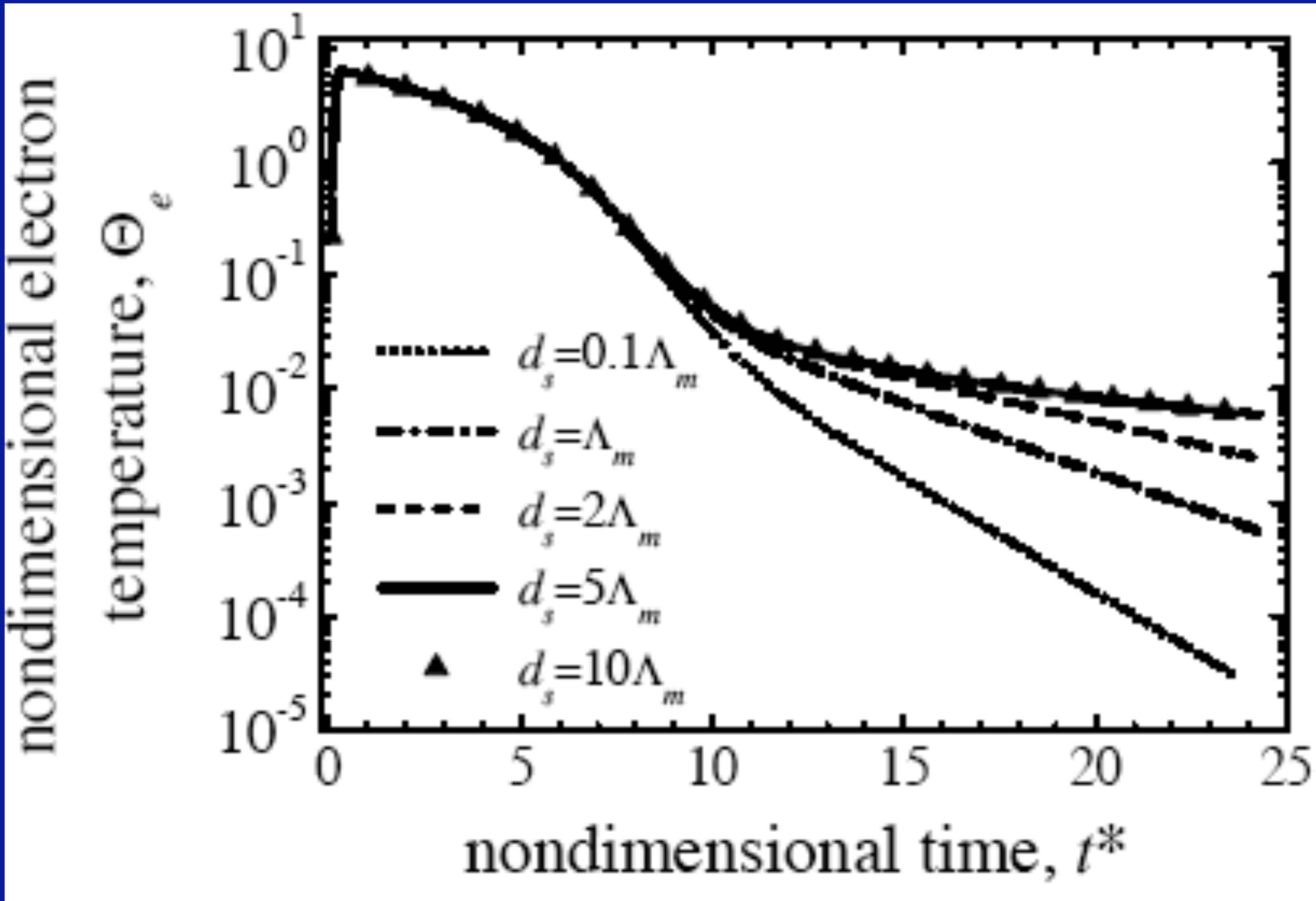
$$\mathbf{q}_b(t, \mathbf{r}) = \frac{1}{4\pi} \int \left[ \int |\mathbf{v}| \hbar \omega D(\omega) f_w[t - (s - s_0)/|\mathbf{v}|, \mathbf{r} - (s - s_0)\hat{\Omega}] \exp\left( - \int_{s_0}^{s} \frac{ds}{|\mathbf{v}|\tau} \right) \cos\theta \, d\Omega \right] d\omega$$

## BDE/FOURIER



$\Theta_e(t^*)$
$\Theta_l(t^*)$
BDE
Fourier
Shell thick.=1 MFP=5.4nm
NP Radius = 10nm
$10^0$
$10^{-2}$
$10^{-4}$
$10^{-6}$
$10^{-8}$
$10^{-10}$
0
5
10
15
20
nondimensional temperature
nondimensional time, $t^*$

# Shell Thickness




STRONG DEPENDENCE TO SHELL THICKNESS

# CONCLUSION on TRANSIENT NON FOURIER

EXPERIMENTAL ACCESS TO
TRANSIENT NON-FOURIER
HEAT CONDUCTION

By USING CORE-SHELL STRUCTURES

WAS NEVER SHOWN AT AMBIENT TEMPERATURE

NEED A SHELL WITH LONG MFP

# Collaborators

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P.-O. Chapuis

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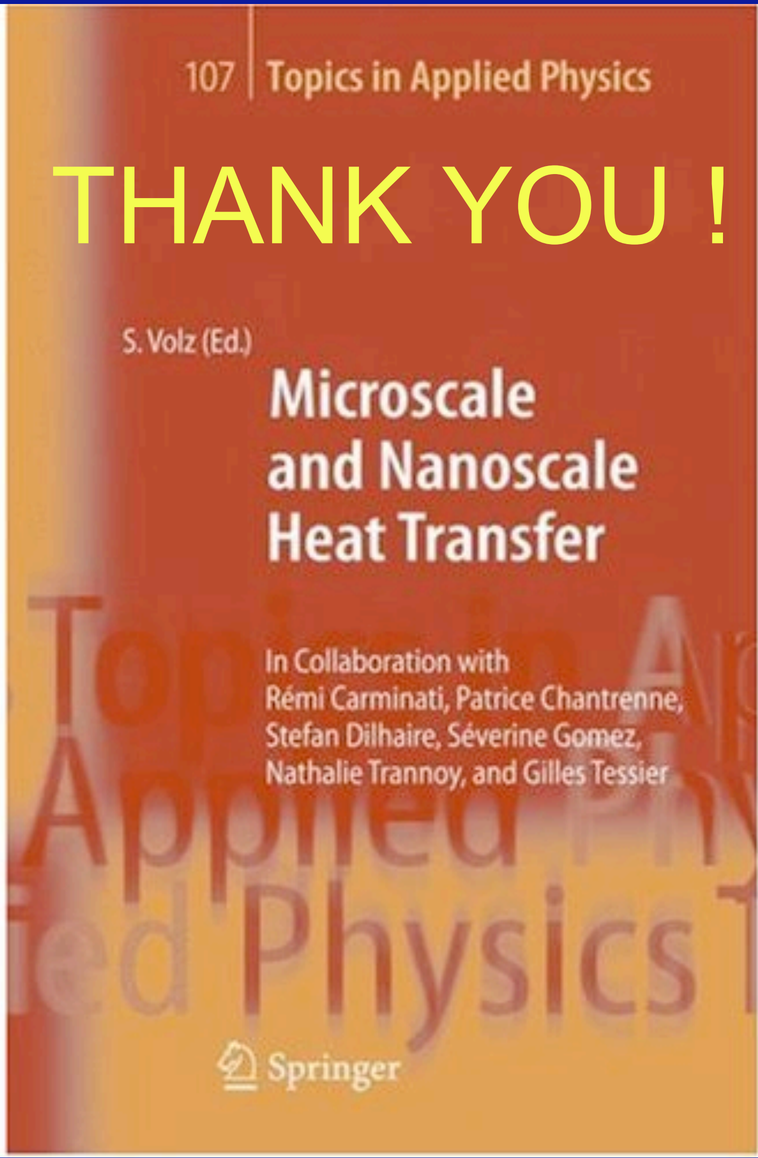
# THANK YOU !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Stefan Dilhaire, Séverine Gomez,
Nathalie Trannoy, and Gilles Tessier
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