Transport de chaleur

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Outline

Introduction - motivations

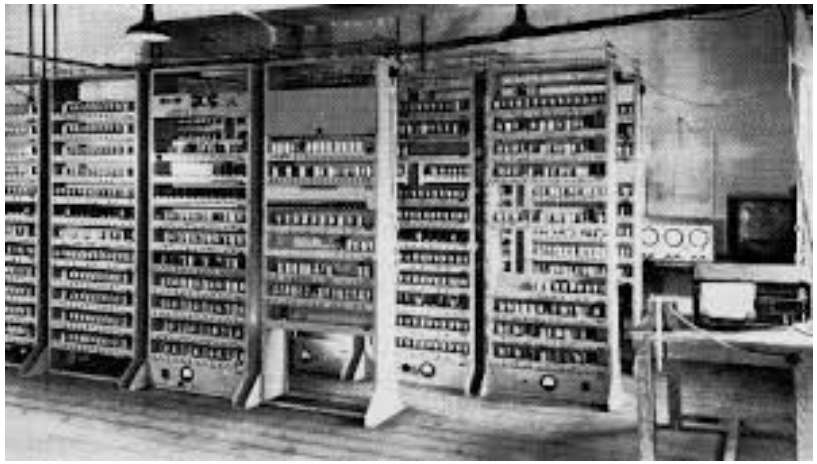
Vibrations

Thermal conductivity

Phonon spectroscopy

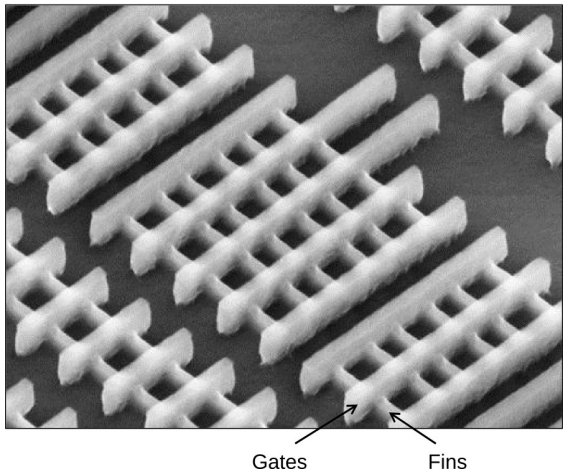
Phonon scattering at interfaces

Nanoscale heat transfer

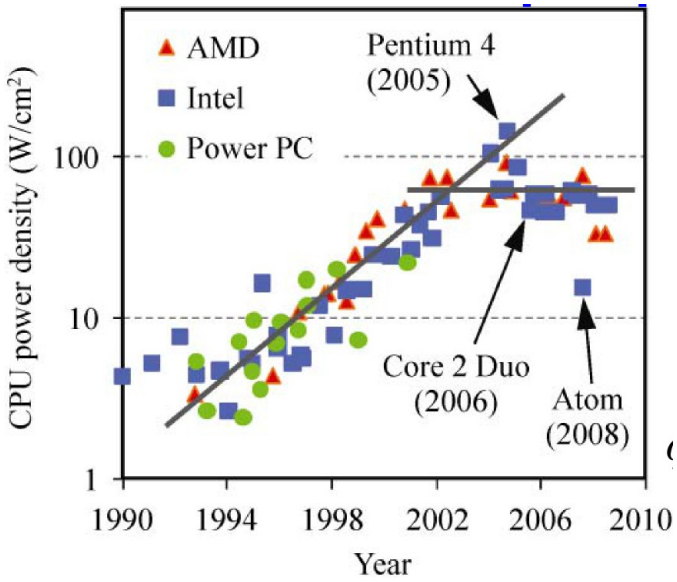


1950's

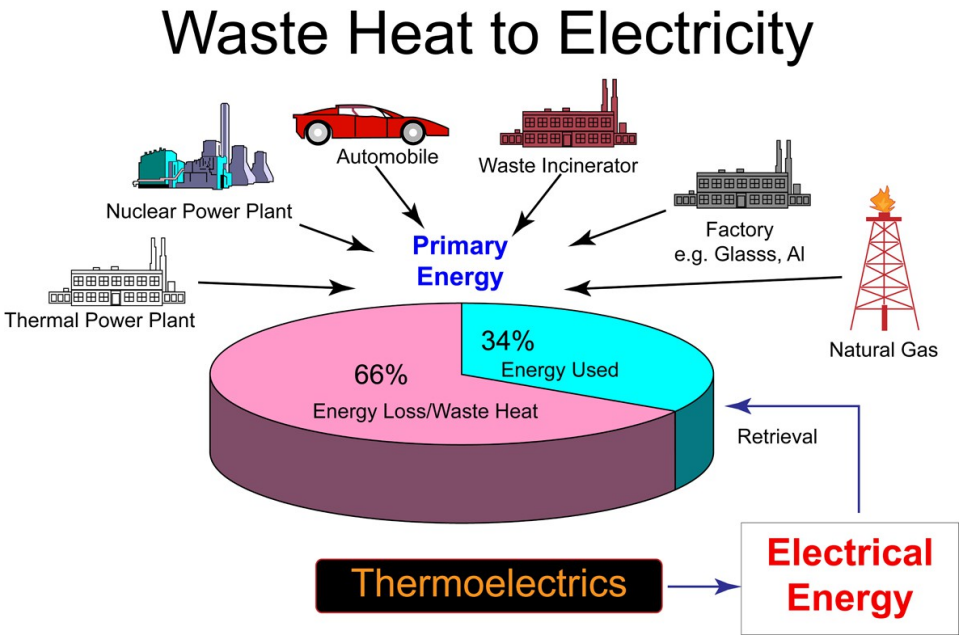
22 nm Tri-Gate Transistor

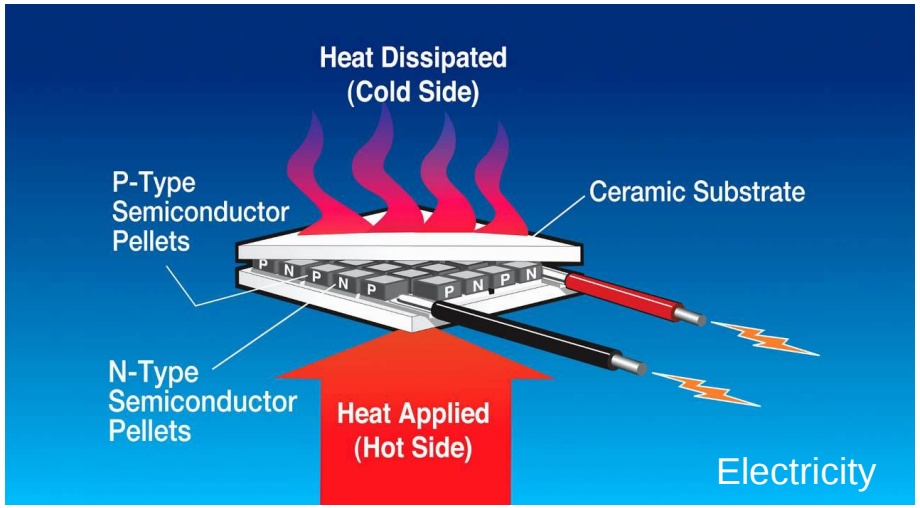


2000's



Materials for thermoelectricity





The ideal thermoelectric material is
a good electronic conductor, but a poor thermal conductor

Thermoelectricity and thermal conductivity

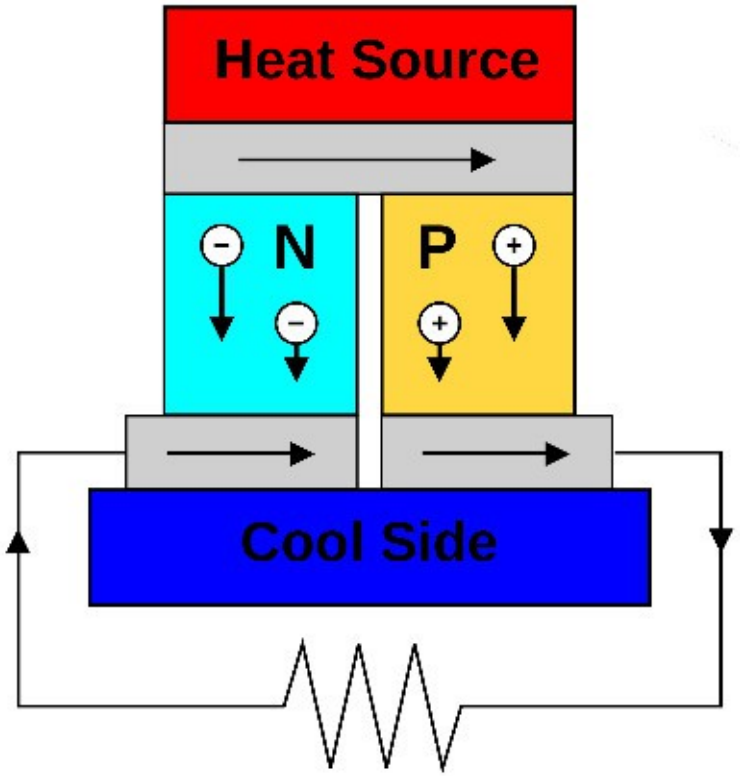


Figure of merit

$$Z = \frac{S^2 \sigma}{\lambda_{ph} + \lambda_e}$$

S Coefficient Seebeck

σ Electronic conductivity

λ Thermal conductivity

Thermoelectricity and thermal conductivity

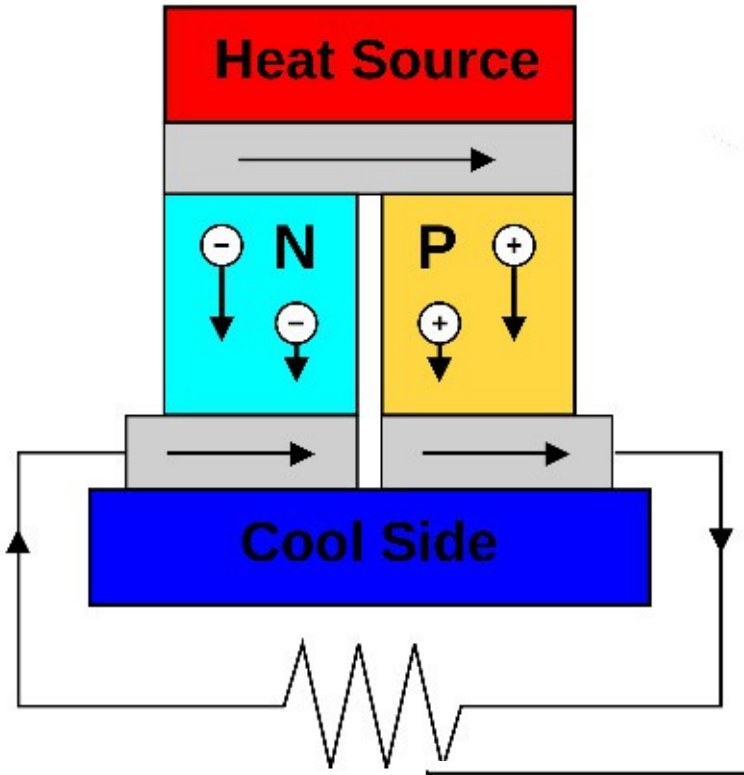
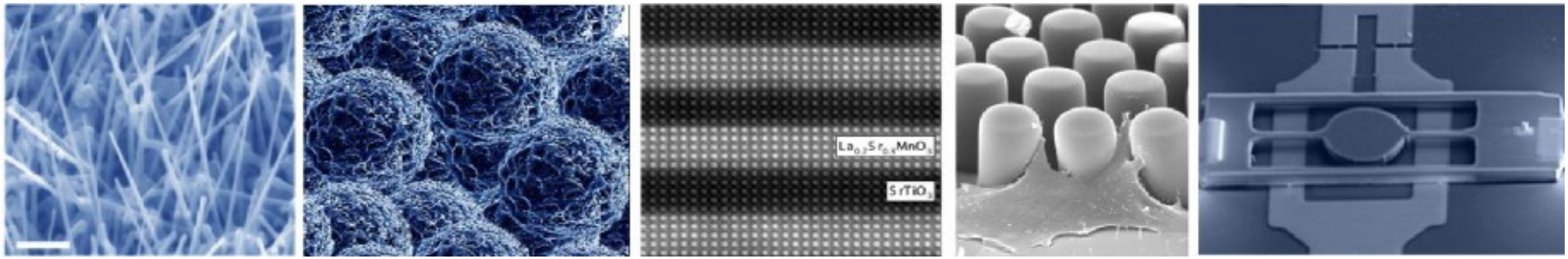


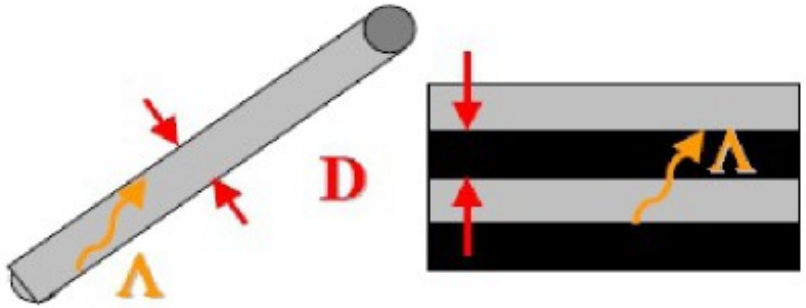
Figure of merit

$$Z = \frac{S^2 \sigma}{\lambda_{ph} + \lambda_e}$$

Property	Metals	Semiconductors	Insulators
S (μVK^{-1})	~ 5	~ 200	~ 1000
σ ($\Omega^{-1}cm^{-1}$)	~ 10^6	~ 10^3	~ 10^{-12}
Z (K^{-1})	~3×10^{-6}	~2×10^{-3}	~5×10^{-17}

Nanostructured materials





D >> Λ, **régime diffusif**

D ≈ Λ, **régime ballistique**

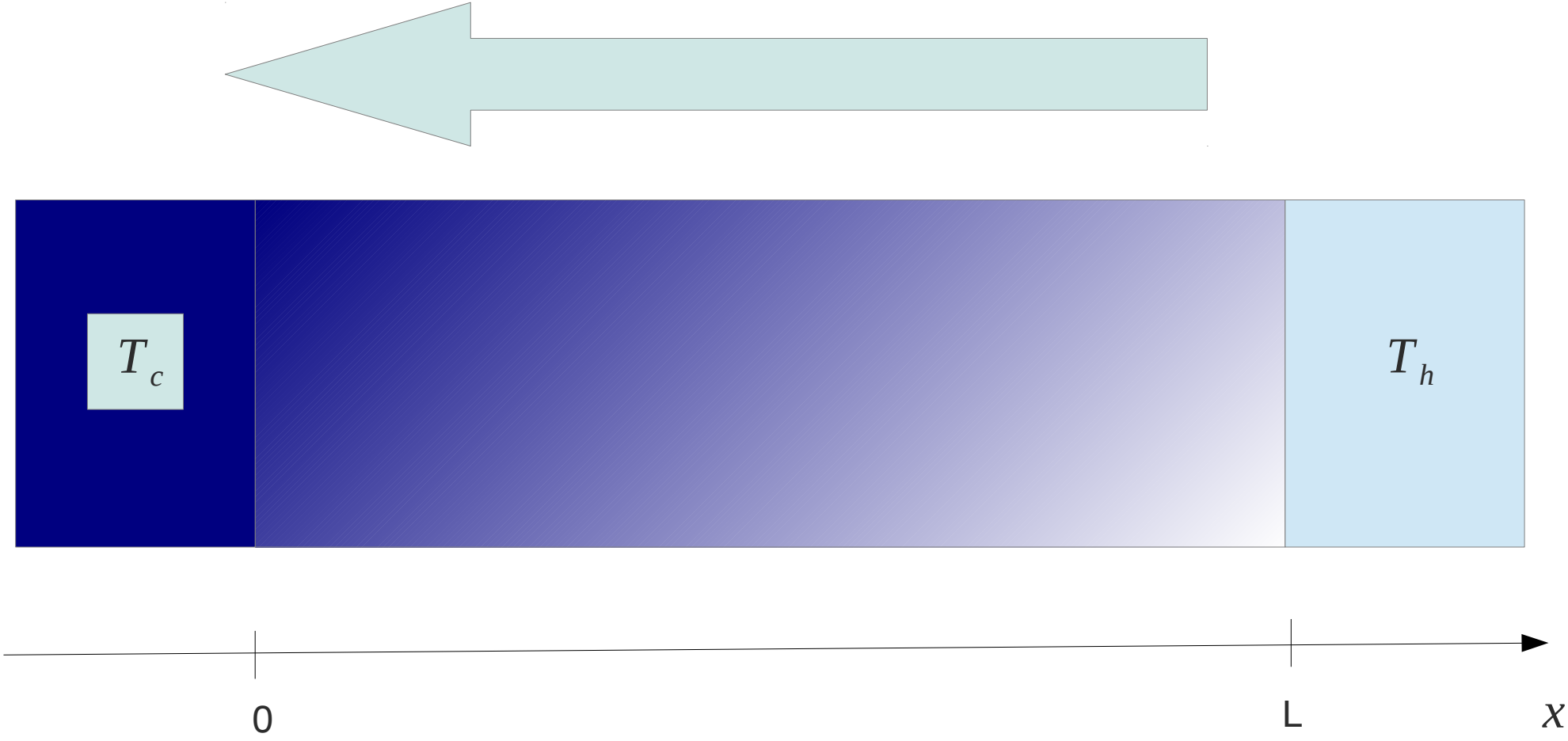
Si @300 K : $\Lambda > 300\,nm$

Fourier

$$\vec{J} = -\Lambda \vec{\nabla} T$$

Fourier law

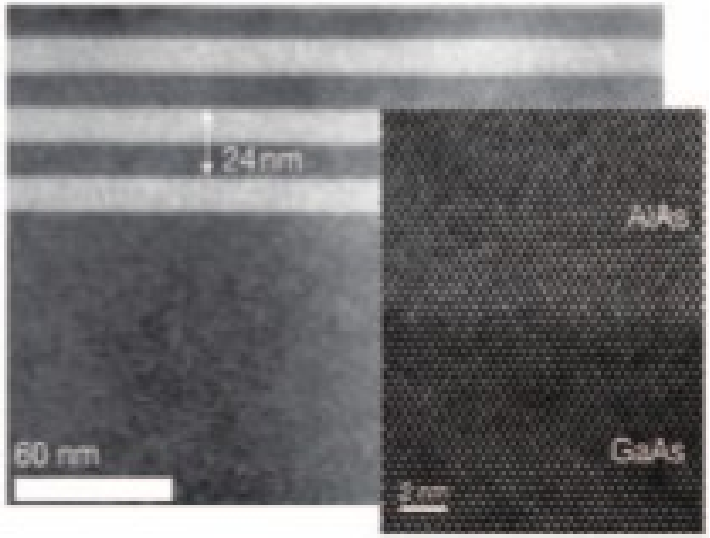
Heat flux



Fourier law : $$q = -\lambda \frac{\partial T}{\partial x} = \lambda \left(\frac{T_h - T_c}{L} \right)$$

Fourier law in anisotropic materials

Superlattices



isotropic

$$\vec{J} = -\lambda \vec{\nabla} T$$

anisotropic

$$J_\alpha = -\lambda_{\alpha,\beta} \partial_\beta T$$

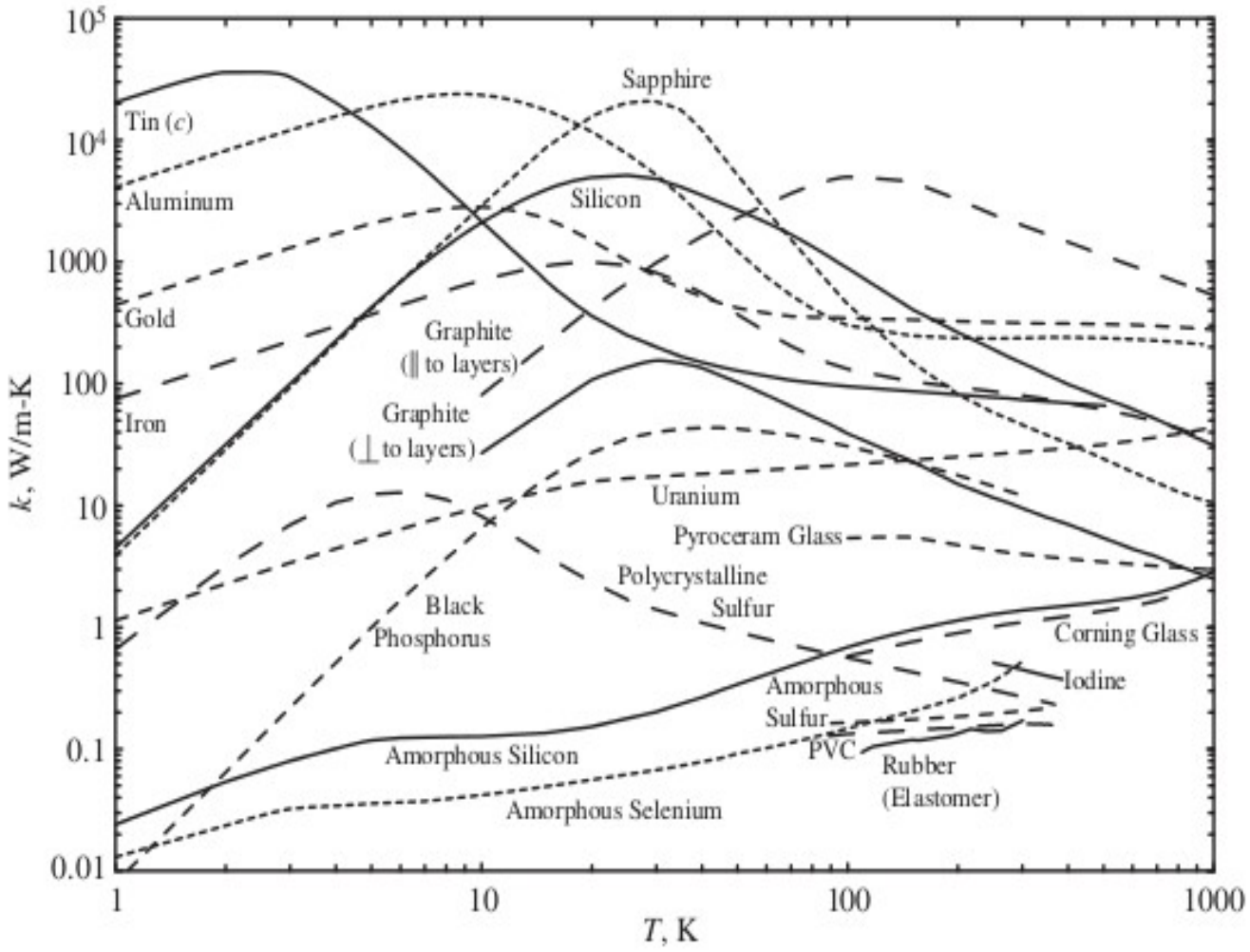
$$\lambda \quad \begin{vmatrix} \lambda_{IP} & 0 & 0 \\ 0 & \lambda_{IP} & 0 \\ 0 & 0 & \lambda_{CP} \end{vmatrix}$$

λ_{IP} In-plane conductivity

λ_{CP} Cross-plane conductivity

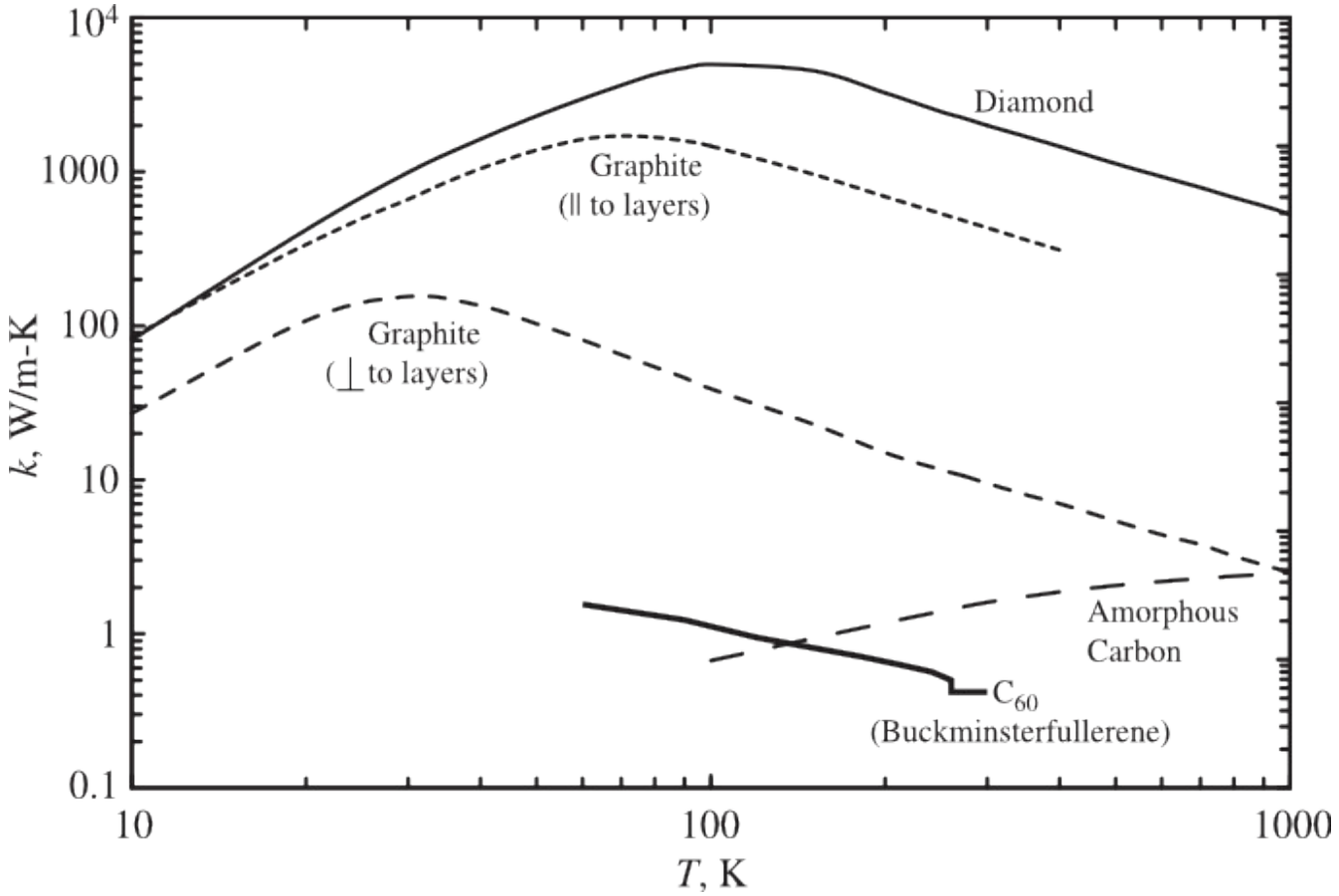
The flux is not always parallel to the temperature gradient !

Thermal conductivity



Y. Touloukian, *Thermophysical properties of matter*

Thermal conductivity



Y. Touloukian, *Thermophysical properties of matter*

Energy carriers

Crystalline phases

Metals : electrons

Less extent phonons

Semi-conductors : mainly phonons

Other excitations : magnons etc
not discussed

Disordered phases

Phonons and diffusons

Electronic thermal conductivity

Thermal conductivity $\lambda = \lambda_e + \lambda_{ph}$

electronic phononic

Wiedemann Franz law $\frac{\lambda_e}{\sigma T} = L$ Lorenz number

$$L_0 = \frac{\pi^2 k_B^2}{3 e^2}$$

$$L_0 = 2.44\,10^{8}\,V^2\,K^{-2}$$

TABLE 1 Thermal Conductivity of Pure Metals at 273 K.[a]

Metal	(W/m-K)	(10^-8 m)	L (10^-8 V²/K²)	Ref.
Ag	436	1.47	2.34	11
Al	237	2.43	2.10	12
Au	318	2.03	2.39	13
Ba	23.3	29.8	2.55	14
Be	230	2.8	2.36	15
Ca	186	3.08	2.13	16
Cd	100	6.80	2.49	15
Ce	11.2 (291 K)	80.0	$ 3.5	17
Co	99 (300 K)	5.99	1.98 (300 K)	18
Cr	95.7 (280 K)	11.8	4.11	19
Cs	37 (295 K)	18.0	2.5 (295 K)	20
Cu	402 (300 K)	1.73 (300 K)	2.31 (300 K)	21
Dy	10.4 (291 K)	93	3.75 (291 K)	22
Er	13.8 (291 K)	79	3.75 (291 K)	22
Fe	80.2 (280 K)	8.64	2.57 (280 K)	23
Ga (jj c)	16.0	50.3	2.95	19
(jj a)	41.0	16.1	2.41	19
(jj b)	88.6	7.5	2.43	24
Gd	9.1 (291 K)	128	4.2 (291 K)	22
Hf	22.4 (293 K)	31.0 (293 K)	2.45 (293 K)	25
Hg (jjÞ	34.1 (197 K)	14.6 (197 K)	2.53 (197 K)	26
(? Þ	25.9 (197 K)	19.3 (197 K)	2.55 (197 K)	26
Ho	11.8 (300 K)	78.0 (300 K)	3.2 (300 K)	27
In	81.0 (280 K)	8.25 (280 K)	2.39 (280 K)	28
Ir	149 (277 K)	4.70	2.57 (277 K)	29
K	98.5	6.20	2.24	30
La	14.0 (291 K)	59	2.9	22
Li	65	8.5	2.05	31
Lu	16.2 (291 K)	$ 50	3.3 (291 K)	22
Mg	153 (301 K)	4.5 (301 K)	2.29 (301 K)	32
Mn (Þ	7.8 (291 K)	137	4.0 (291 K)	22
Mo	143	4.88	2.56	33
Na	142	4.29	2.23	34
Nb	51.8 (280 K)	13.3	2.53 (280 K)	35
Nd	16.5 (291 K)	58	3.7 (291 K)	22
Ni	93 (280 K)	6.24	2.19 (280 K)	36
Os	87 (323 K)	8.3	2.7 (323 K)	29
Pb	35.5	19.2	2.50	37
Pd	71.7	9.74	2.57	38
Pr	12.8	65	3.1 (280 K)	39
Pt	71.9 (280 K)	9.82	2.59 (280 K)	23
Pu	5.2 (298 K)	$ 130	2.48 (298 K)	40
Rb	55.8	11.3	2.30	41
Re	49	16.9	3.05	42
Rh	153 (280 K)	4.35	2.46 (280 K)	43
Ru	110 (280 K)	6.7	2.72 (280 K)	43
Sc	21.8	44	4.3	44
Sm	13.4 (291 K)	90	4.3 (291 K)	22
Sn	64	10.6	2.48	15
Sr	51.9	11.0	2.18	14
Ta	57.7 (280 K)	12.1	2.56 (280 K)	45
Tb	10.4 (291 K)	110	4.25 (291 K)	22
Tc	51 (300 K)	16.7	$ 3.4 (300 K)	46

Lorenz number

$$L_0 = 2.44\,10^{8} V^2 K^{-2}$$

Tritt, thermal conductivity

What is a phonon ?

Vibrations

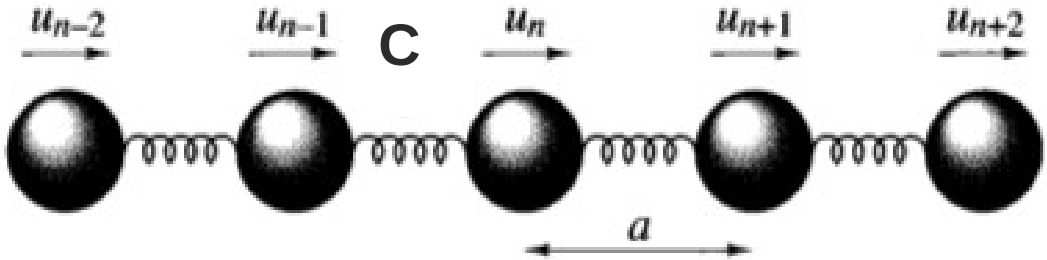
Vibrations : assumptions

-adiabatic assumption

-harmonic approximation

-quasi-classical treatment

Dynamics of a monoatomic chain

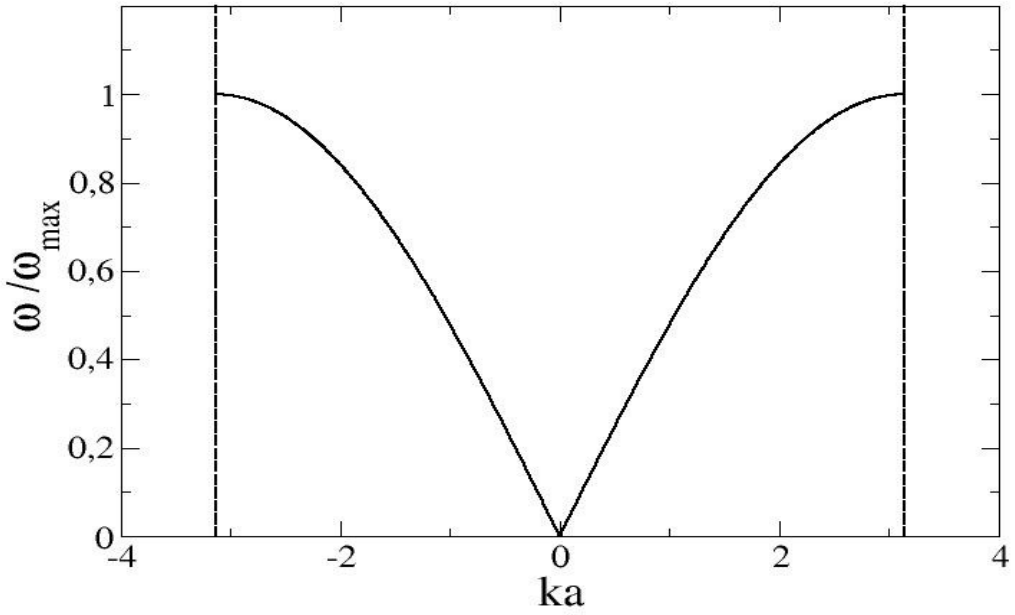


Equations of motion : $m\frac{d^2u_n}{dt^2}=C\left(u_{n+1}+u_{n-1}-2u_n\right)$

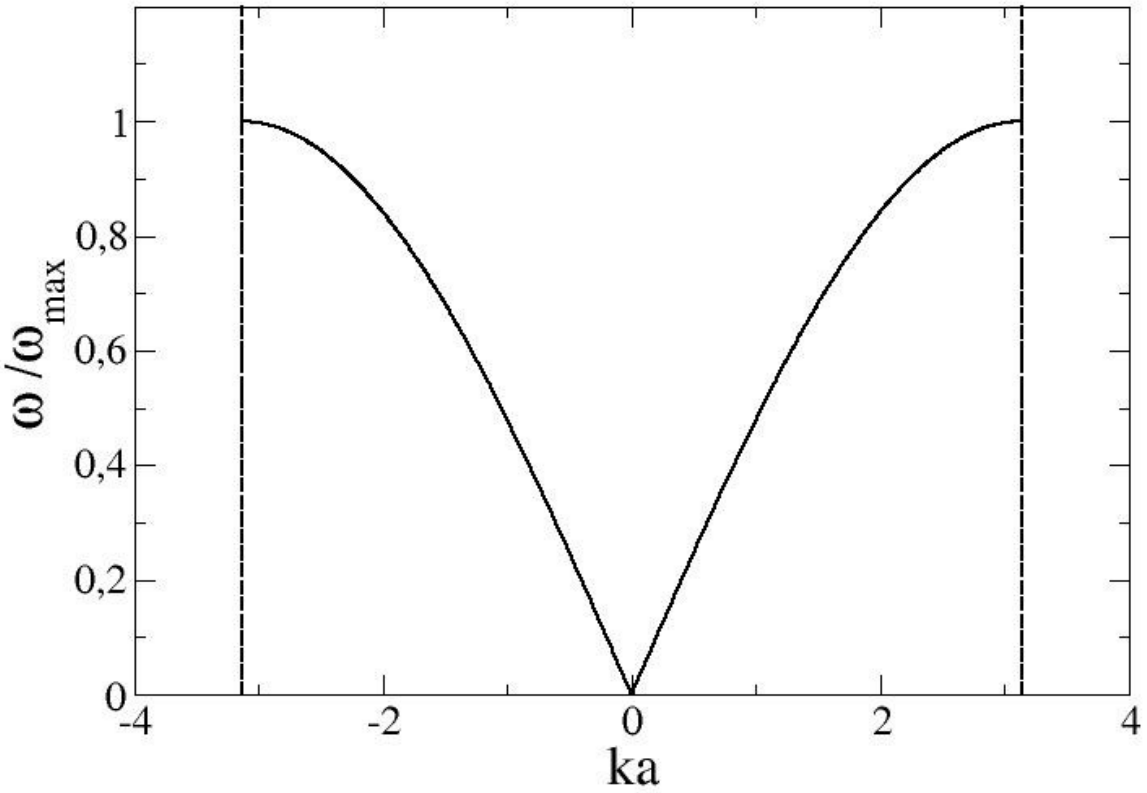
Solutions : $u_n(t)=q_k\exp\left(i\left(kna-\omega(k)t\right)\right)$ $\qquad k=\frac{2\pi p}{N}\ \ (p\ integer)$

Dispersion relation :

$$\omega(k)=\left(\frac{4C}{m}\right)^{1/2}\left|\sin\left(\frac{ka}{2}\right)\right|$$



Dynamics of a monoatomic chain



Dispersion relation

$$\omega(k) = \left(\frac{4C}{m}\right)^{1/2} \left|\sin\left(\frac{ka}{2}\right)\right|$$

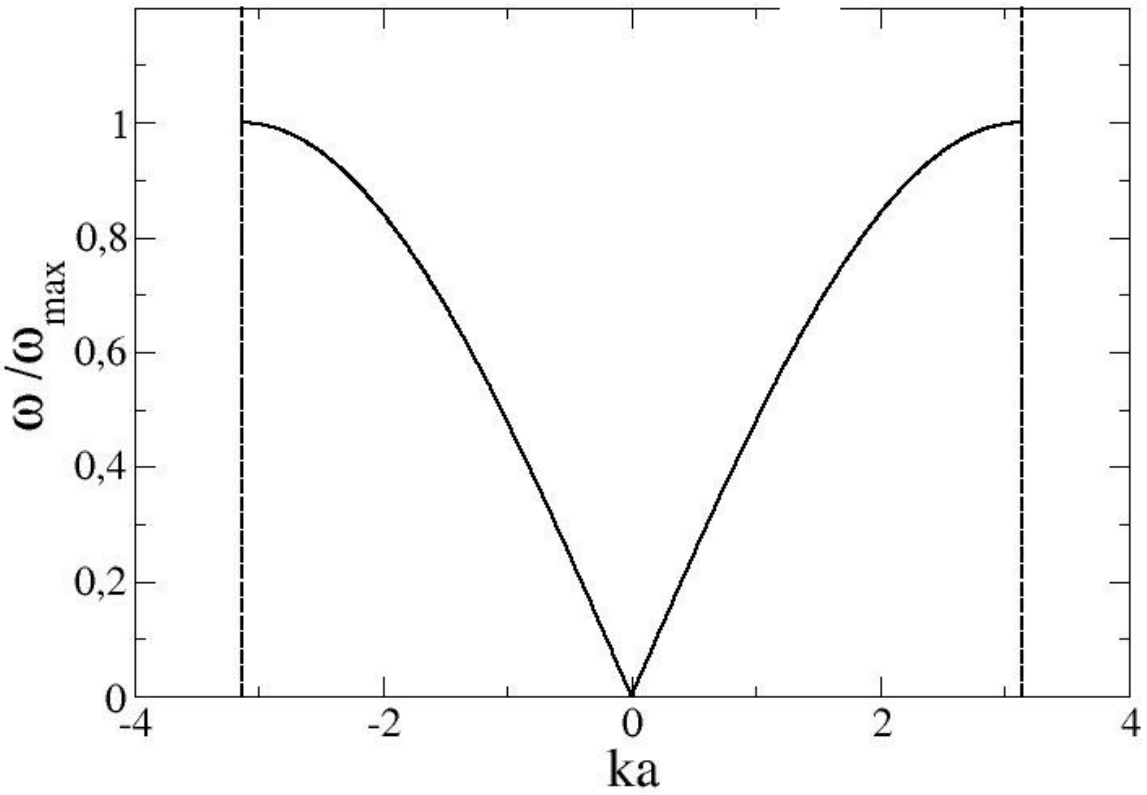
Phase velocity

$$v_\varphi(k) = \left(\frac{4C}{m}\right)^{1/2} \sin\left(\frac{ka}{2}\right)/k$$

Group velocity

$$v_g(k) = \left(\frac{C}{m}\right)^{1/2} a\cos\left(\frac{ka}{2}\right)$$

Dynamics of a monoatomic chain



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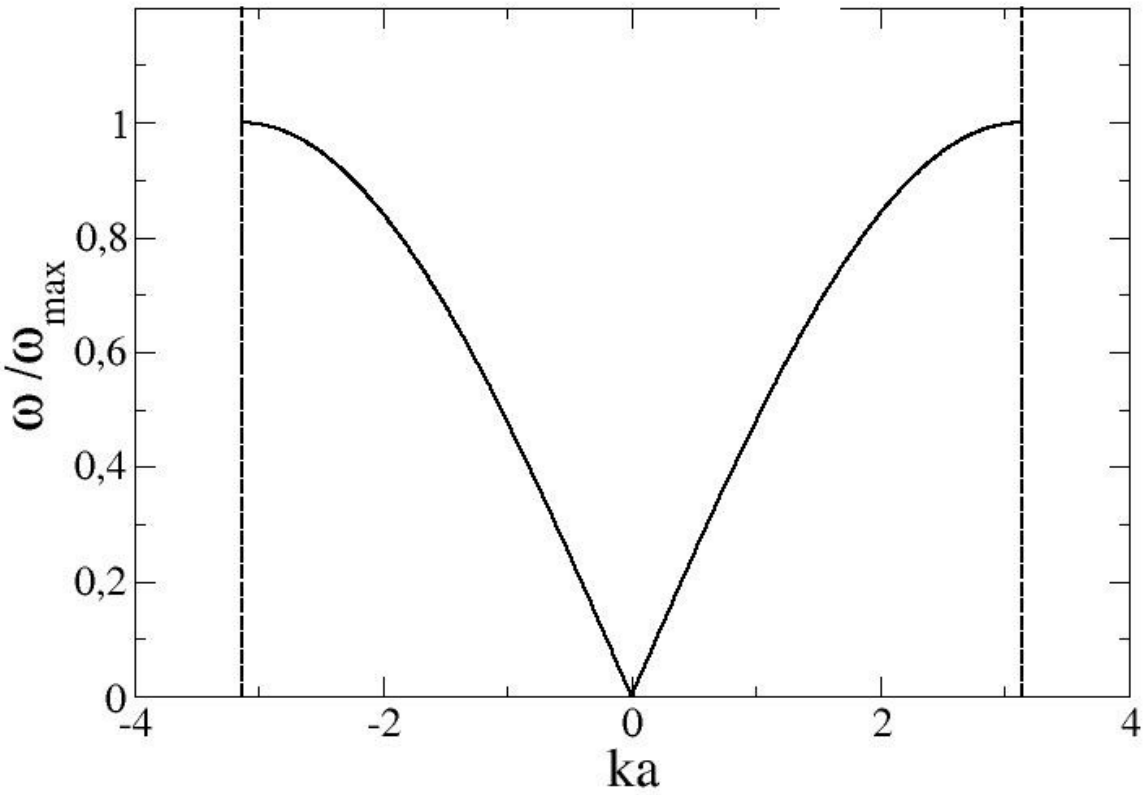
Vibrational density of states

$$g(\omega)=\frac{dN}{d\omega}\sim\frac{1}{v_g(\omega)}\sim\frac{1}{\left(\omega_{max}^2-\omega^2\right)^{1/2}}$$

Dynamics of a monoatomic chain



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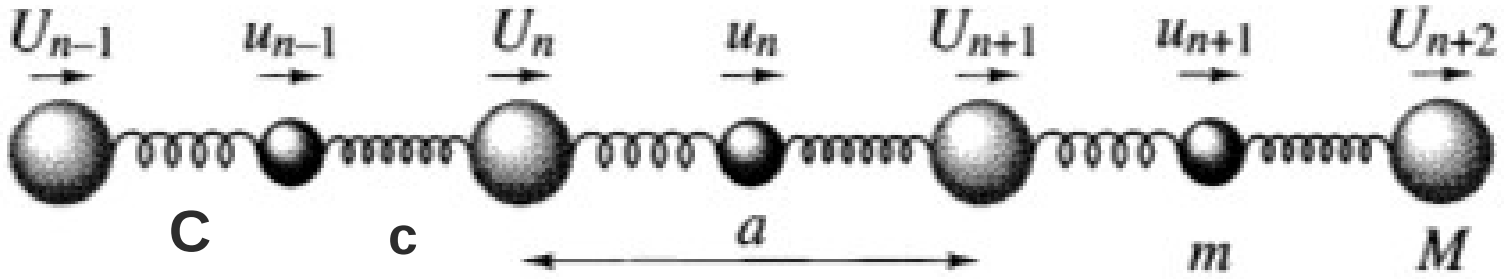
Vibrational density of states $g(\omega)=\frac{dN}{d\omega}\sim\frac{1}{v_g(\omega)}\sim\frac{1}{(\omega_{max}^2-\omega^2)^{1/2}}$

Acoustic limit : $k\to 0\ v_\varphi(k)\simeq v_g(\vec{k})\simeq v_s k\quad v_s=\left(\frac{C}{m}\right)^{1/2}a$

Dynamics of a diatomic chain



Equations of motion :

$$M\frac{d^2U_n}{dt^2}=-C(U_n-u_n)-c(U_n-u_{n-1})$$

$$m\frac{d^2u_n}{dt^2}=-c(u_n-U_{n+1})-C(u_n-U_n)$$

Solutions :

$$U_n(t)=Q_k\exp(i(kna-\omega(k)t))$$

$$k=\frac{2\pi p}{N}\quad(p\,integer)$$

$$u_n(t)=q_k\exp(i(k(n+\frac{1}{2})a-\omega(k)t))$$

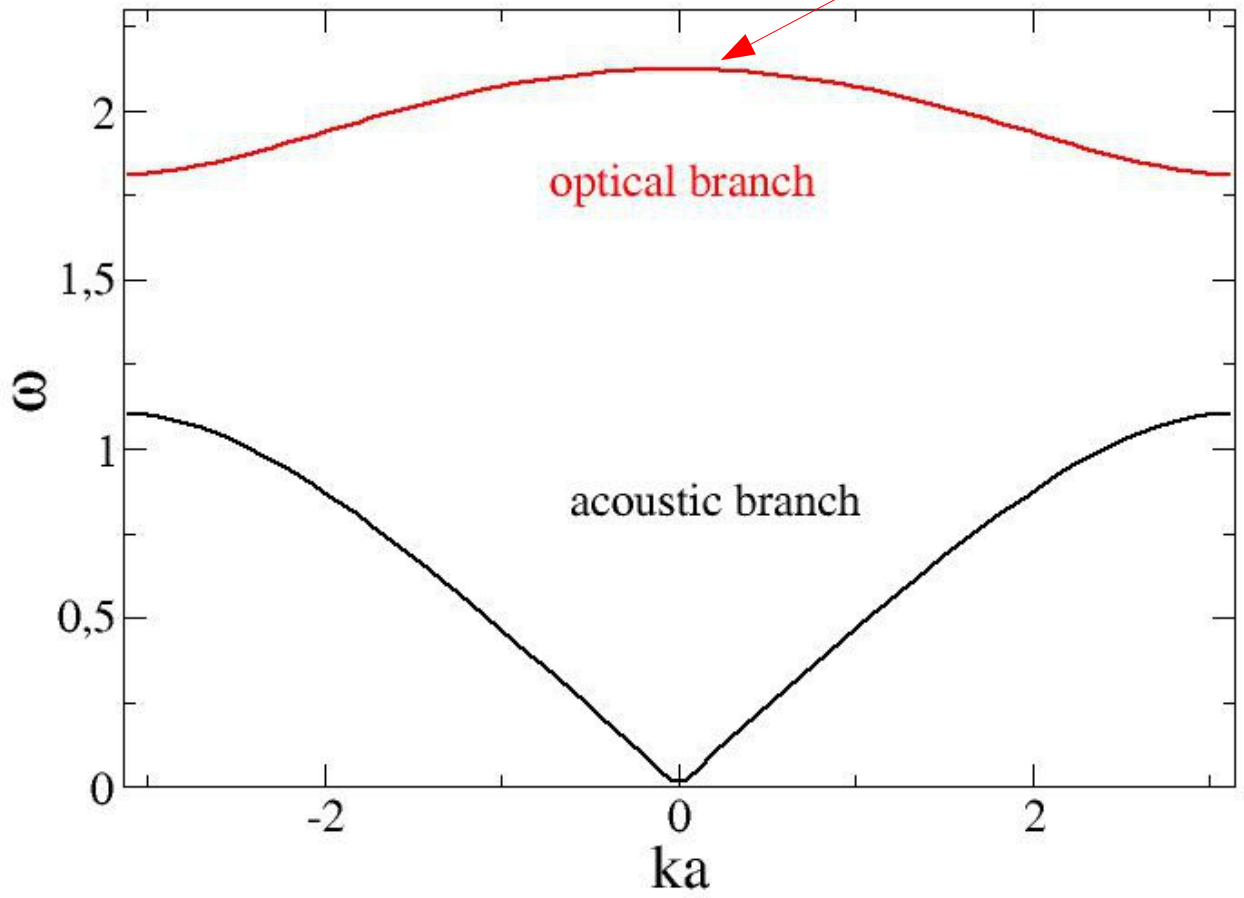
Dispersion relation :

$$\omega^2(k)=(M+m)\frac{(C+c)}{2Mm}\pm\frac{((M+m)^2(C+c)^2-16MmCc\sin^2(ka/2))^{1/2}}{2Mm}$$

Dynamics of a diatomic chain

Case $C = c$

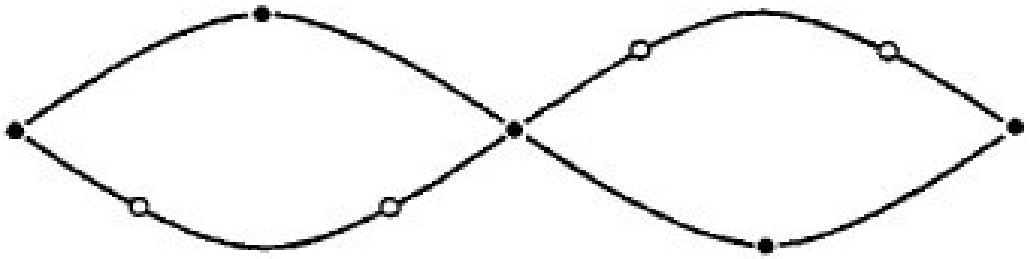
$$\left(2C\frac{(M+m)}{Mm}\right)^{1/2}$$



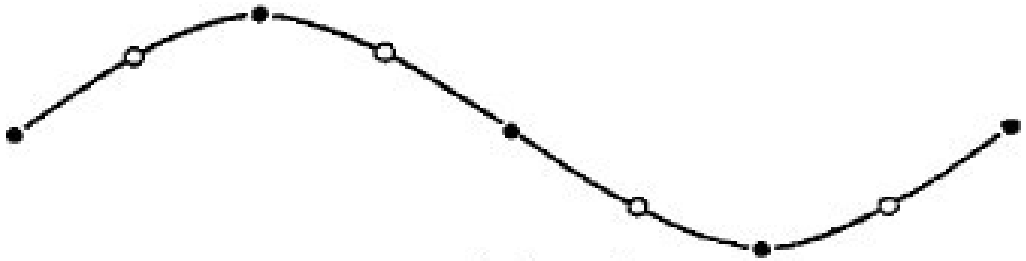
$$\left(\frac{2C}{m}\right)^{1/2}$$

$$\left(\frac{2C}{M}\right)^{1/2}$$

Optical vs acoustic modes



Optical mode



Acoustical mode

Three dimensional dispersion curve

Harmonic Hamiltonian : $H = H_0 + \frac{1}{2}\sum_{i,j} \Phi_{ij}^{\alpha\beta} u_i^{\alpha} u_j^{\beta}$ $\quad \alpha, \beta \in x, y, z$

Harmonic force constants

Equations of motion : $m_i \frac{d^2 u_i^{\alpha}}{dt^2} = -\sum_j \Phi_{ij}^{\alpha,\beta} u_j^{\beta}$

Solution : $u_i^{\alpha} = \frac{Q_{\vec{k}}}{\sqrt{m_i}} e_{\alpha}(\vec{k}) \exp\left(i\left(\vec{k}\cdot\vec{r}_i - \omega t\right)\right)$

Polarisation vector

$$D_{\alpha,\beta}(\vec{k}) e_{\beta}(\vec{k}) = \omega^2(\vec{k}) e_{\alpha}(\vec{k})$$

Dynamic matrix :

$$D_{ij}^{\alpha,\beta} = \frac{1}{\sqrt{m_i m_j}} \Phi_{ij}^{\alpha\beta}$$

$$D_{\alpha\beta}(\vec{k}) = \Sigma_j D_{ij}^{\alpha\beta} \exp\left(i\vec{k}\cdot(\vec{r}_j - \vec{r}_i)\right)$$

Dynamic matrix and dispersion relations

Dynamic matrix : $D_{ij}^{\alpha,\beta}=\frac{1}{\sqrt{m_i m_j}}\Phi_{ij}^{\alpha\beta}$ $D_{\alpha\beta}(\vec{k})=\Sigma_j D_{ij}^{\alpha\beta}\exp\left(i\vec{k}\cdot(\vec{r}_j-\vec{r}_i)\right)$

$$D_{\alpha,\beta}(\vec{k})e_\beta(\vec{k})=\omega^2(\vec{k})e_\alpha(\vec{k})$$

Properties : $D_{ij}^{\alpha,\beta}=D_{ji}^{\beta,\alpha}$ $D_{\alpha\beta}(\vec{k})=D_{\beta\alpha}^{*}(-\vec{k})$ (Taylor)

$D_{ij}^{\alpha,\beta}=D_{ji}^{\alpha,\beta}$ $D_{\alpha\beta}(\vec{k})=D_{\alpha\beta}^{*}(-\vec{k})$ (inversion symmetry)

$\forall i,\Sigma_j D_{ij}^{\alpha\beta}=0 \rightarrow D_{\alpha\beta}(\vec{k}=\vec{0})=0$ (acoustic rule)

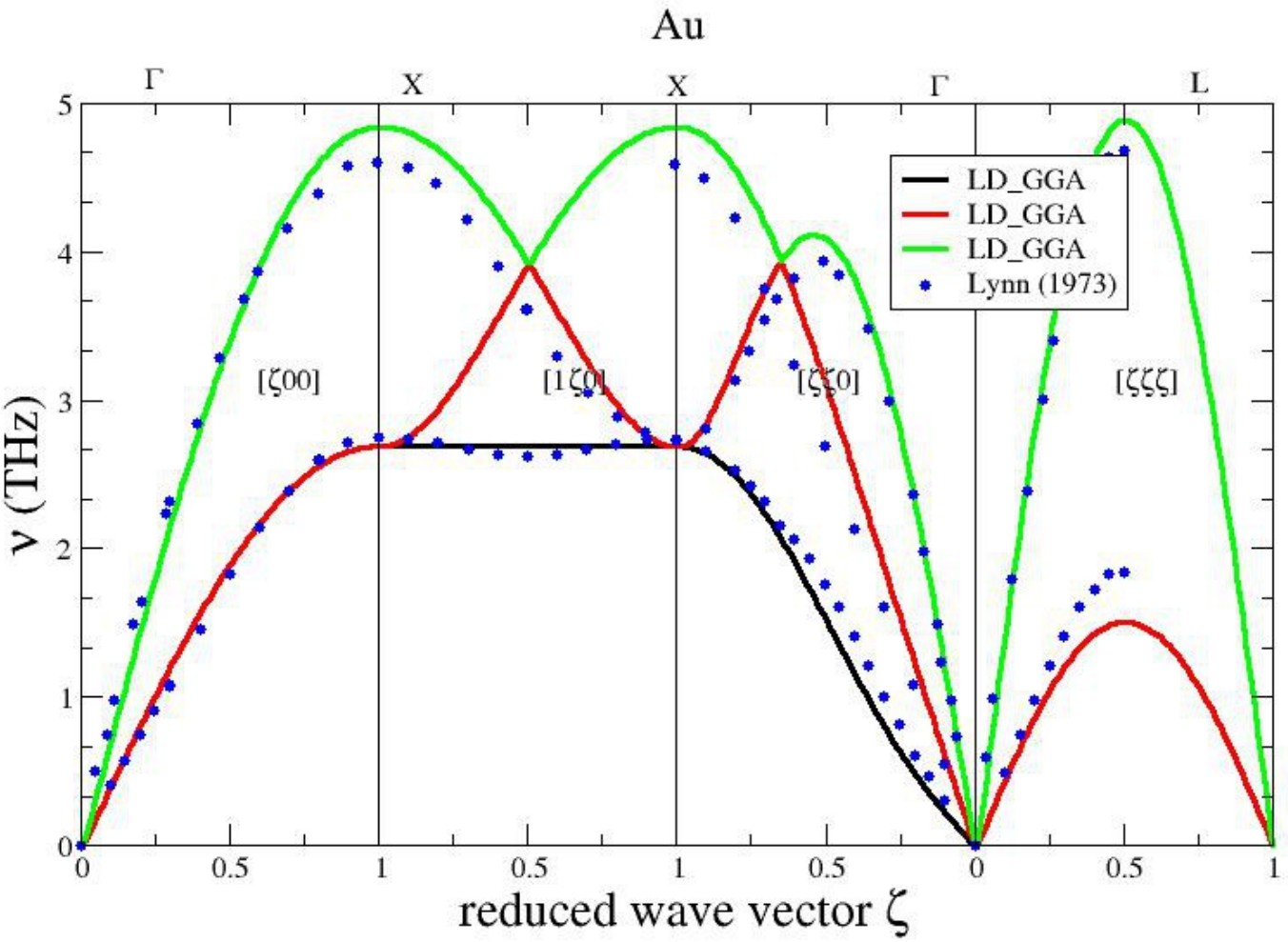
Phonon dispersion in gold

Transverse modes

Displacement perpendicular to k

Longitudinal mode

Displacement parallel to k

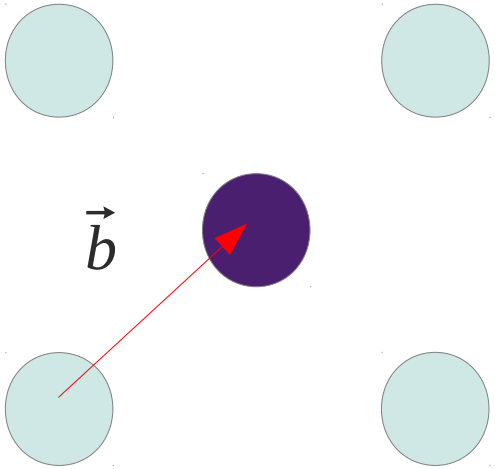


A. Alkurdi, C. Adessi *et al.*

Dispersion relations for complex crystals

Eigenmodes : $u_i^{\alpha}(\vec{b}) = \frac{Q_{\vec{k}}}{\sqrt{m_i}} e_{\alpha}(\vec{k},\vec{b}) \exp\left(i\left(\vec{k}\cdot\vec{r}_i(\vec{b}) - \omega t\right)\right)$

vector defining the position in the primitive cell



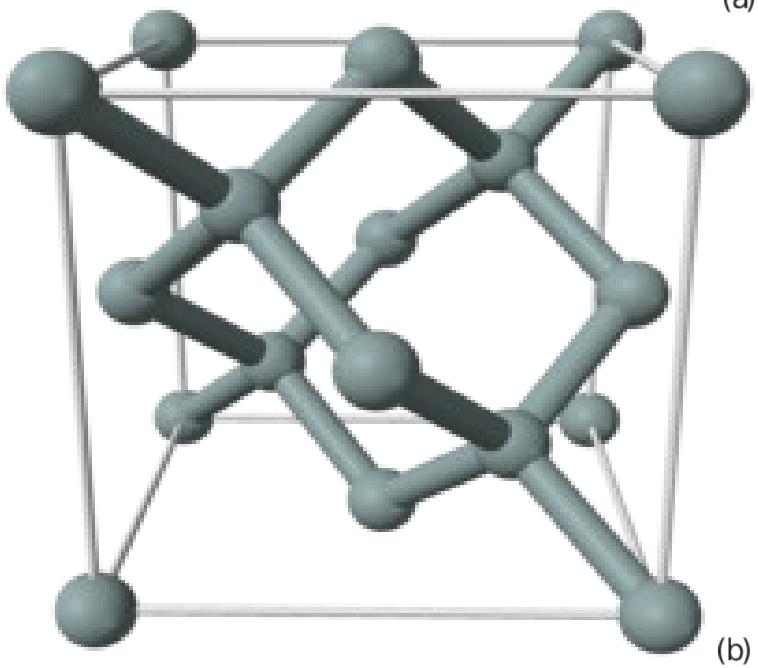
Eigenvalues :

$$\omega^2(\vec{k}) e_{\alpha}(\vec{k},\vec{b}) = \sum_{\vec{b}'} D_{\alpha\beta}(\vec{k};\vec{b},\vec{b}') e_{\beta}(\vec{k},\vec{b}')$$

$\omega_s^2(\vec{k}); e_{\alpha,s}(\vec{k},\vec{b})$

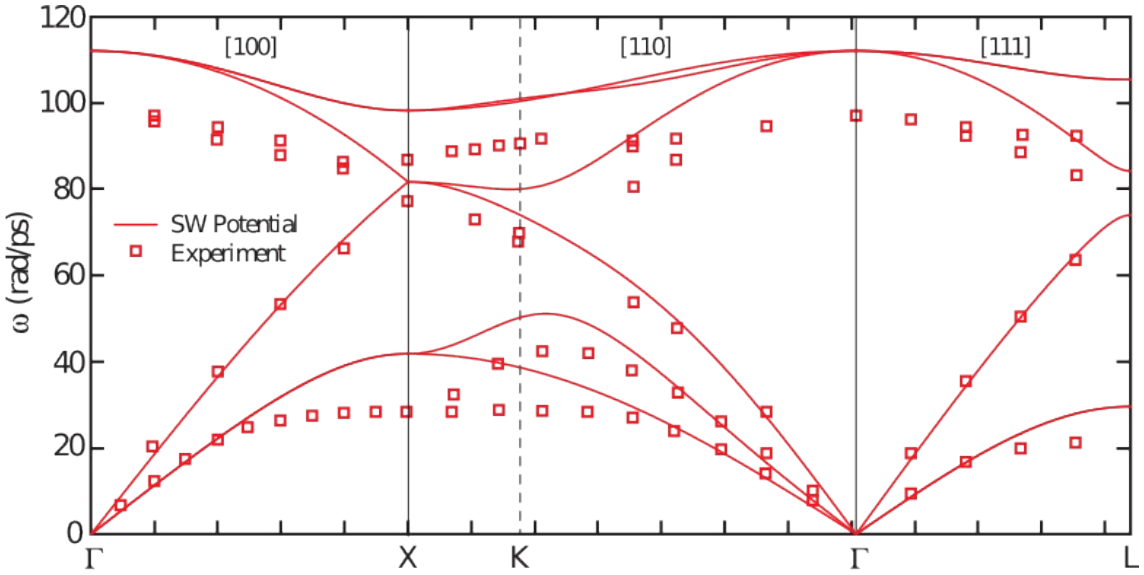
Three dimensional crystal : index s
Total = 3*p branches with p = number of atoms in the primitive cell

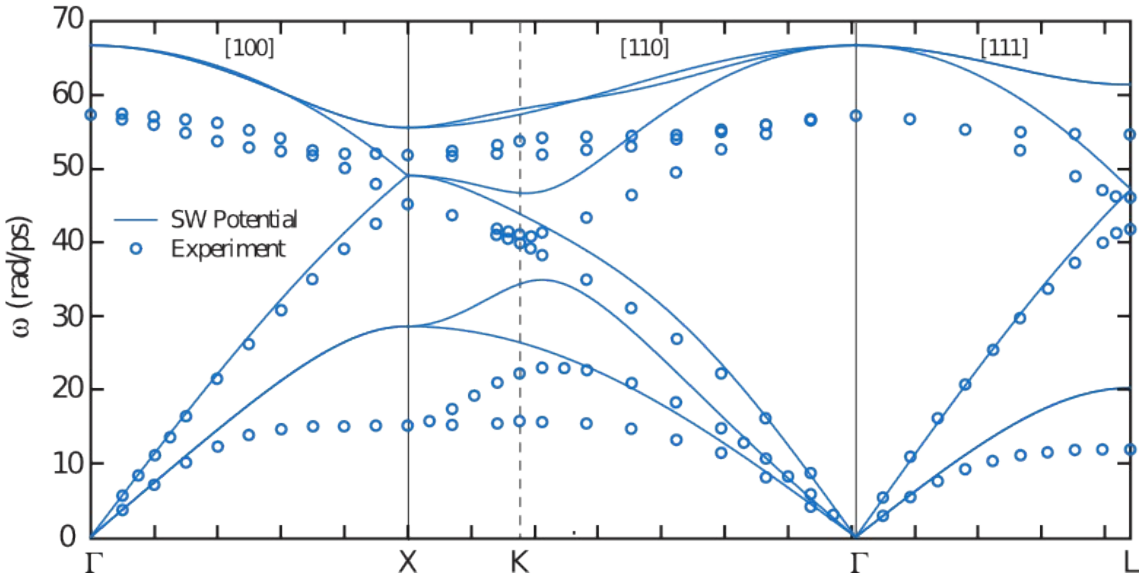
Phonon dispersion in Si



(a) Si

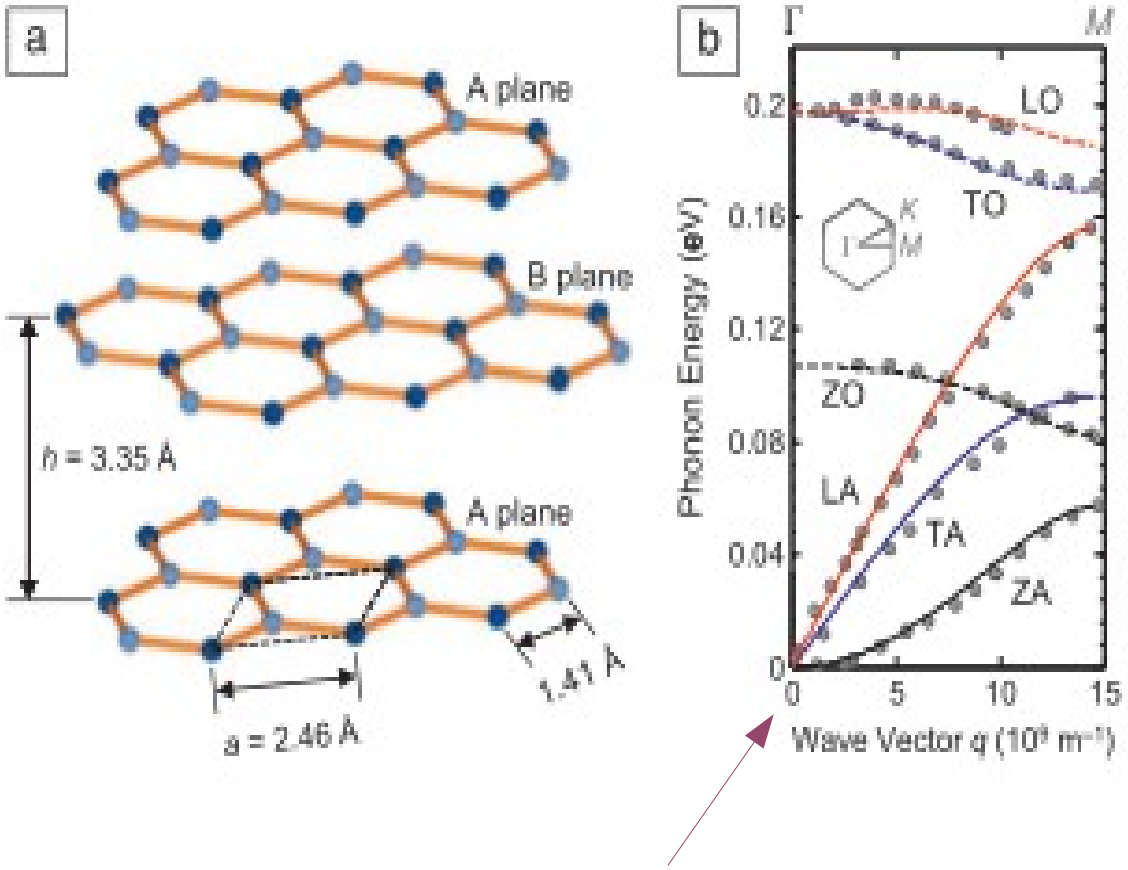
(b) Ge





Landry, phD thesis 2009

Phonon dispersion in graphene



2D material

$$g(\omega)=\frac{\omega}{v_{\varphi}(\omega)\,v_{g}(\omega)}$$

Bending modes dominant at low q

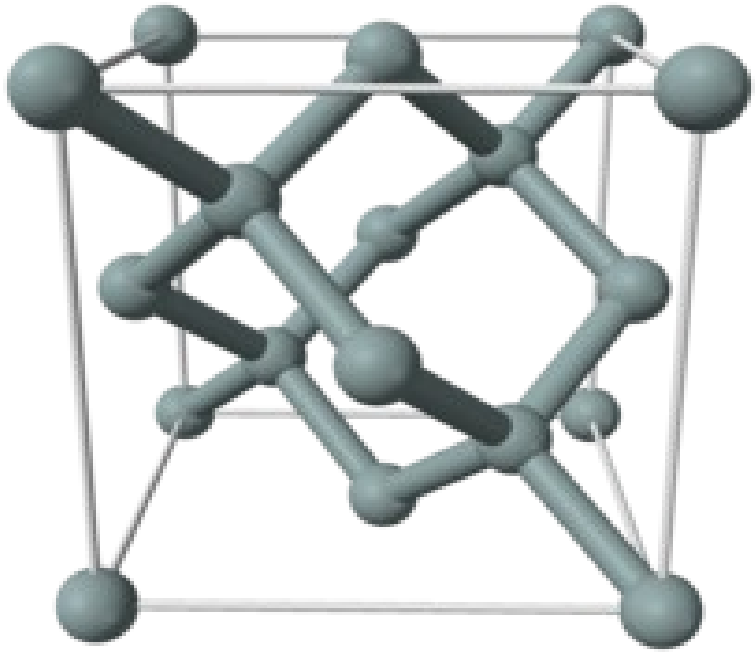
E. Pop, V. Varshney and A.K. Roy, MRS Bull., 37 (2012) 1273

Molecular dynamics

Molecular dynamics : $m\frac{d^2\vec{r}_i}{dt^2}=-\frac{\partial\Phi}{\partial\vec{r}_i}$ + thermal bath

Interatomic potential :

$$\Phi=\sum_{i<j}V_2(\vec{r}_{ij})+\sum_{i<j<k}V_3(\vec{r}_i,\vec{r}_j,\vec{r}_k)$$



Stilinger-Weber potential (Si) :

$$\Phi=\sum_i\sum_{i>j}\nu_1(r_{ij})+\sum_i\sum_{j\neq i}\sum_{k>j}\nu_2(r_{ij},r_{ik},\theta_{ijk})$$

$$\upsilon_1(r_{ij})=A\epsilon\left(B\left(\frac{\sigma}{r_{ii}}\right)^p-1\right)e^{\frac{\sigma}{r_{ij}-a\sigma}}$$

$$\upsilon_2(r_{ij},r_{ik},\theta_{ijk})=\lambda\epsilon\left(\cos\theta_{ijk}-\frac{1}{3}\right)^2 e^{\frac{\sigma\gamma}{r_{ij}-a\sigma}}e^{\frac{\sigma\gamma}{r_{ik}-a\sigma}}$$

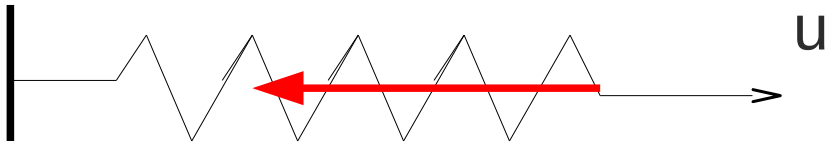
Dispersion from molecular dynamics

We use the property : $\Phi_{\alpha,\beta}(\vec{k}) = k_B T\, G^{-1}_{\alpha,\beta}(\vec{k})$

Harmonic force constants

Atomic displacement Green's function

F=-Hu



Equipartition : $H = \dfrac{k_B T}{\langle u^2 \rangle}$

$$\Phi_{\alpha,\beta}(\vec{k}) = \sum_j \Phi_{\alpha,\beta}(i,j) \exp\left(i\vec{k}\cdot(\vec{r}_i - \vec{r}_j)\right)$$

$$D_{\alpha,\beta}(\vec{k}) = \frac{1}{m}\Phi_{\alpha,\beta}(\vec{k})$$

$$G_{\alpha,\beta}(\vec{k}) = \langle u_\alpha(\vec{k})\, u^{cc}_\beta(\vec{k})\rangle$$

$$u_\alpha(\vec{k}) = \Sigma_i u_{\alpha,i} \exp\left(i\vec{k}\cdot\vec{r}_i\right)$$

$$G_{\alpha,\beta}(\vec{k}) = \langle r_\alpha(\vec{k})\, r^{cc}_\beta(\vec{k})\rangle - \langle r_\alpha(\vec{k})\rangle\langle r^{cc}_\beta(\vec{k})\rangle$$

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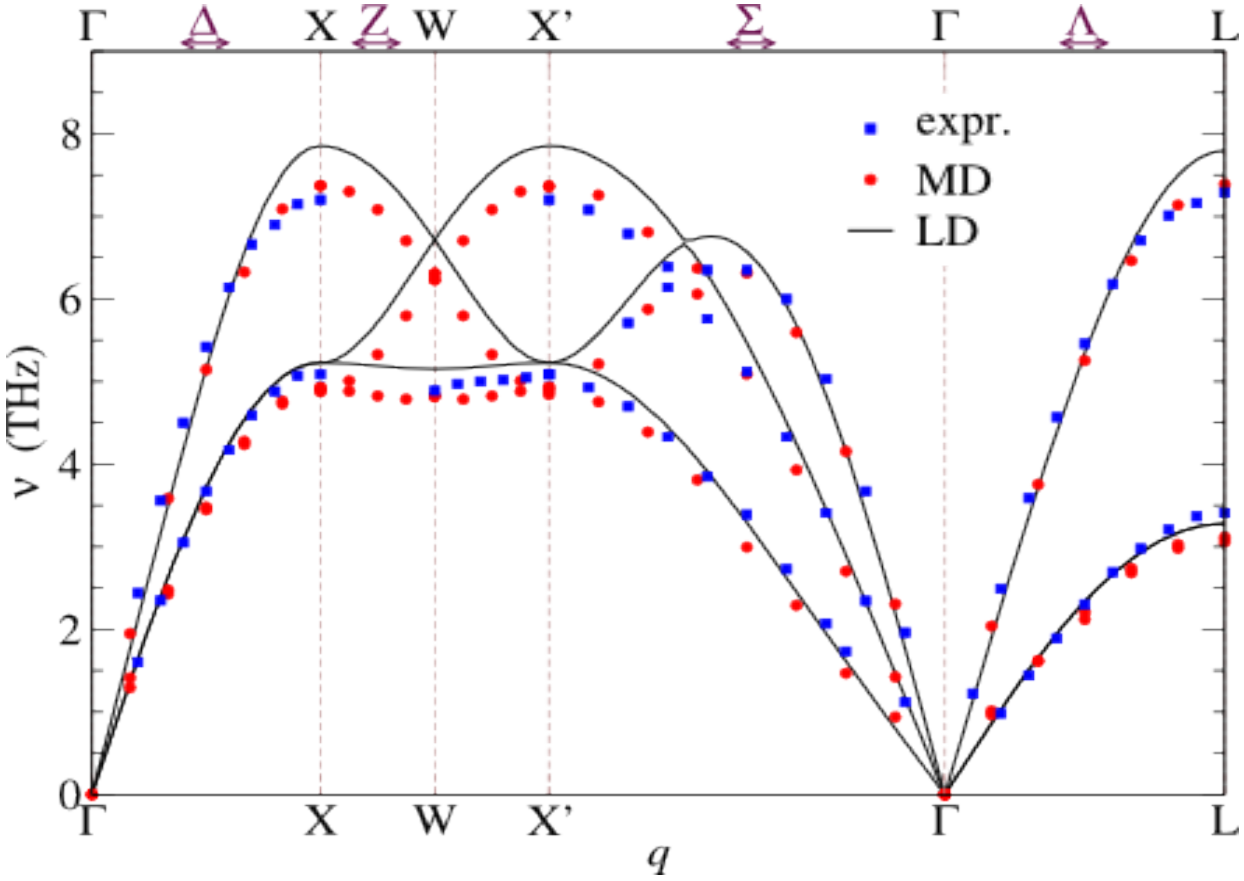
Phonon dispersion measured directly from molecular dynamics simulations ☆

Ling Ti Kong

School of Materials Science and Engineering, Shanghai Jiao Tong University, 800 Dongchuan Road, Minhang, Shanghai 200240, China

FCC Cu



Implemented in LAMMPS

« fix phonon« command

Vibrational density of states

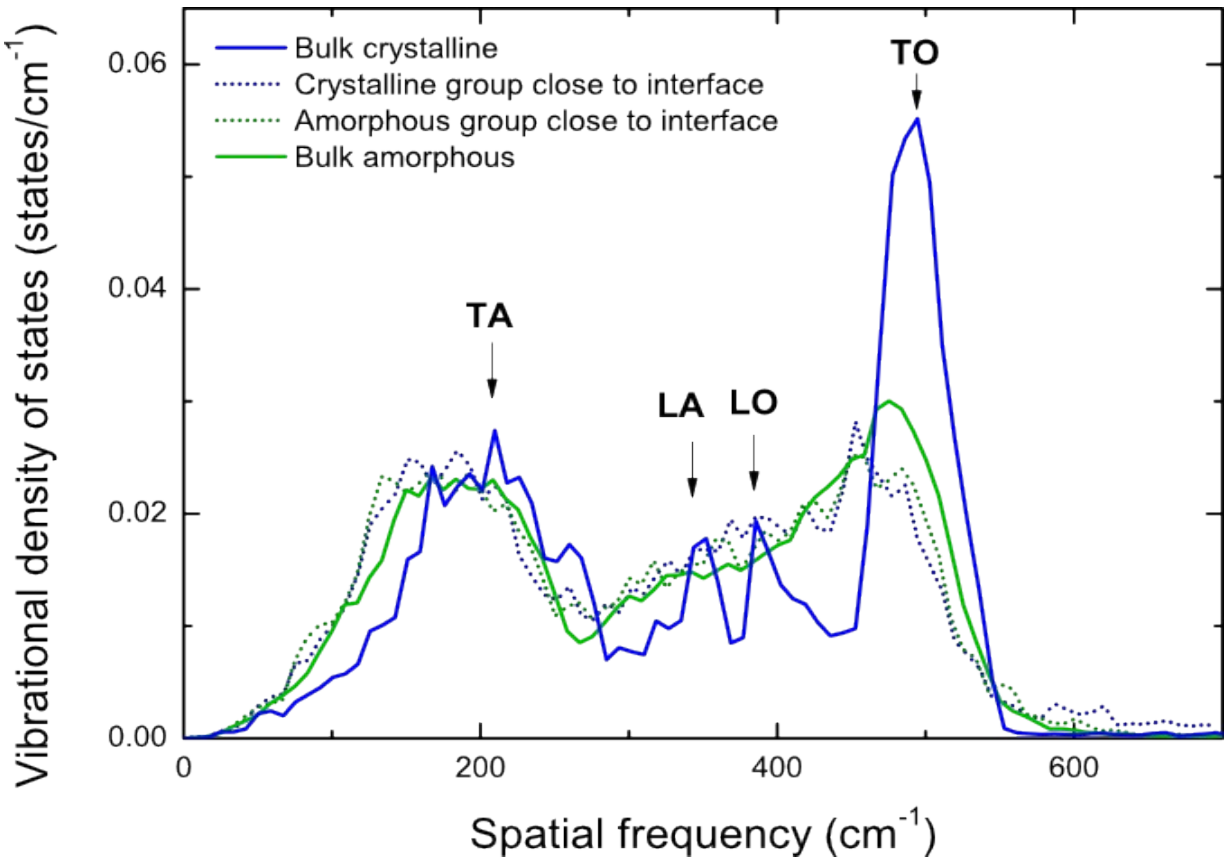
Definition $$g(\omega)=\frac{1}{V}\sum_k \delta(\omega-\omega_k)$$

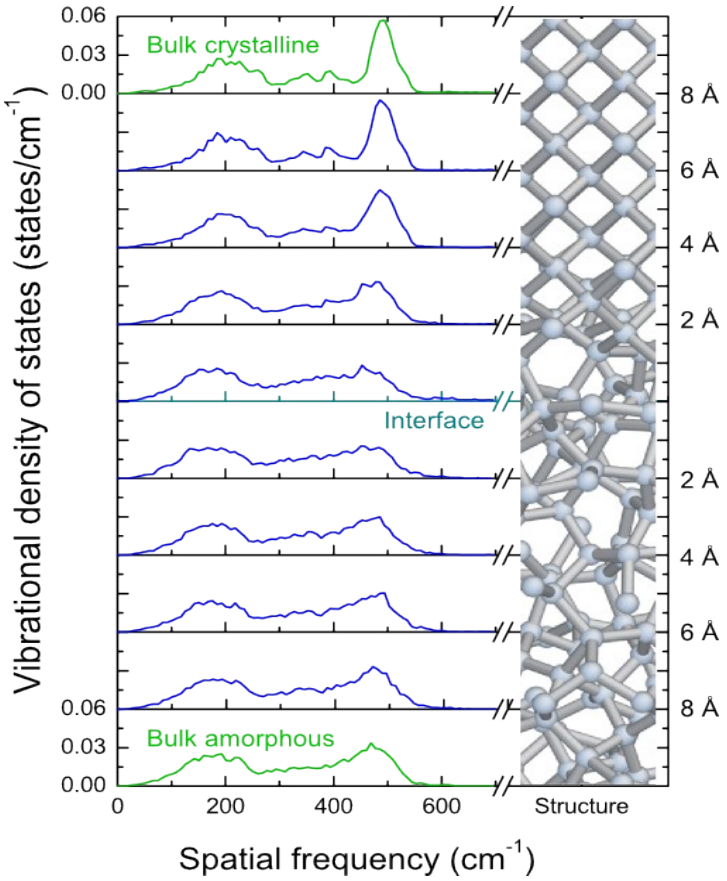
Identity $$g(\omega)\propto\int_0^{+\infty} C_{vv}(t)\exp(i\omega t)d\omega$$

$$C_{vv}(t)=\langle \vec{v}_i(t)\cdot\vec{v}_i(0)\rangle$$

See Dove « Introduction to lattice dynamics »

Silicon crystalline and amorphous





A. France-Lanord et al., *J.Phys. Cond. Mat.*, 2014

Thermal conductivity

Thermal conductivity

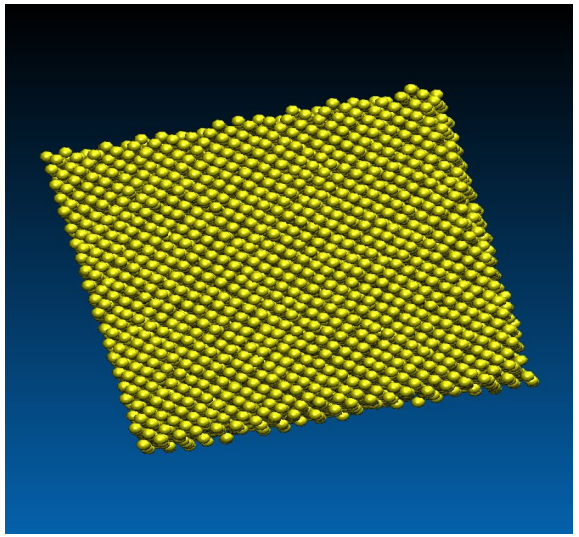
Essentially, two methods :

1. the « direct » method

Apply a temperature gradient or energy flux
and calculate the conductivity with Fourier law

2. equilibrium method

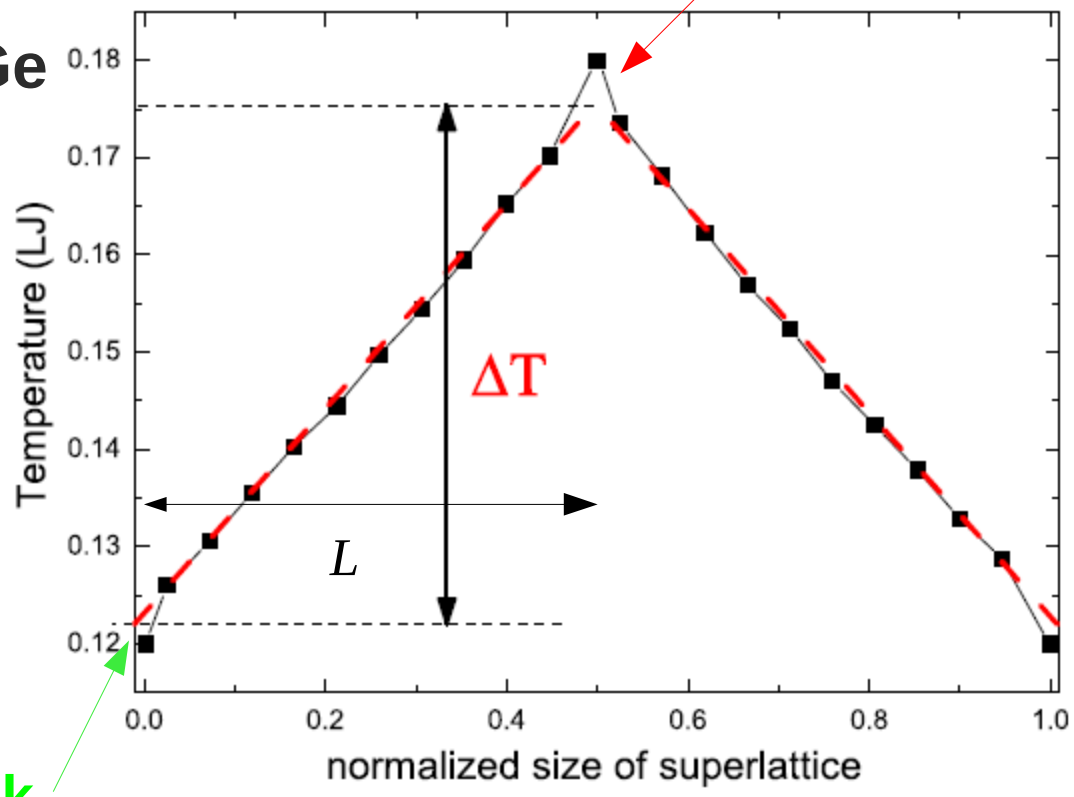
Probe the fluctuations around equilibrium
of the energy flux vector



1. Thermal conductivity : the direct method

Steady state temperature profile

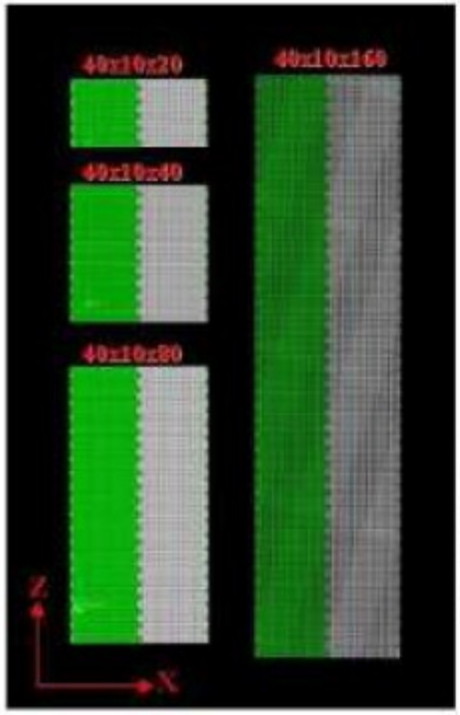
Example Si/Ge

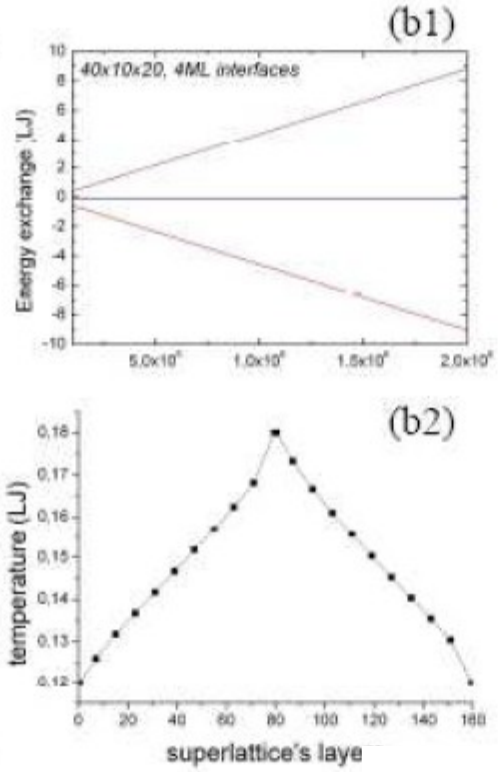


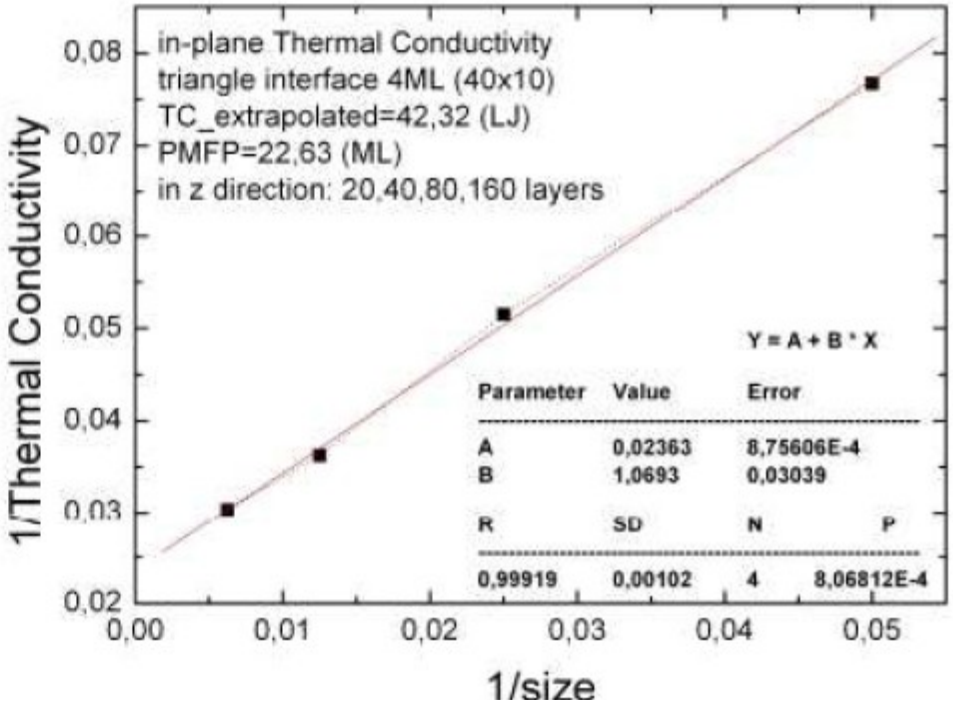
Fourier law : $$J = -\lambda \frac{\Delta T}{L}$$

Thermal conductivity : the direct method

Finite size effect analysis







« Bulk » thermal conductivity $1/\Lambda(L) = 2/L + 1/\Lambda(L \to \infty)$

Thermal conductivity : direct method

Advantages : - relatively easy to implement using open sources codes (LAMMPS)
-may be used also to compute the thermal boundary resistance

Inconvenients : -need to check if we are in the linear regime
=> analyze different heat fluxes
-severe finite size effects !
=> analyze different system sizes to properly extrapolate a « bulk » conductivity

Thermal conductivity : Green-Kubo equilibrium simulations

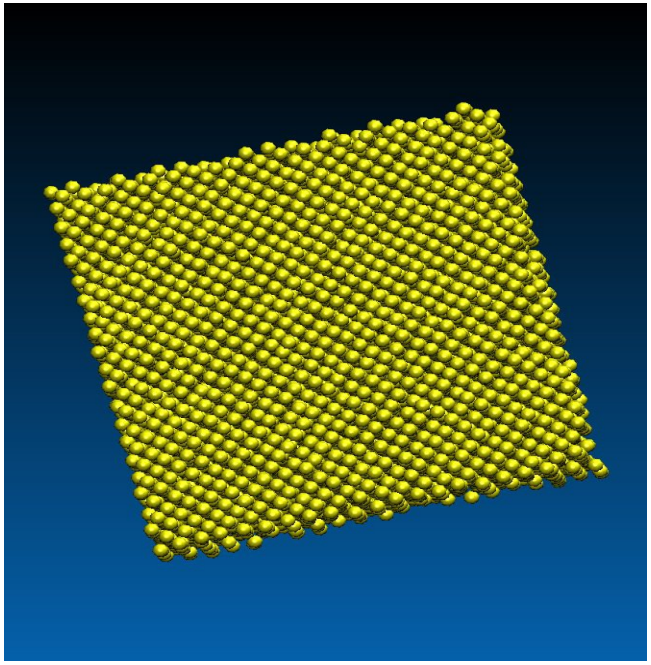
Green-Kubo formula :

$$\lambda_{\alpha,\beta} = \frac{1}{V k_B T^2} \int_0^{+\infty} \langle J_\alpha(t) J_\beta(0) \rangle \, dt$$

Heat flux vector : $\vec{J} = \frac{d}{dt}\left(\sum_i E_i \vec{r}_i\right)$

$$\vec{J} = \sum_i E_i \vec{v}_i + \frac{1}{2} \sum_{i \neq j} \vec{F}_{ij} \cdot (\vec{v}_i + \vec{v}_j)$$

In practice, run in NVE ensemble



Thermal conductivity : Green-Kubo equilibrium simulations

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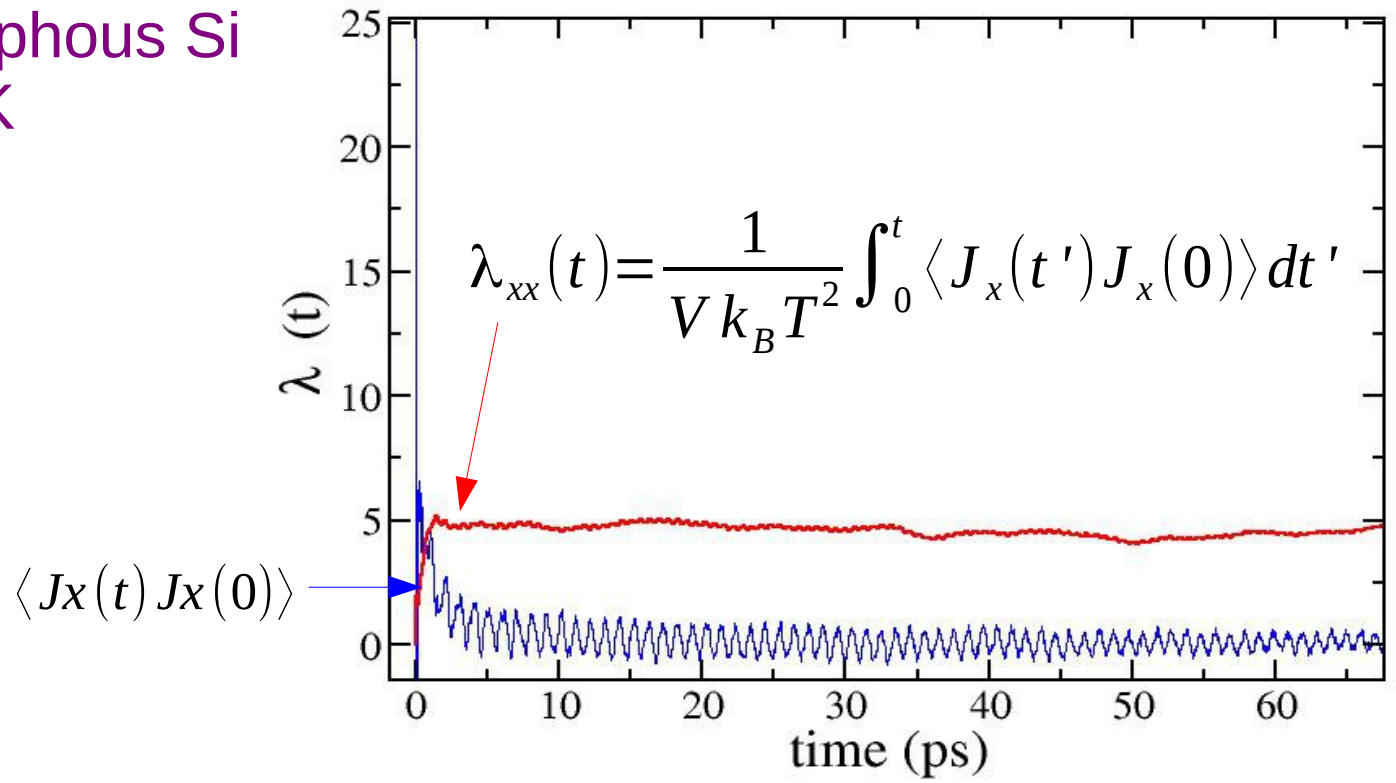
Example amorphous Si
300 K



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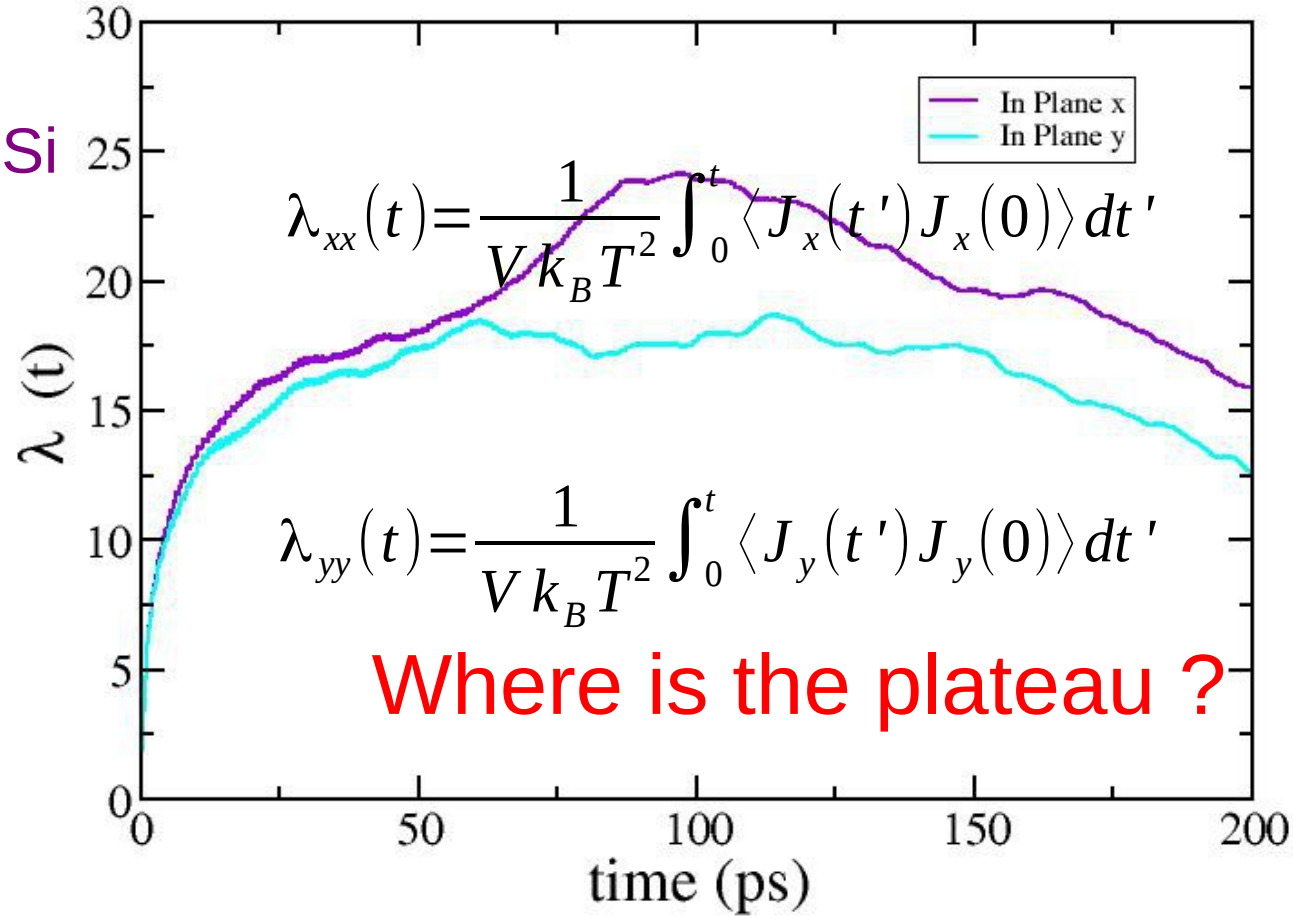
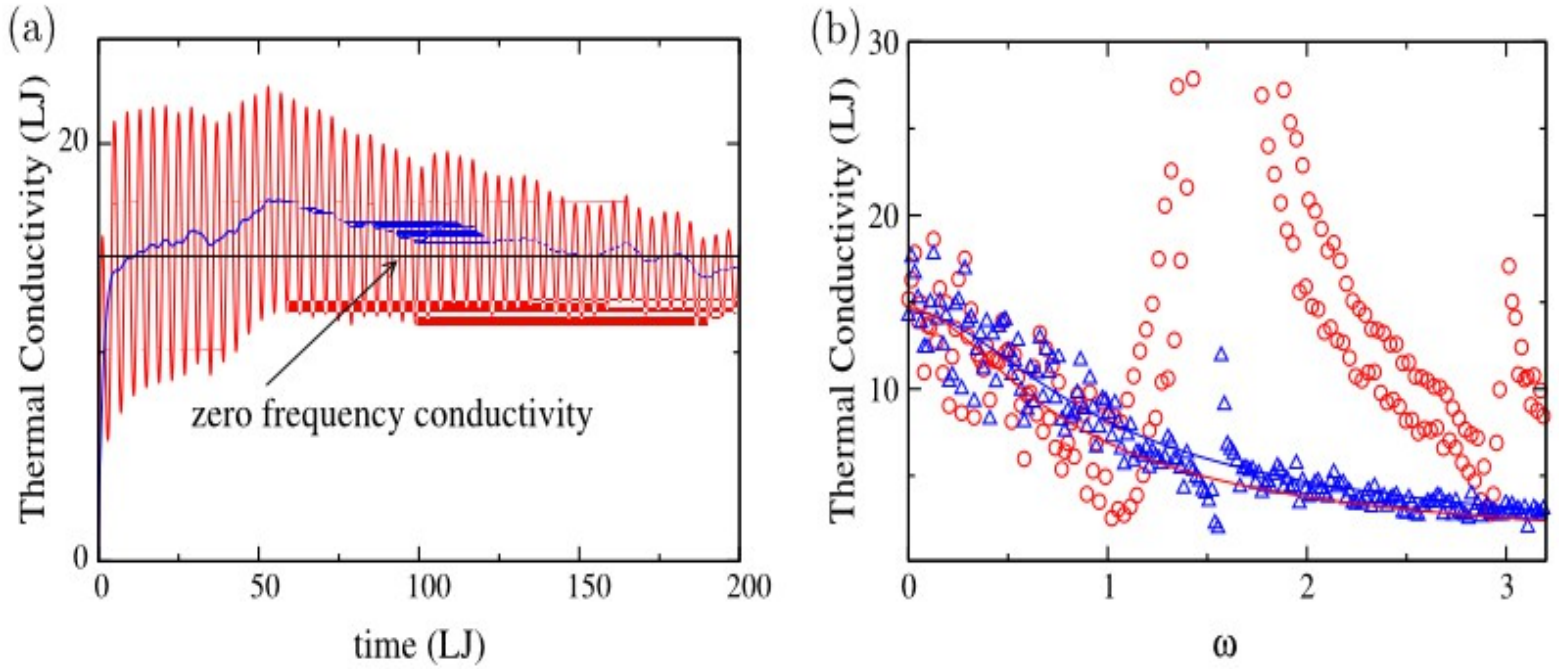
$$\lambda_{\alpha,\beta} = \frac{1}{V k_B T^2} \int_0^{+\infty} \langle J_\alpha(t) J_\beta(0) \rangle \, dt$$

Example amorphous Si
300 K



Optical modes



$$\lambda(\omega) = \frac{1}{V k_B T^2} \int_0^\infty \langle J(t) J(0) \rangle \exp(i \omega t) dt$$

Termentzidis, SM, Chantrenne IJHMT 2011

Thermal conductivity : Green-Kubo equilibrium simulations

Advantages : - less severe finite size effects

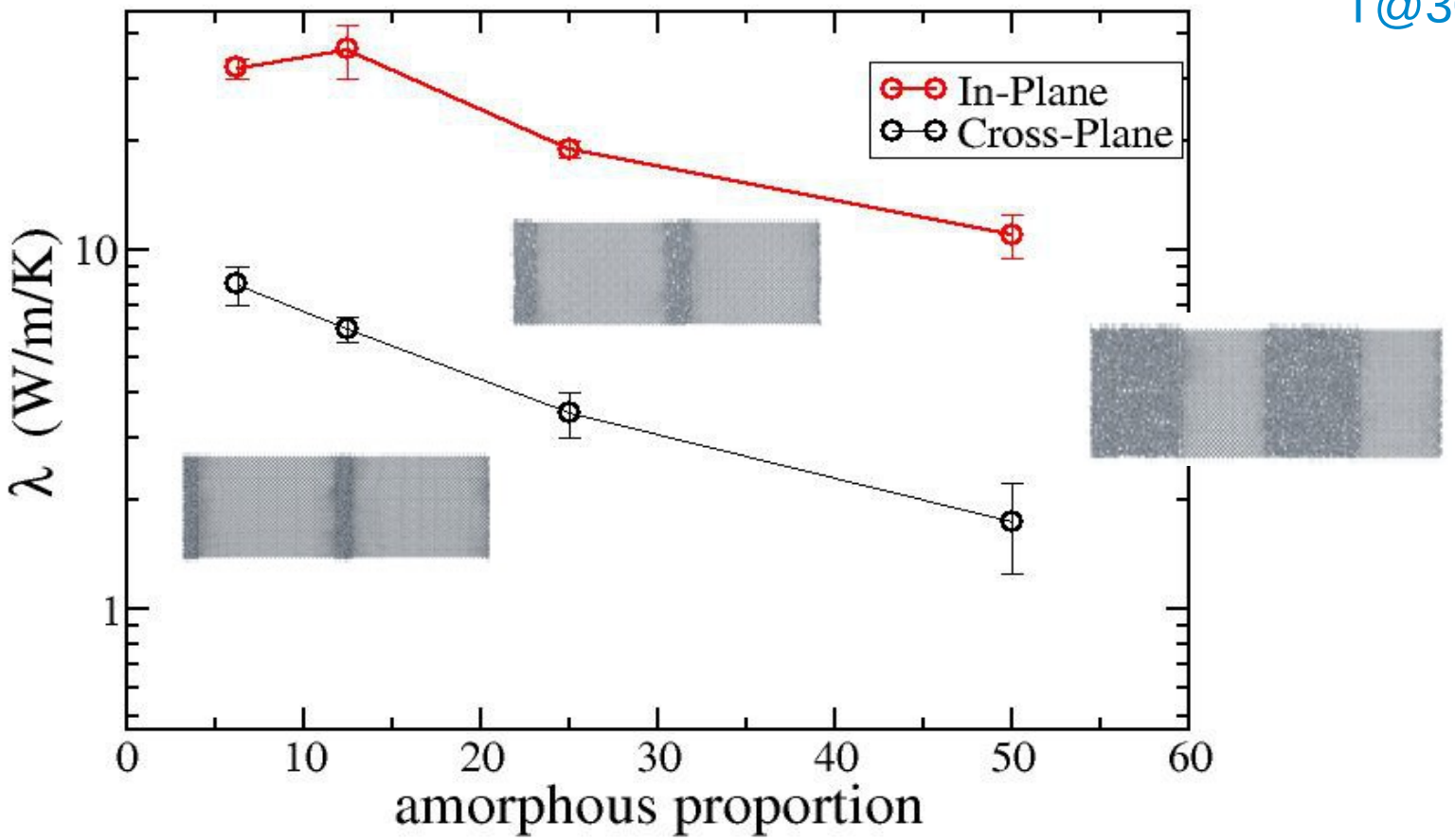
- access to the full thermal conductivity tensor in a single simulation (anisotropic materials, superlattices)

Inconvenients : -need to run several independent simulations (usually 10 to 20)

-the plateau is sometimes difficult to identity (in principle, in a finite system the Green-Kubo formula should give a vanishing conductivity ...)

Thermal anisotropy

T@300 K



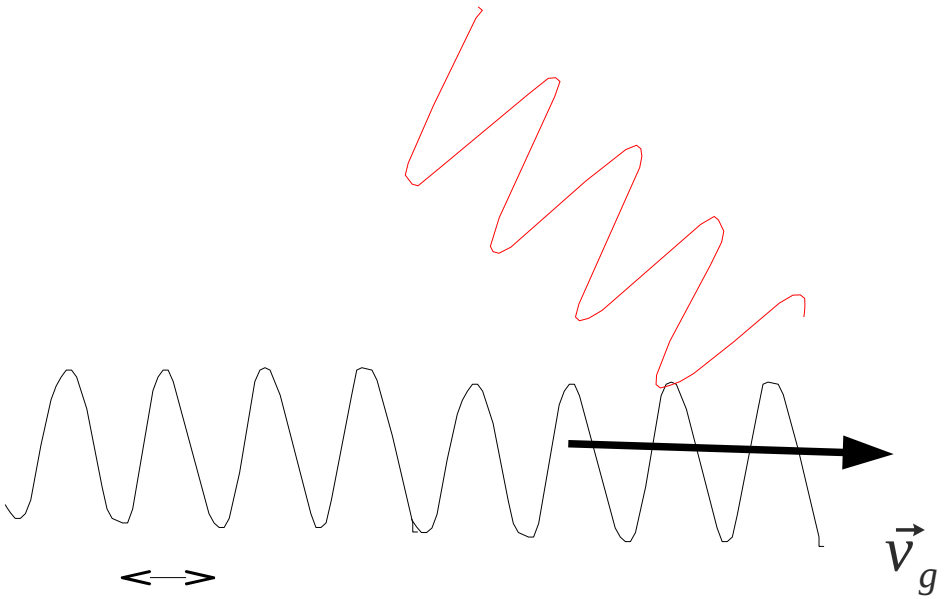
A.F. Lannord, SM, T. Albaret, D. Lacroix, K. Termentzidis, 2014

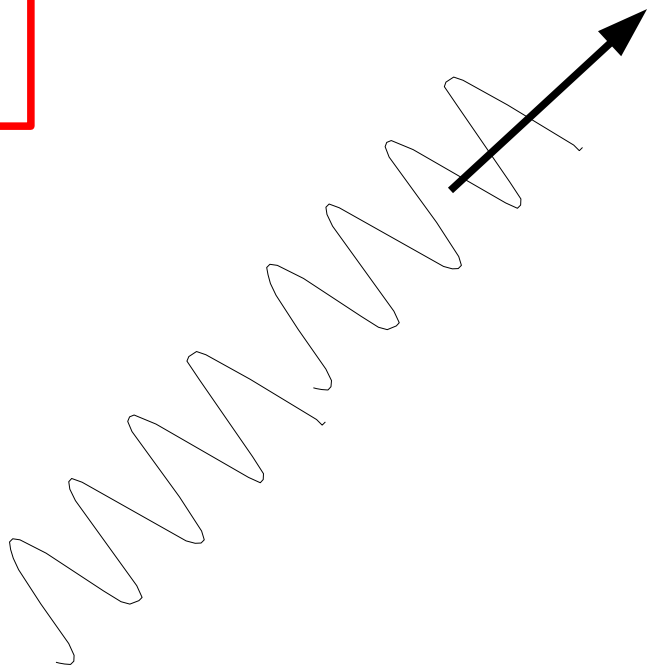
Thermal conductivity

Kinetic formula : $\lambda = \frac{1}{3} \Sigma_{\vec{k}} c_v v_g \Lambda_{\vec{k}}$

Phonon lifetime $\tau(\omega)$

Mean Free path $\Lambda(\omega) = v_g \tau(\omega)$





$\Lambda(\omega)$

Thermal conductivity

Local phonon occupation number : $n \equiv n(\vec{k}, s, \vec{r}, t)$

Boltzmann transport equation : $\frac{\partial n}{\partial t} + \vec{v}_g \cdot \vec{\nabla} n = \left(\frac{\partial n}{\partial t} \right)_{coll}$

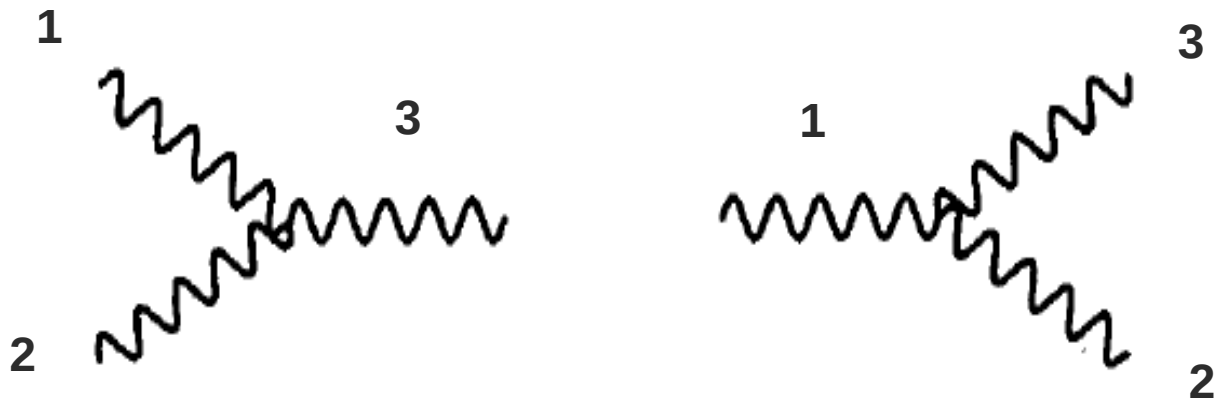
Single relaxation time approximation : $\frac{\partial n}{\partial t} + \vec{v}_g \cdot \vec{\nabla} n = -\frac{(n - n_{eq})}{\tau(\vec{k}, s)}$

Thermal conductivity : $\lambda = \frac{\rho}{3} \int_0^{\omega_{max}} g(\omega) C_v(\omega) v_g^2(\omega) \tau(\omega) d\omega$

$$\lambda = \frac{1}{3} \Sigma_{\vec{k}} c_v v_g \Lambda_{\vec{k}}$$

Mean free path $\Lambda(\omega) = v_g \tau(\omega)$

Relaxation times : phonon-phonon scattering



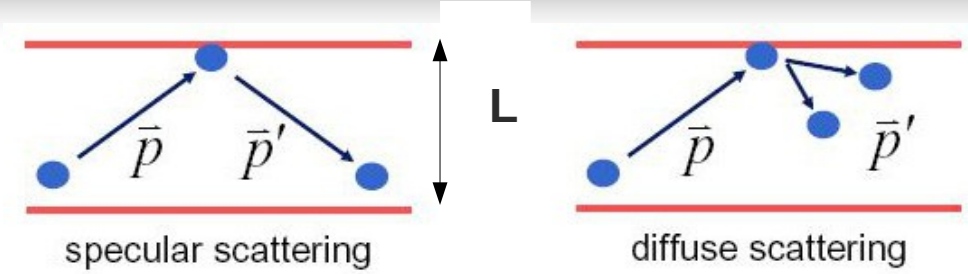
Three phonons Umklapp processes : $\tau^{-1}(\omega,T)=A\,\omega^2 T\exp(-B/T)$

Klemens formula $\tau^{-1}(\omega,T)=\gamma^2\frac{k_B T}{Mv^2}\frac{\omega^2}{\omega_D^2}$

P.G. Klemens, « Solid State Physics » Academic Press New-York 1958

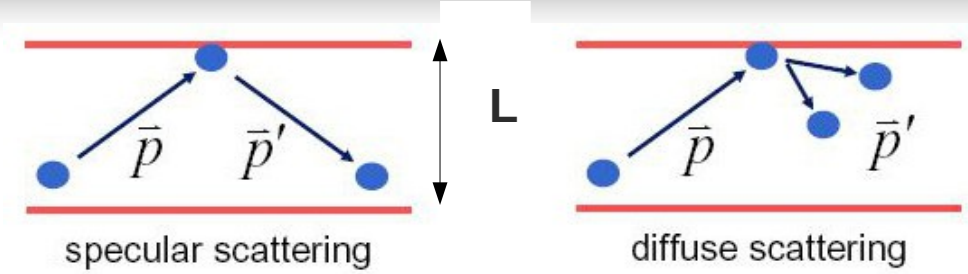
Other relaxation mechanisms

Boundary scattering $\tau_b = \frac{v}{L}$

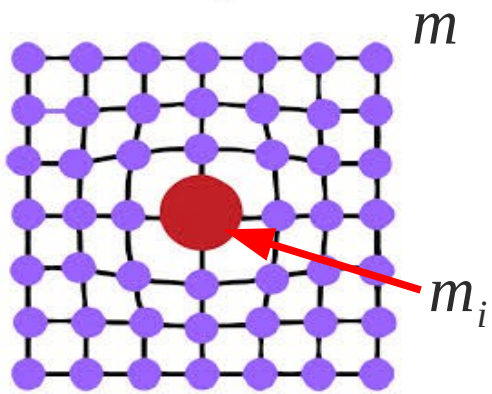


Other relaxation mechanisms

Boundary scattering $\tau_b = \frac{v}{L}$

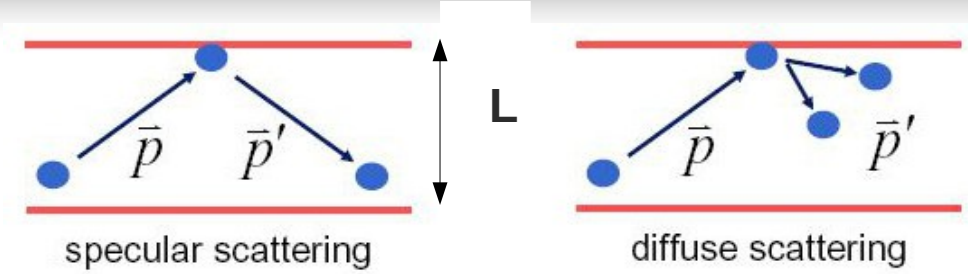


Point defects $\tau_m^{-1} = V\left(\frac{m_i - m}{m}\right)^2 \frac{\omega^4}{4\pi v^3}$



Other relaxation mechanisms

Boundary scattering $\tau_b = \frac{v}{L}$



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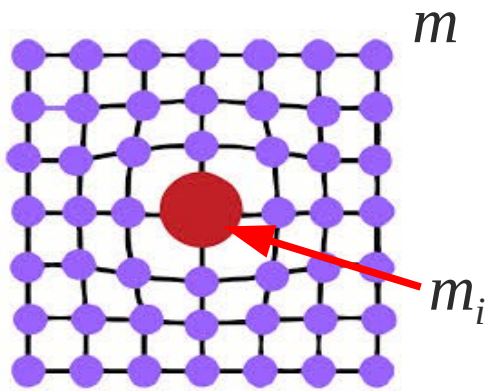
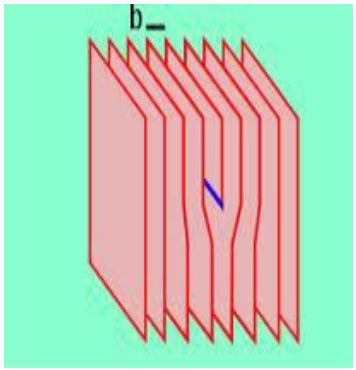


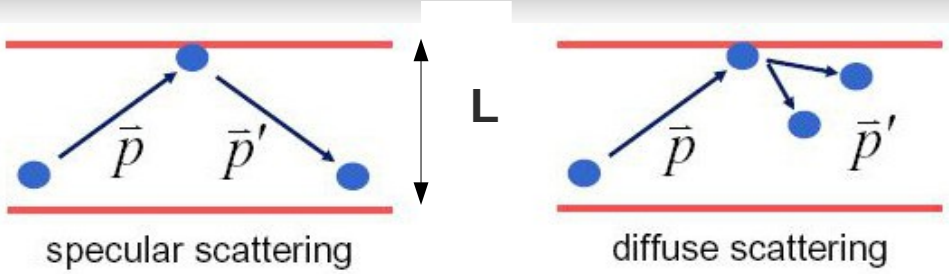
Dislocations $\tau_d^{-1} = N_d b^2 \omega$



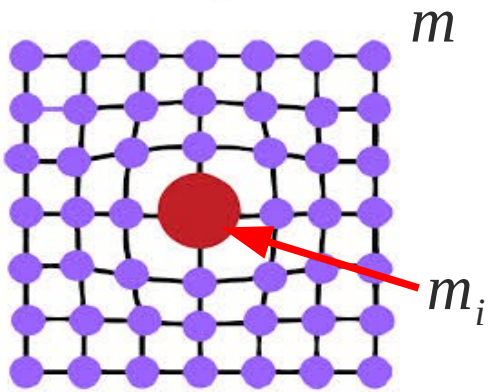
number of dislocation lines per unit area

Other relaxation mechanisms

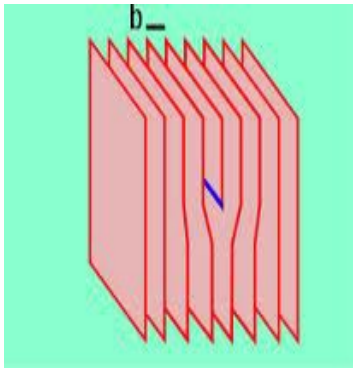
Boundary scattering $\tau_b = \frac{v}{L}$



Point defects $\tau_m^{-1} = V\left(\frac{m_i - m}{m}\right)^2 \frac{\omega^4}{4\pi v^3}$

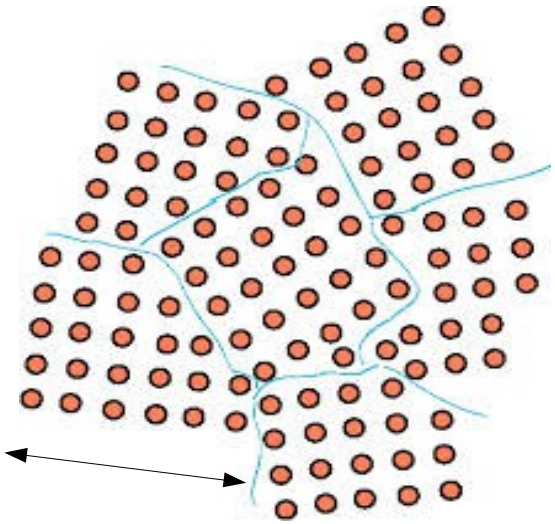


Dislocations $\tau_d^{-1} = N_d b^2 \omega$



number of dislocation lines per unit area

Grain boundaries $\tau_g \simeq \frac{v}{d}$



Thermal conductivity

Matthiessen's rule

$$\frac{1}{\tau}=\frac{1}{\tau_{3\,ph}}+\frac{1}{\tau_b}+\frac{1}{\tau_m}+\frac{1}{\tau_d}+\frac{1}{\tau_g}$$

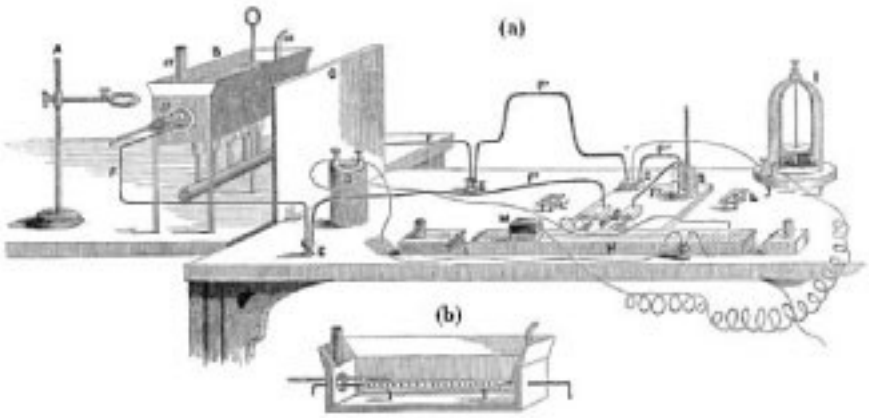
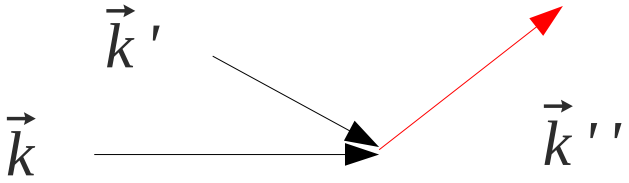
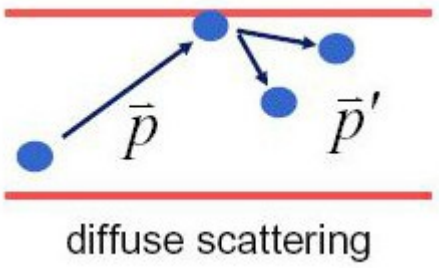
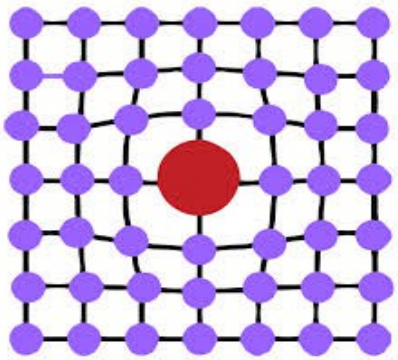
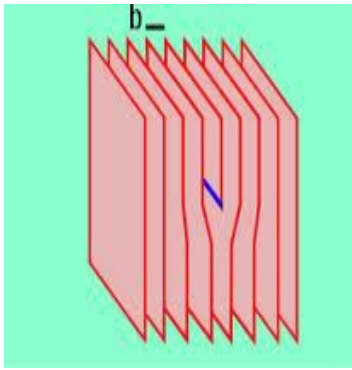


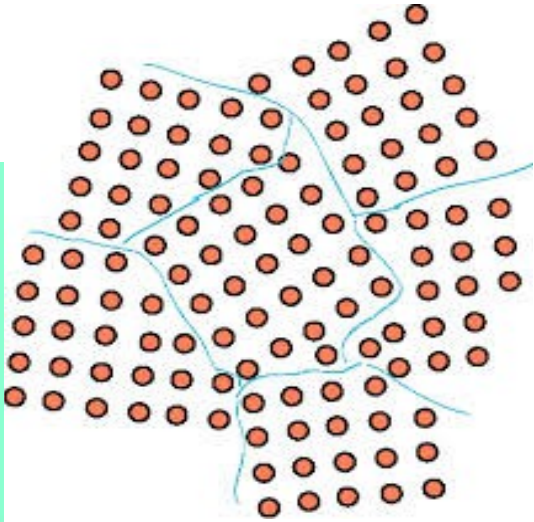
Figure 7 – Matthiessen's apparatus. Credit: Ref. [32].



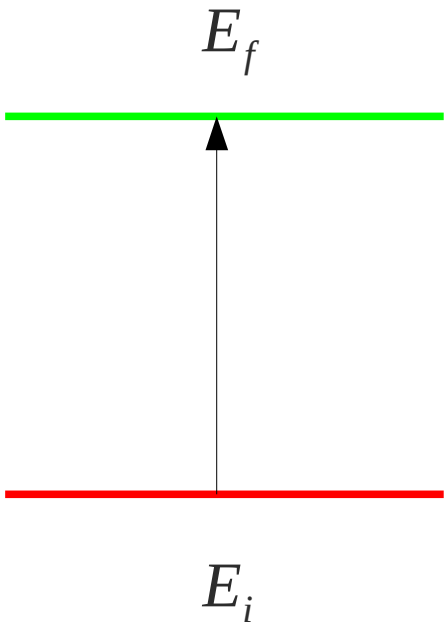








Phonon-phonon scattering :Perturbation theory

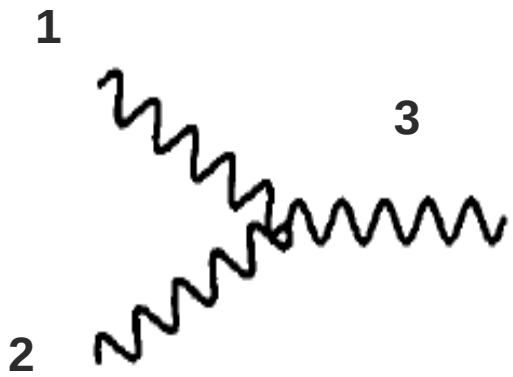


Hamiltonian :

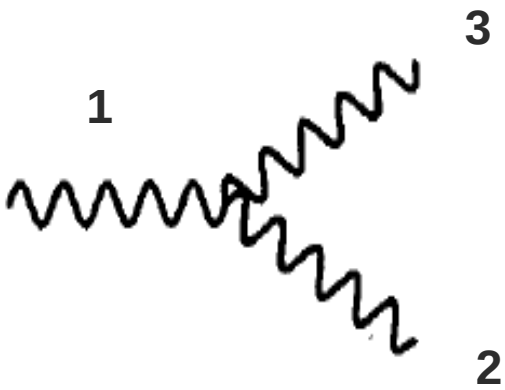
$$H = H_0 + H'$$

$$P_i^f = \frac{2\pi}{\hbar} |\langle i|H'|f\rangle|^2 \rho(E_i)\delta(E_f - E_i)$$

E. Fermi



Initial state Final state



Initial state Final state

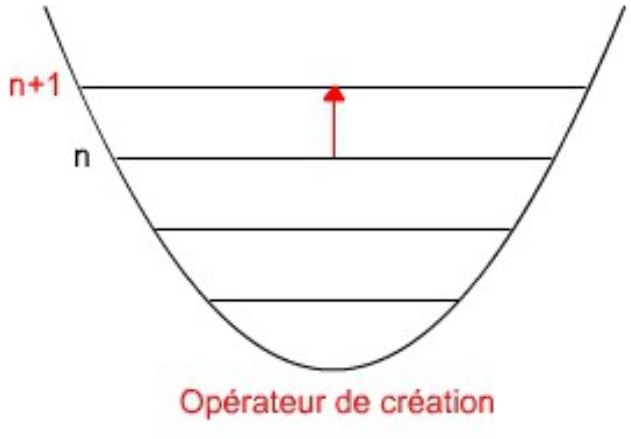
Thermal conductivity : perturbation Hamiltonian

Reference Hamiltonian : (harmonic crystal)

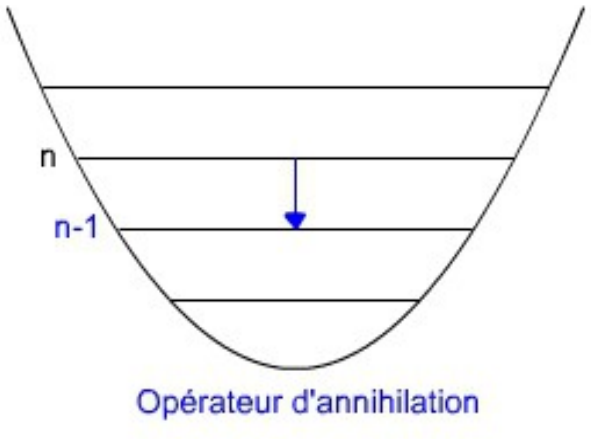
$$H_0 = \frac{1}{2}\sum_{i,j,\alpha,\beta} \Phi_{ij}^{\alpha,\beta} u_{i,\alpha} u_{j,\beta}$$

$$H_0 = \sum_{\vec{k},s} \hbar\omega(\vec{k},s)\left(\hat{a}^{+}(\vec{k},s)\hat{a}(\vec{k},s) + \frac{1}{2}\right)$$

operator $\hat{a}^{+}$



operator $\hat{a}$



Thermal conductivity : perturbation Hamiltonian

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$$H_0 = \sum_{\vec{k},s} \hbar \omega(\vec{k},s) \left(\hat{a}^{+}(\vec{k},s) \hat{a}(\vec{k},s) + \frac{1}{2} \right)$$

Perturbation Hamiltonian :

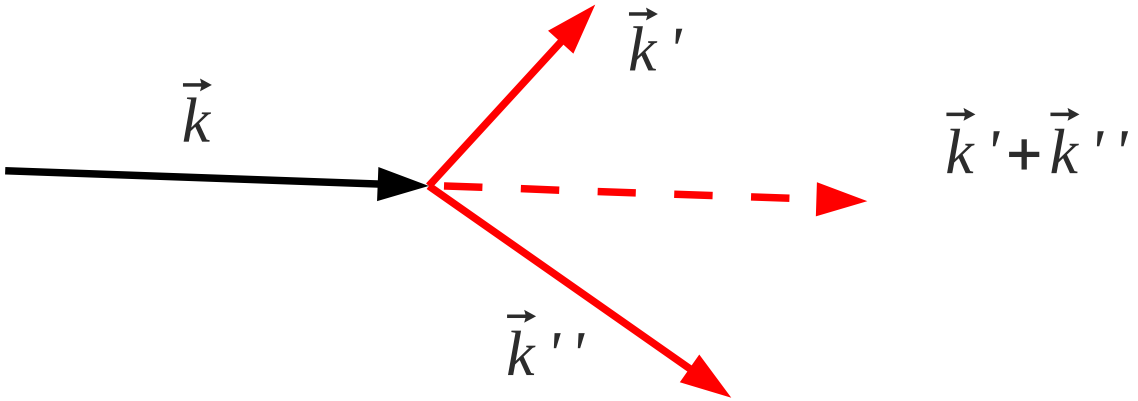
$$H' = \frac{1}{6} \sum_{i,j,k,\alpha,\beta,\gamma} X_{ijk}^{\alpha,\beta,\gamma} u_{i,\alpha} u_{j,\beta} u_{k,\gamma}$$

$$H' = \Sigma_{\vec{k},s,\vec{k}',s',\vec{k}'',s''} \delta_{\vec{G},\vec{k}+\vec{k}'+\vec{k}''} V(\vec{k},s,\vec{k}',s',\vec{k}'',s'')$$
$$(\hat{a}^{+}(\vec{k},s) - \hat{a}(-\vec{k},s))(\hat{a}^{+}(\vec{k}',s') - \hat{a}(-\vec{k}',s'))(\hat{a}^{+}(\vec{k}'',s'') - \hat{a}(-\vec{k}'',s''))$$

$\vec{G}$: Reciprocal lattice vector

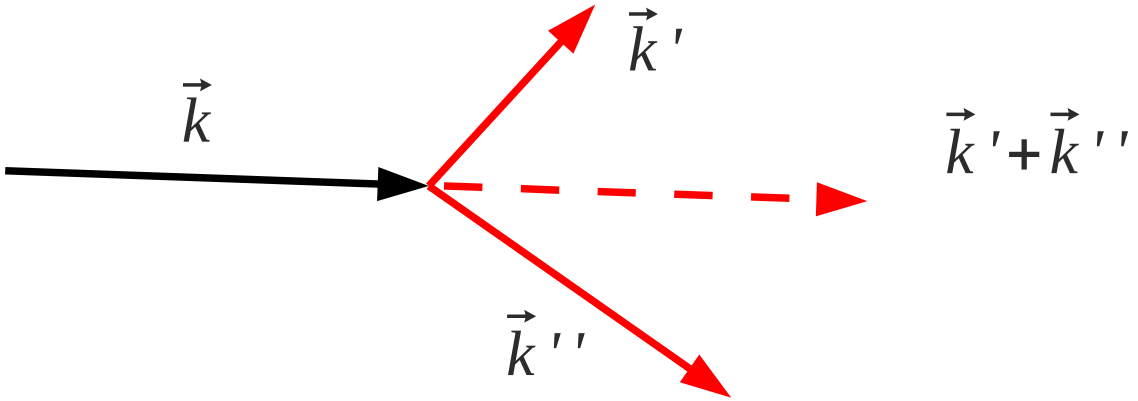
Momentum (non) conservation

Normal processes $\vec{k} = \vec{k}' + \vec{k}$

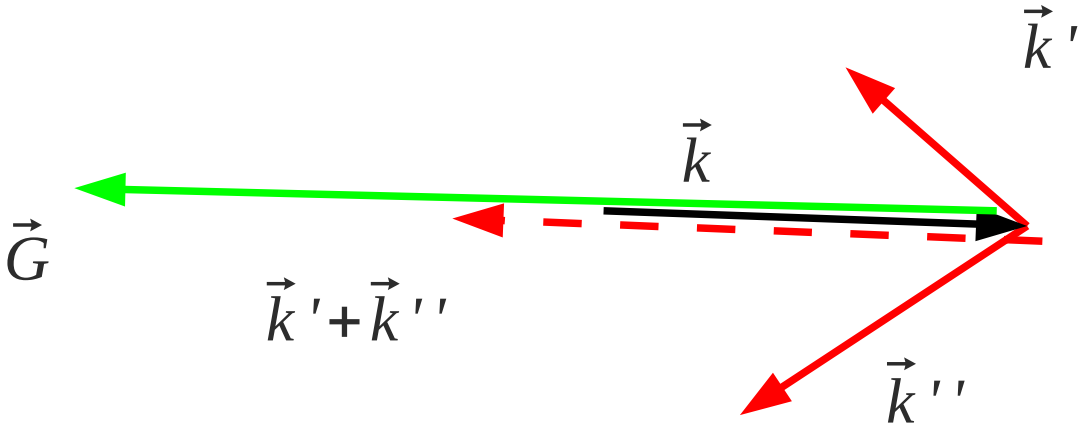


Momentum (non) conservation

Normal processes $\vec{k} = \vec{k}' + \vec{k}$



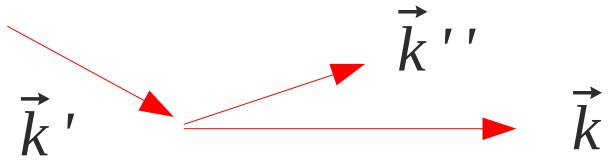
Umklapp processes $\vec{k} = \vec{k}' + \vec{k}'' + \vec{G}$



Three phonon processes

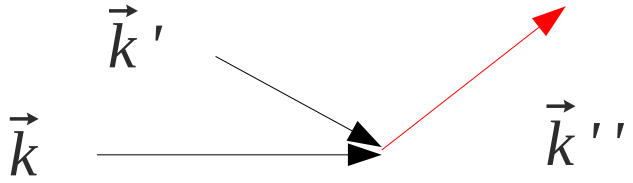
$\hat{a}^{+}(\vec{k})\hat{a}^{+}(\vec{k}')\hat{a}^{+}(\vec{k}'')$

Simultaneous creation of three phonons



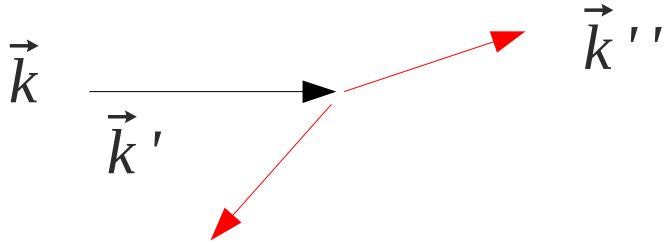
$\hat{a}^{+}(\vec{k})\hat{a}^{+}(\vec{k}')\hat{a}(\vec{k}'')$

Destruction of two phonons and creation of one phonon



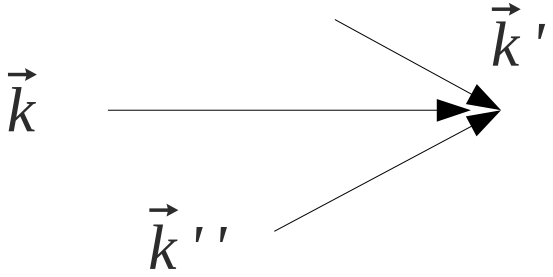
$\hat{a}^{+}(\vec{k})\hat{a}(\vec{k}')\hat{a}(\vec{k}'')$

Destruction of one phonon and creation of two phonons



$\hat{a}(\vec{k})\hat{a}(\vec{k}')\hat{a}(\vec{k}'')$

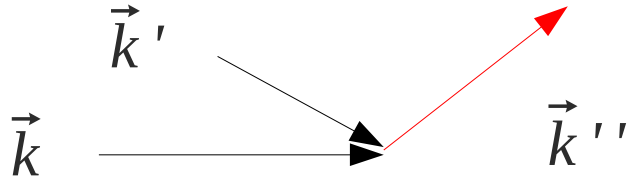
Simultaneous destruction of three phonons



Three phonon processes

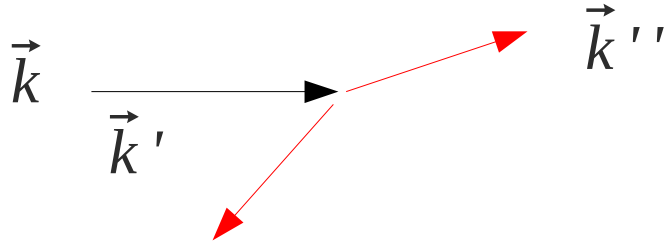
$\hat{a}^{+}(\vec{k})\hat{a}^{+}(\vec{k}')\hat{a}(\vec{k}'')$

Destruction of two phonons and creation of one phonon



$\hat{a}^{+}(\vec{k})\hat{a}(\vec{k}')\hat{a}(\vec{k}'')$

Destruction of one phonon and creation of two phonons



Only these processses do not violate energy conservation !!

Single relaxation time

Class 1 events : $$\frac{1}{\tau(\vec{k})} = \Sigma^{\vec{G}}_{\vec{k}',\vec{k}''} |\gamma|^2 n'_{eq} \frac{(n''_{eq}+1)}{(n_{eq}+1)} \delta(\omega+\omega'-\omega'')$$

Single relaxation time

Class 1 events : $$\frac{1}{\tau(\vec{k})} = \Sigma^{\vec{G}}_{\vec{k}',\vec{k}''} |\gamma|^2 n'_{eq} \frac{(n''_{eq}+1)}{(n_{eq}+1)} \delta(\omega+\omega'-\omega'')$$

High temperature regime : $n'_{eq} \simeq \frac{k_B T}{\hbar \omega'}$ $n_{eq}+1 \simeq \frac{k_B T}{\hbar \omega'}$

$$\frac{1}{\tau(\vec{k})} = k_B T \Sigma^{\vec{G}}_{\vec{k}',\vec{k}''} |\gamma|^2 \frac{\omega}{\omega'\omega''} \delta(\omega+\omega'-\omega'')$$

Difficult to estimate because Dispersion : $\omega' \equiv \omega'(\vec{k}')$

Crystal anisotropy : $\omega' \neq \omega'(|\vec{k}'|)$

Polarisation : $\vec{k}' \equiv (\vec{k}', s)$

Some references

Isotropic crystal, no polarisation

P.G. Klemens, « Solid State Physics » Academic Press New-York 1958

J. Callaway, « Model for lattice thermal conductivity at low temperatures », Phys. Rev. 1958

Effect of the crystal anisotropy

C. Herring, « Role of low-energy phonons in thermal conduction », Phys. Rev. 1954

Effect of the normal processes :

P. Carruthers,
« Theory of thermal conductivity of solids at low temperatures »
Rev. Mod. Phys. 1961

Effect of the polarisation

M.G. Holland, « Analysis of lattice thermal conductivity », Phys. Rev. 1963

'Exact' model for a model crystal

A.A. Maradudin and A.E. Fein,
« Scattering of neutrons by an anharmonic crystal »,
Phys. Rev., 1962

Phonon spectroscopy

Phonon lifetimes

Thermal conductivity :
(single relaxation time approximation)

$$\lambda = \sum_{\vec{k},\nu} c_\nu(\vec{k},\nu)\, v_g(\vec{k},\nu)\, \Lambda(\vec{k},\nu)$$

Phonon mean free path : $\Lambda(\vec{k},\nu) = |\vec{v}_g(\vec{k},\nu)|\,\tau(\vec{k},\nu)$

Importance to calculate the phonon lifetimes :
-understand the physical mechanisms at play in Umklapp and/or normal process
-use the phonon lifetimes in a Monte-Carlo simulation based on the solution of Boltzmann's equation :

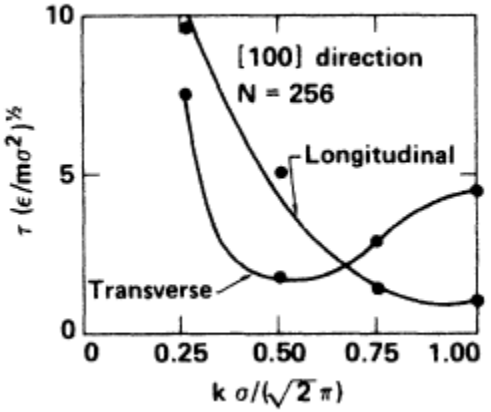
$$\frac{\partial f(\vec{k},\nu)}{\partial t} + \vec{v}_g \cdot \vec{\nabla} f(\vec{k},\nu) = -\frac{f - f_{eq}(\vec{k},\nu)}{\tau(\vec{k},\nu)}$$

allows large scale simulations-> nanowires, superlattices ...

Phonon lifetimes : some elements of history

First computation of phonon lifetimes in MD goes back to 1986 !

Ladd, Moran and Hoover,
Phys. Rev. B, 34 (1986) 5058



Small system sizes => limited range of k values, but this idea was there

Phonon lifetimes : some elements of history

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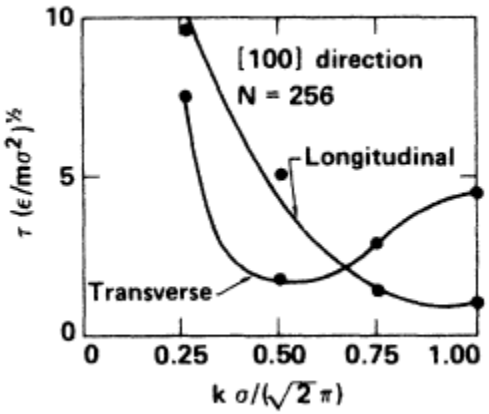
Ladd, Moran and Hoover,
Phys. Rev. B, 34 (1986) 5058



Small system sizes => limited range of k values, but this idea was there

Until 2004....almost nothing .... !
McGaughey, Kaviany, *Phys. Rev. B* 69 (2004) 094303

Since then, considerable amount of work to describe :
-silicon (Henry and Chen, *J. Comp. Theo. Nanores.*, 2008)
-alloys (Larkin and Mcgaughey, *J. App. Phys.* 114 (2013) 023507)
-amorphous solids (He, Donadio, Galli, *App. Phys. Lett.*, 98 (2011)144101
-polymers (Henry and Chen, *Phys. Rev. B* 79 (2009) 144305)

Phonon lifetimes

How to put it in practice ?

1. Determine the harmonic frequencies and eigenvectors :

$$\omega^2(\vec{k})\vec{e}(\vec{k}) = D(\vec{k})\cdot\vec{e}(\vec{k})$$ dynamic matrix

2. Run MD simulations and compute the normal coordinates :

$$Q(\vec{k},t) = \Sigma_i \left(\frac{m_i}{N}\right)^{(1/2)} \exp\left(i\vec{k}\cdot r_i^0\right)\vec{e}_i(\vec{k})\vec{u}_i(t)$$

3. Calculate the kinetic and potential energies :

$$T(\vec{k},t) = \frac{1}{2}\frac{dQ}{dt}(\vec{k})\frac{dQ}{dt}(-\vec{k})$$

$$U(\vec{k},t) = \frac{1}{2}\omega^2(\vec{k})Q(\vec{k})Q(-\vec{k})$$

$$E(\vec{k},t) = T(\vec{k},t) + U(\vec{k},t)$$

$$\tau(\vec{k}) = \int_0^\infty \frac{\langle E(\vec{k},t)E(\vec{k},0)\rangle}{\langle E(\vec{k},t)^2\rangle}dt$$

But this route doesnot give access to the anharmonic frequencies $\omega_a(\vec{k})$!!

Phonon lifetimes

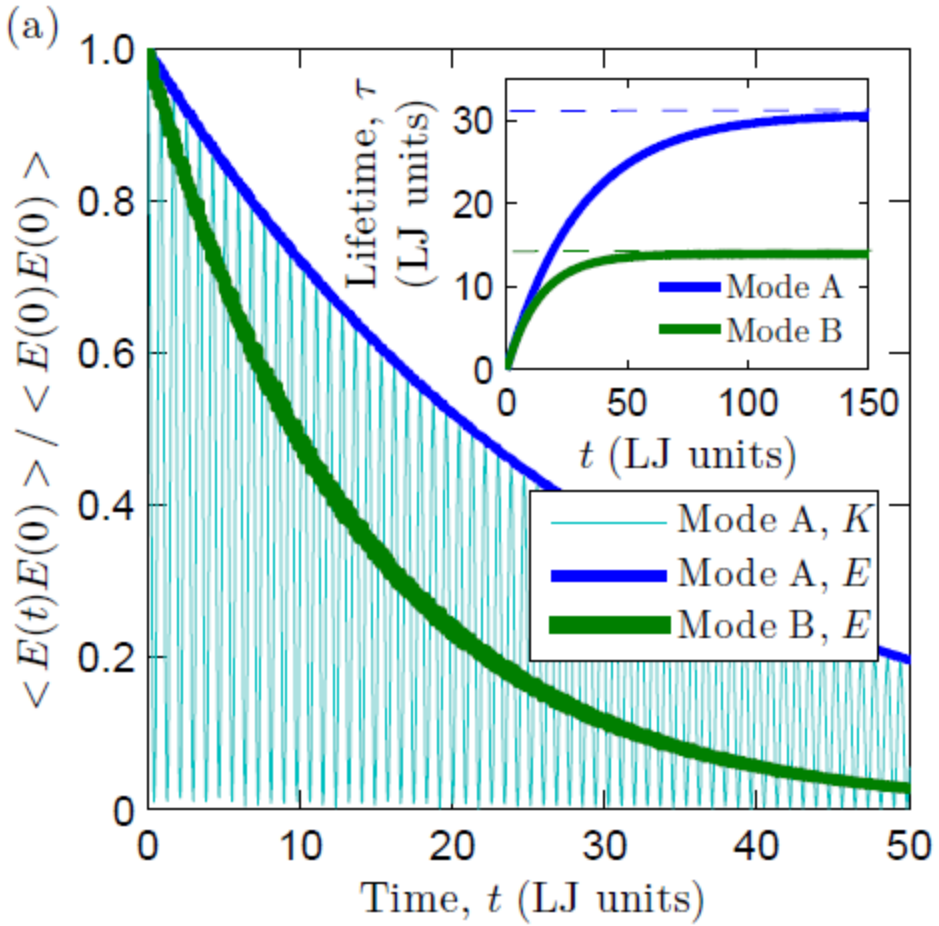
How to extract the phonon lifetime of mode k ?

$$\frac{\langle T(\vec{k},t)T(\vec{k},0)\rangle}{\langle T^2(\vec{k},t)\rangle} = \cos^2(\omega_a(\vec{k})t)\exp(-t/\tau(\vec{k}))$$

$$\frac{\langle E(\vec{k},t)E(\vec{k},0)\rangle}{\langle E^2(\vec{k},t)\rangle} = \exp(-t/\tau(\vec{k}))$$

$$\tau(\vec{k}) = \int_0^\infty \frac{\langle E(\vec{k},t)E(\vec{k},0)\rangle}{\langle E(\vec{k},t)^2\rangle} dt$$

Example LJ Argon, 10 K



Turney, Landry, McGaughey, Amon, Phys. Rev. B, 2009

Phonon lifetimes

Alternative computation : the frequency domain decomposition

3. Calculate the kinetic and potential energies : $T(\vec{k},t)=\frac{1}{2}\frac{dQ}{dt}(\vec{k})\frac{dQ}{dt}(-\vec{k})$

Expectation value : $\langle T(\vec{k},t)\rangle=\lim_{\tau_0\to\infty}\frac{1}{2\tau_0}\int_0^{\tau_0}\frac{dQ}{dt}(\vec{k},t)\frac{dQ}{dt}(-\vec{k},t)dt$

Parseval theorem : $\langle\tilde{T}(\vec{k},\omega)\rangle=\omega^2|\tilde{Q}(\vec{k},\omega)|^2$

$$\tilde{Q}(\vec{k},\omega)=\lim_{\tau_0\to\infty}\frac{1}{\sqrt{2\pi}}\int_0^{\tau_0}Q(\vec{k},t)\exp(-i\omega t)dt$$

Spectral energy density

$$\langle\tilde{T}(\vec{k},\omega)\rangle=C(\vec{k})\frac{1/2\pi\tau(\vec{k})}{(\omega_a(\vec{k})-\omega)^2+(1/4\pi\tau(\vec{k}))^2}$$

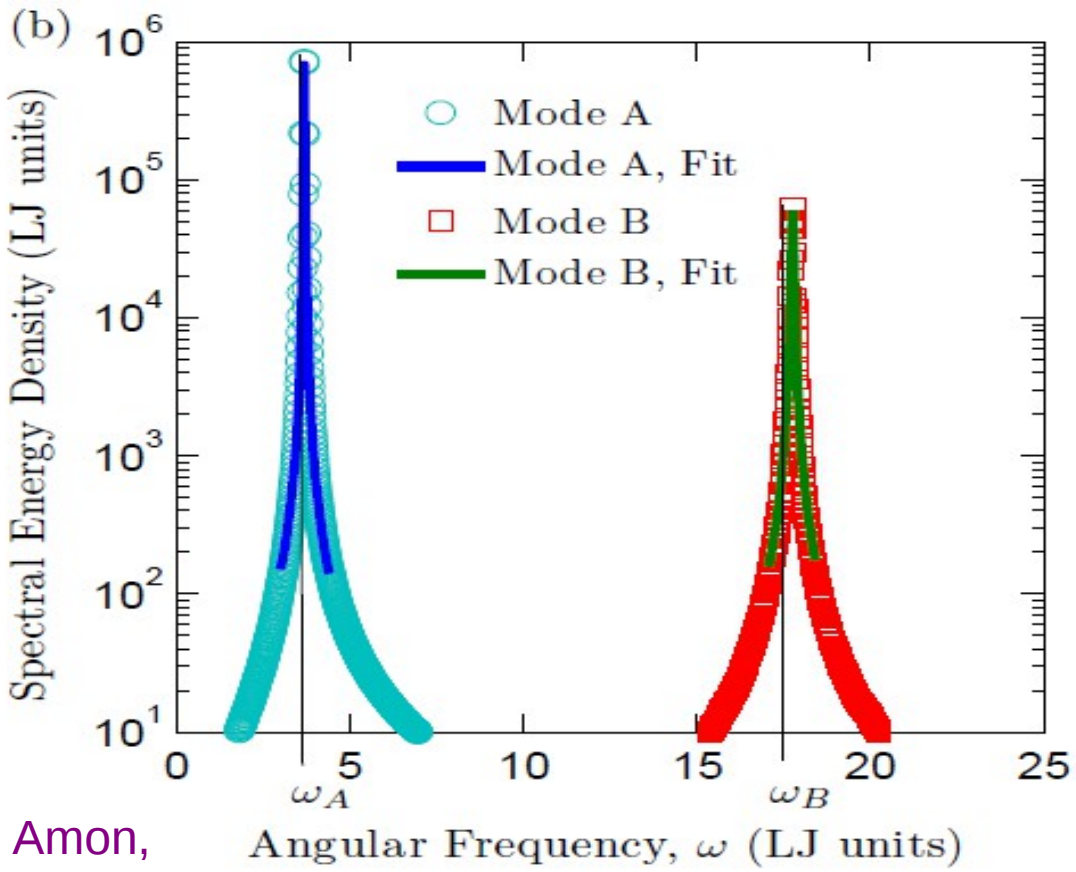
Phonon lifetimes

Alternative computation : the frequency domain decomposition

Spectral energy density

$$\langle \tilde{T}(\vec{k},\omega)\rangle = C(\vec{k})\frac{1/2\pi\tau(\vec{k})}{(\omega_a(\vec{k})-\omega)^2+(1/4\pi\tau(\vec{k}))^2}$$

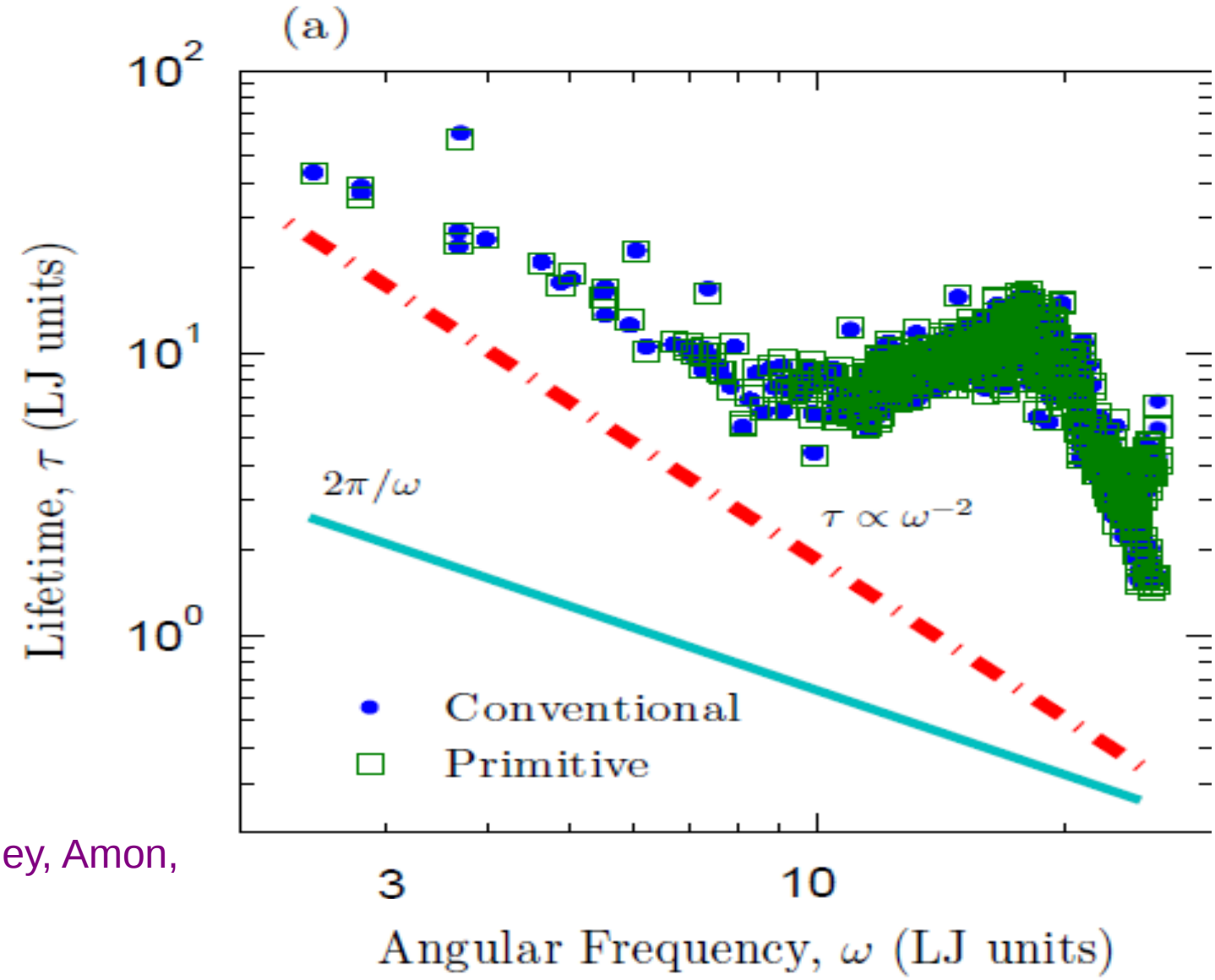
Example LJ Argon, 10 K



Turney, Landry, McGaughey, Amon, Phys. Rev. B, 2009

Phonon lifetimes

Example LJ Argon, 10 K

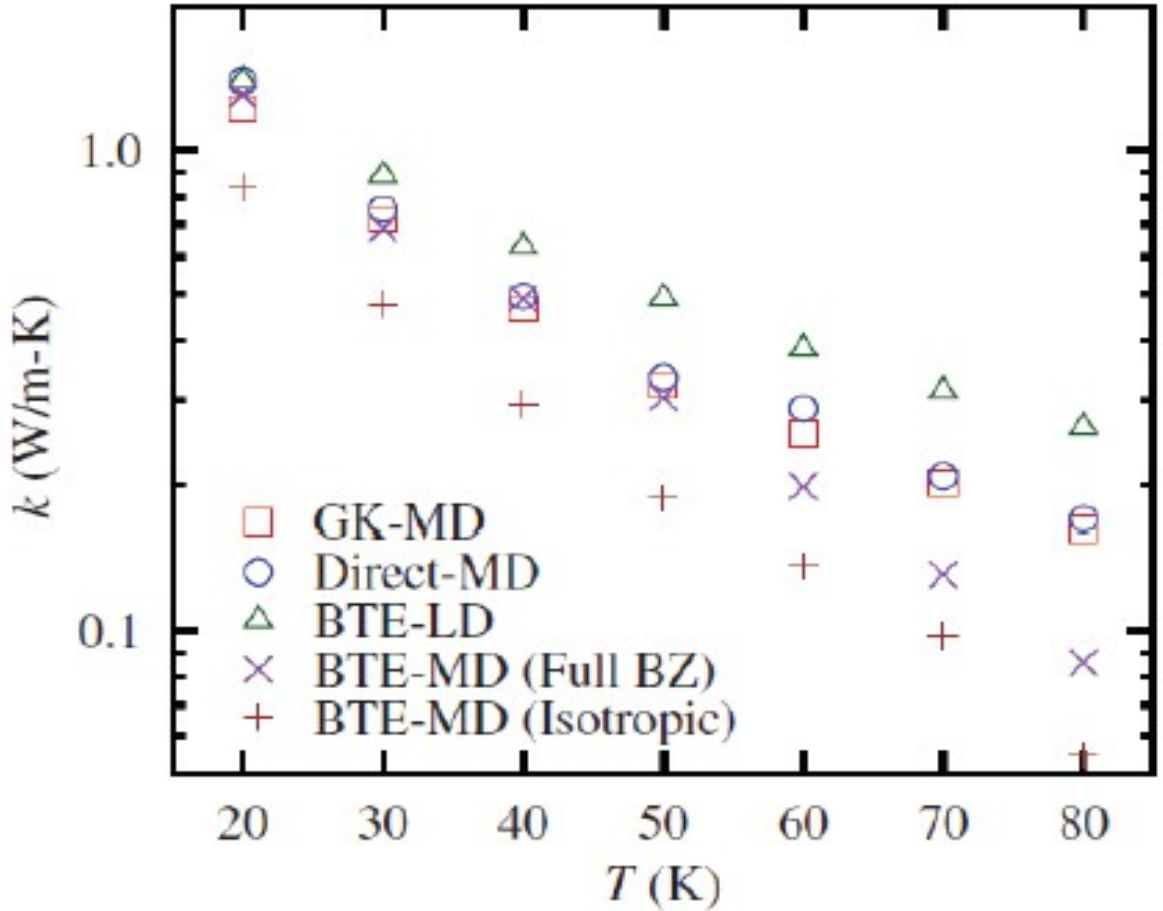


Turney, Landry, McGaughey, Amon, Phys. Rev. B, 2009

Phonon lifetimes

Thermal conductivity $\lambda = \sum_{\vec{k}} c_v(\vec{k}) |v_g(\vec{k})| \tau(\vec{k})$

Example LJ Argon, 10 K



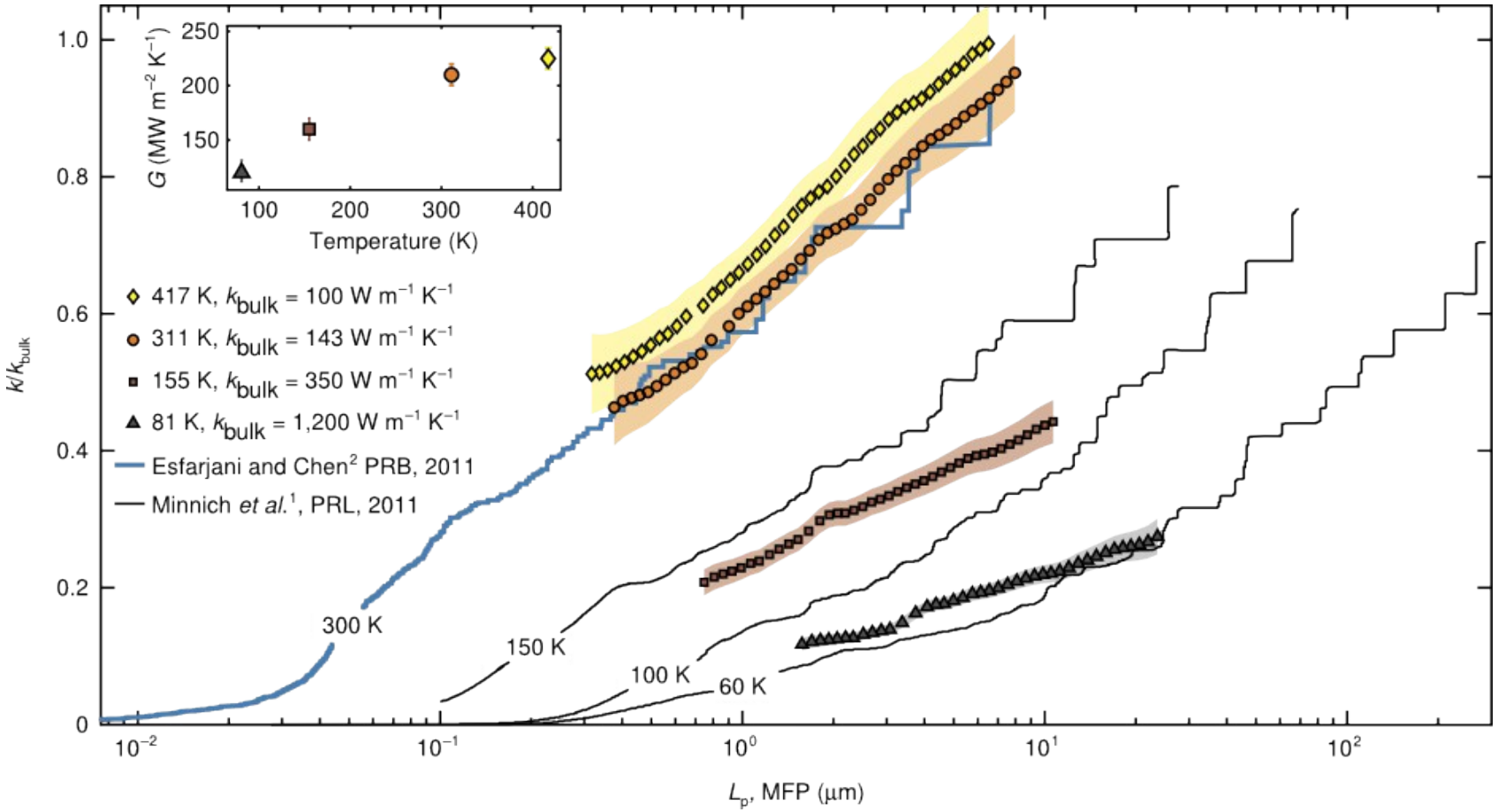
Towards large scale simulations :

Boltzmann transport equation :

$$\frac{\partial n}{\partial t} + \vec{v}_g \cdot \vec{\nabla} n = -\frac{(n - n_{eq})}{\tau(\vec{k}, s)}$$

Accumulation function : phonon spectroscopy

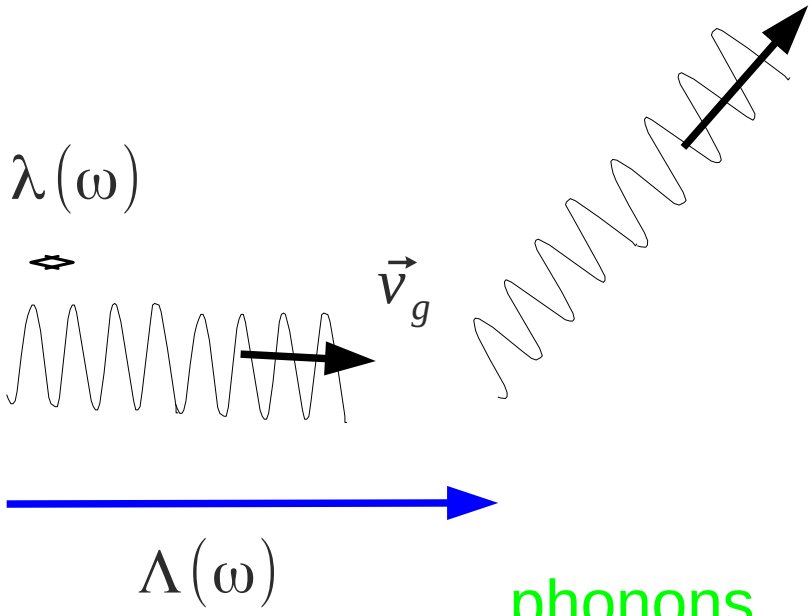
Crystal Si



$$acc(\omega) = \int_0^{\omega} c_v(\omega)\, vg(\omega)\, \Lambda(\omega)\, d\omega$$

Regner et al., *Nat. Comm.* 2013

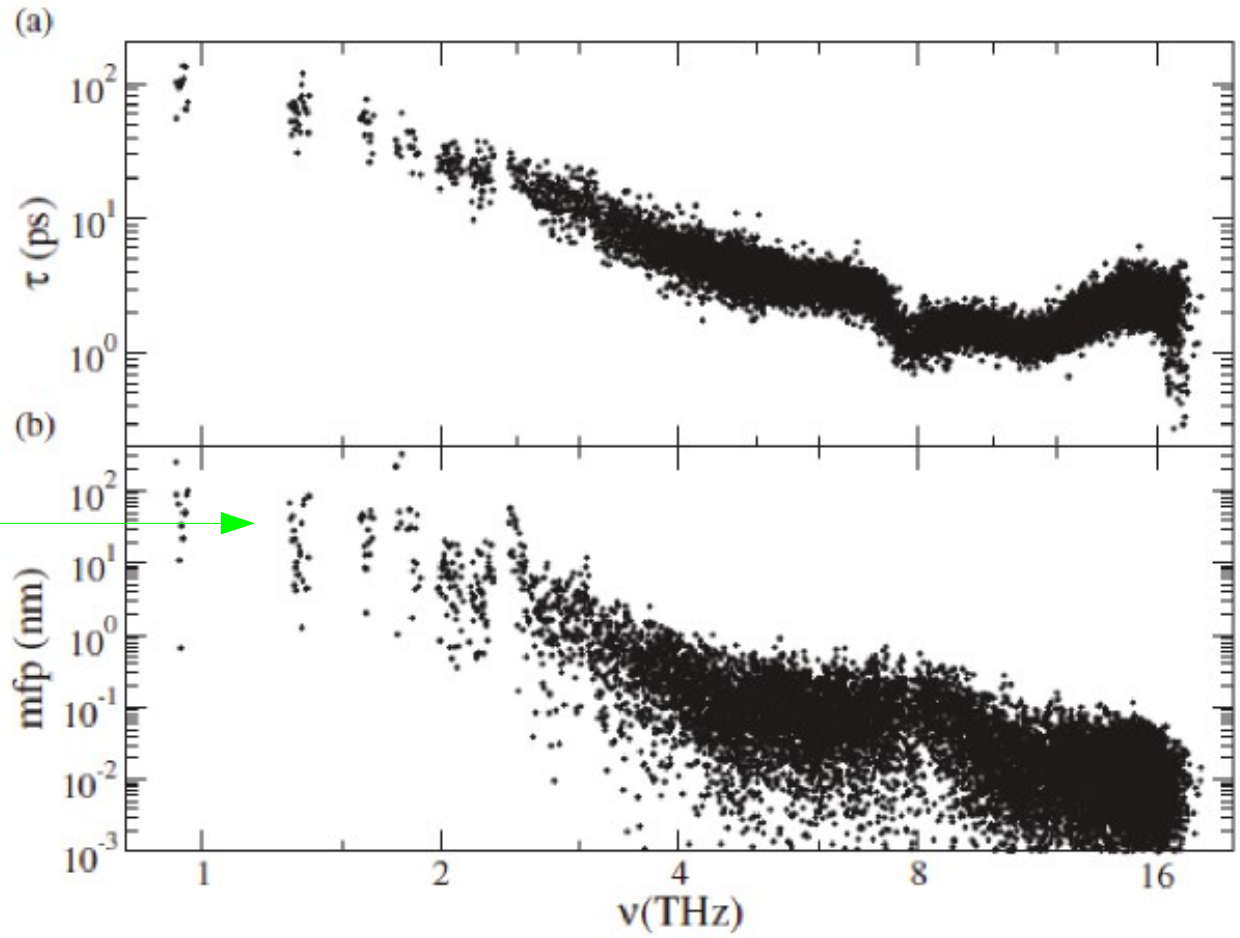
Amorphous materials



phonons

phonons $\Lambda > \lambda$

Amorphous Si

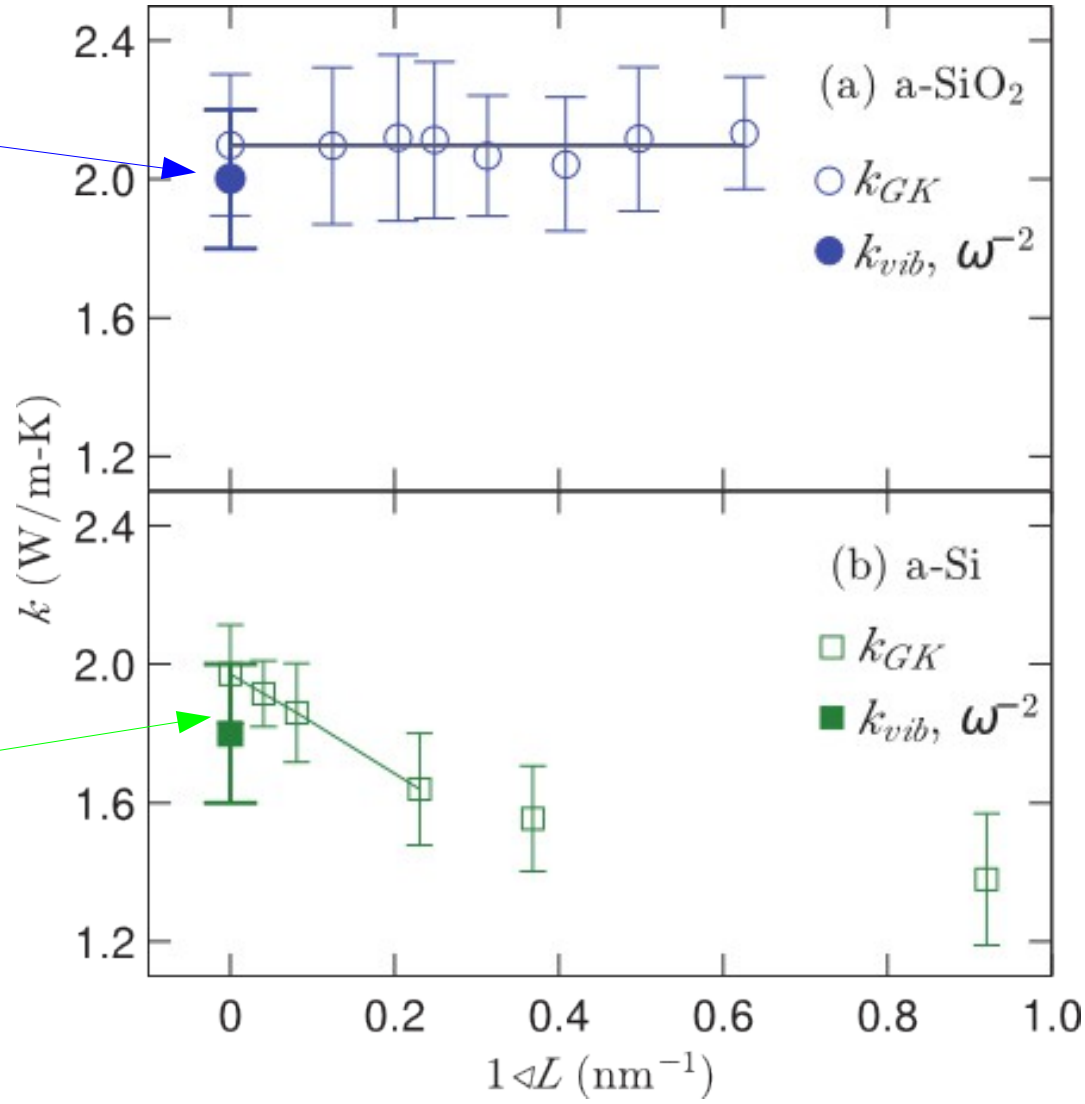


He, Donadio and Galli, *APL* 2011

Amorphous materials

Only localized modes

phonons

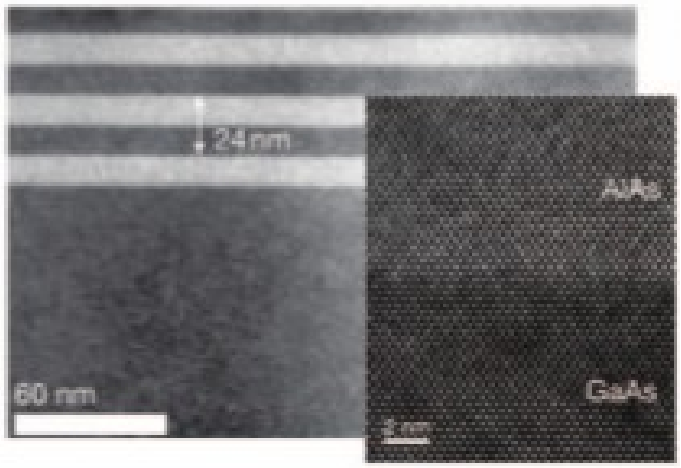


Larkin and McGaughey, *PRB* 2014

Phonon scattering at interfaces

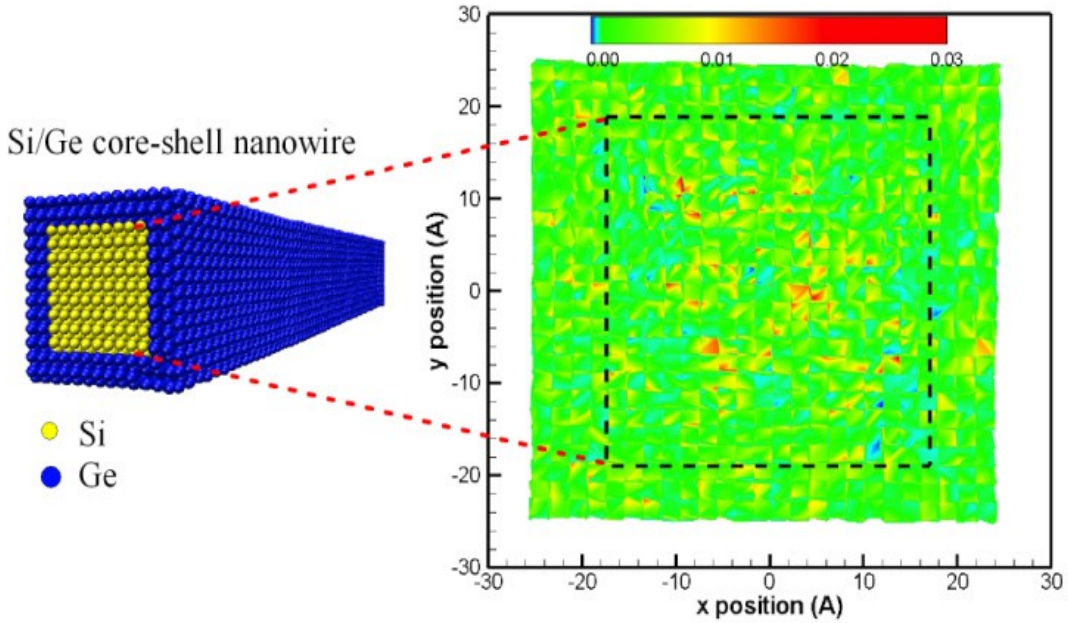
Heat Transfer at the nanoscale

Superlattices



Dresselhaus, Chen, Science 2012

Nanocomposites-nanowires

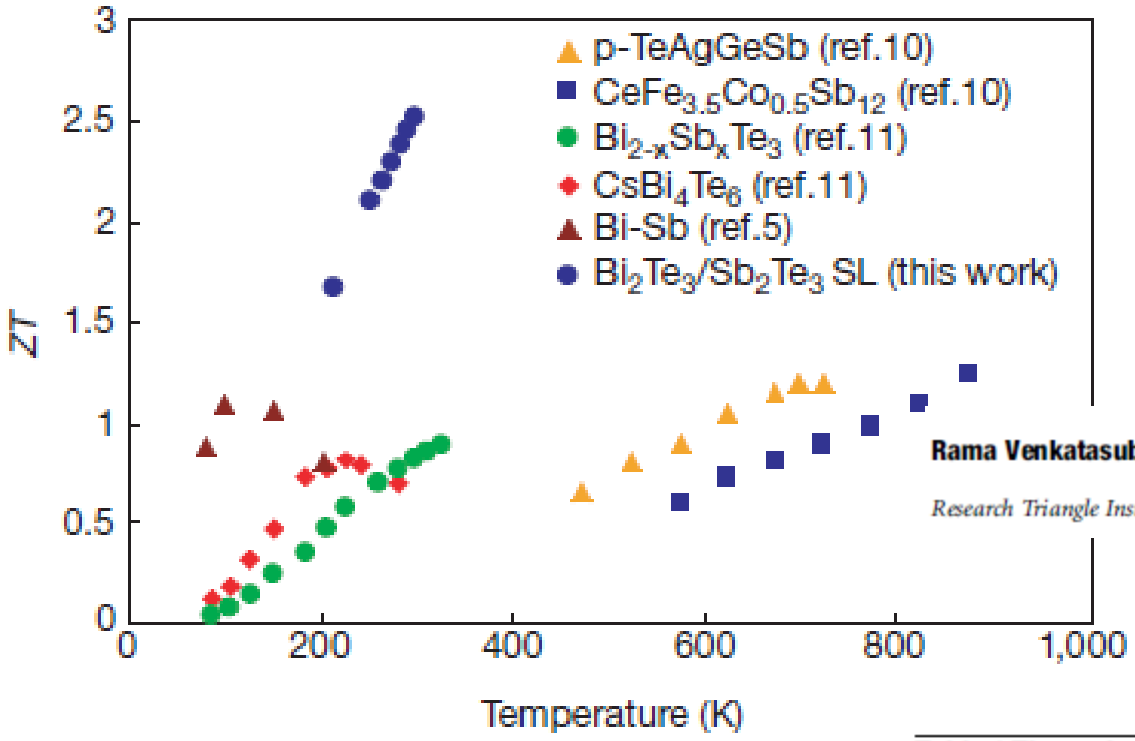


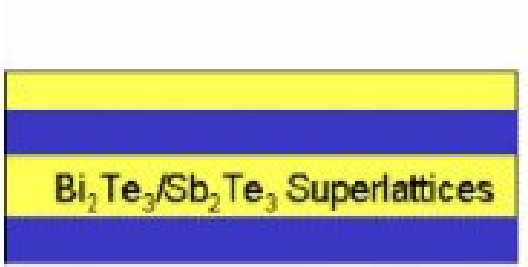
Poulikakos, NanoLetters 2011

-Deviations from Fourier's law (dimensions < phonon mean free path)

-Thermal boundary resistance

Superlattices as high ZT materials





NATURE | VOL 413 | 11 OCTOBER 2001 | www.nature.com

Rama Venkatasubramanian, Edward Siivola, Thomas Colpitts & Brooks O'Quinn

Research Triangle Institute, Research Triangle Park, North Carolina 27709, USA

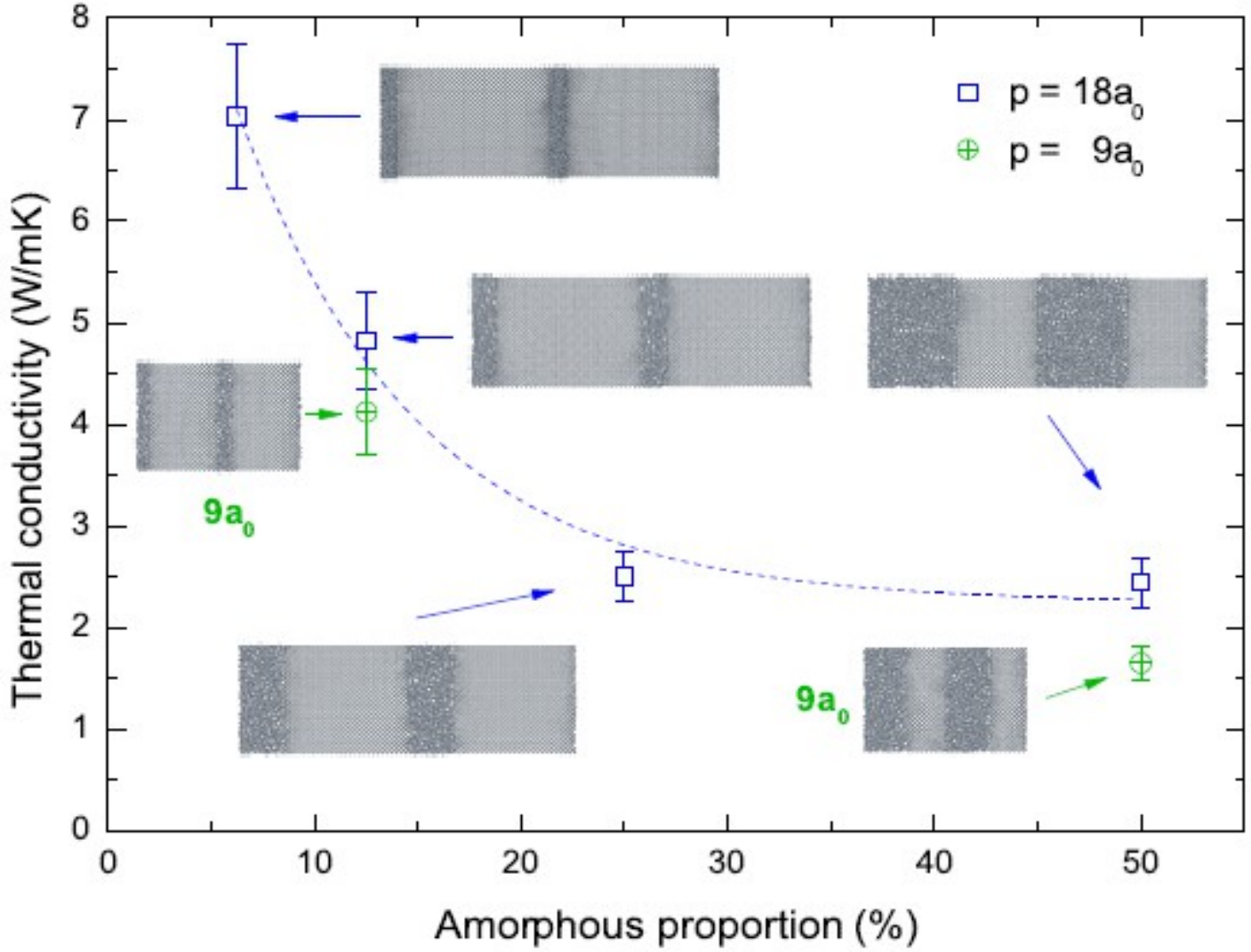
$$Z = \frac{\alpha^2 \sigma}{K_L + K_e} \simeq \frac{\alpha^2}{\left(\frac{K_L}{\mu_P \eta}\right) + L_0 T}$$

Table 1 Theoretical and experimental lattice thermal conductivities

Material	Thermal conductivity ($W\,m^{-1}\,K^{-1}$)
K_{min} of Bi_2Te_3 (*a*-*b* axis), Slack model[34]	0.55
K_{min} of Bi_2Te_3 (*c* axis), Slack model[34]	0.28
K_{min} of Bi_2Te_3 (*a*-*b* axis), Cahill model[35]	0.28
K_{min} of Bi_2Te_3 (*c* axis), Cahill model[35]	0.14
K_L of $Bi_{2-x}Sb_xTe_3$ alloy (*a*-*b* axis)	0.97
K_L of $Bi_{2-x}Sb_xTe_3$ alloy (*c* axis)	0.49
K_L of Bi_2Te_3/Sb_2Te_3 superlattice (*c* axis)	0.22

Lattice thermal conductivity (K_L) of the Bi_2Te_3/Sb_2Te_3 superlattice (period ~50 Å) compared with K_L observed in the respective alloys and the theoretical minimum lattice thermal conductivity (K_{min}) from various models.

Crystalline/amorphous superlattices



Bulk crystalline Si @300 K

$\lambda = 148\, W/K/m$

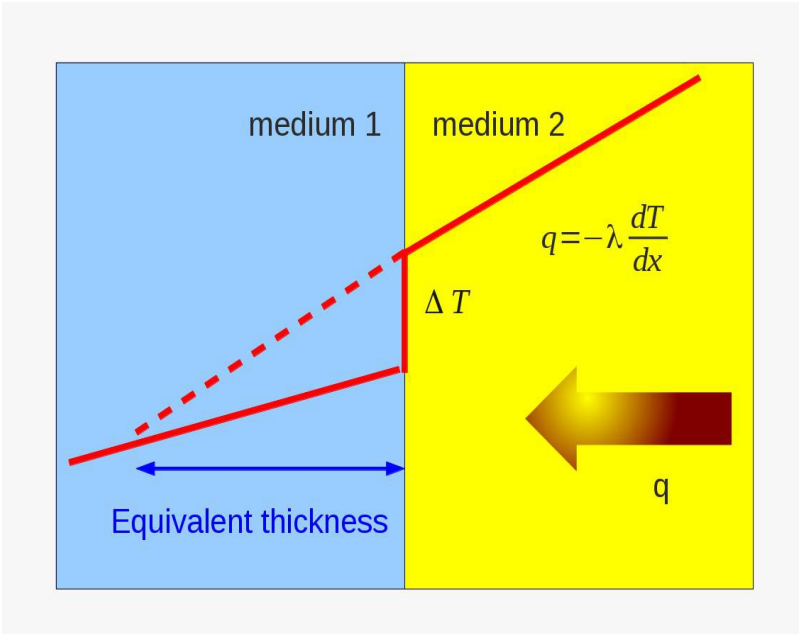
Bulk amorphous Si @300 K

$\lambda = 0.68\, W/K/m$

6% amorphised Silicon
=> 20 fold drop in the thermal conductivity

A. France Lanord et al.,
J. Phys. Cond. Mat. 2014

Thermal boundary (Kapitza) resistance



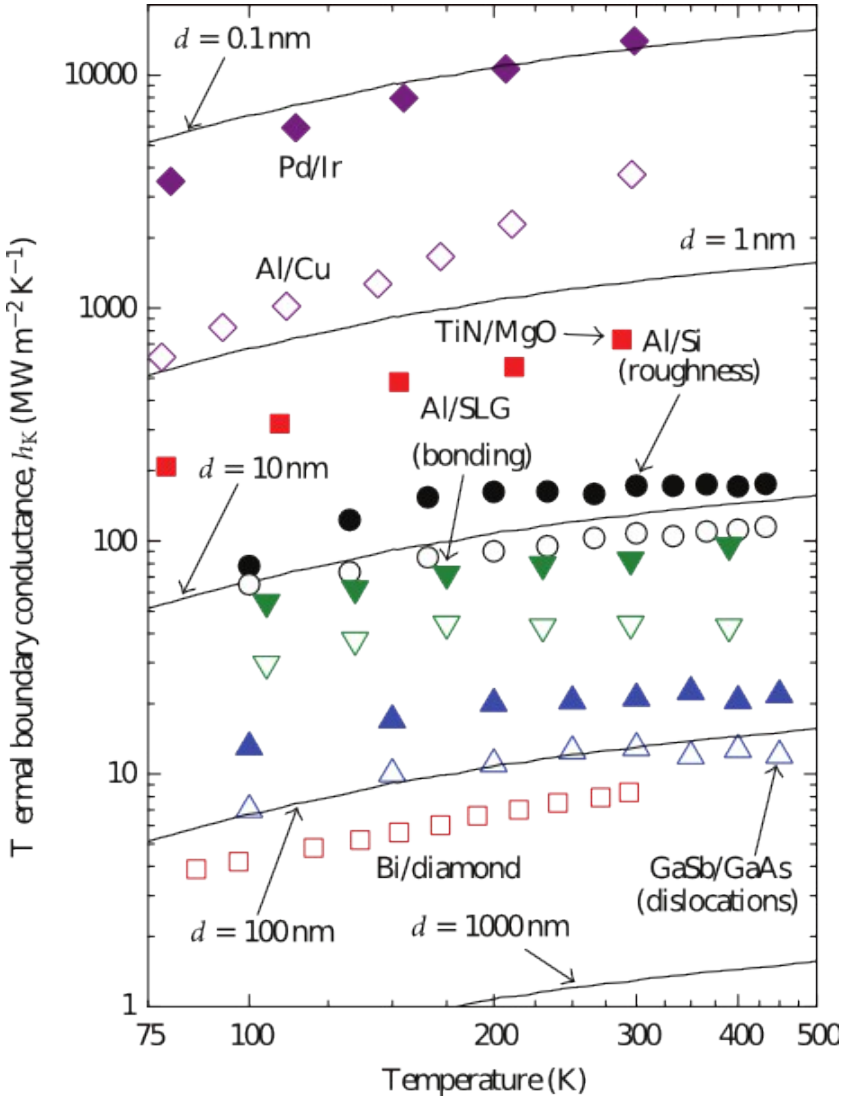
Thermal boundary conductance $G=q/\Delta T$

$$G=1/R=\int C_v(\omega)v_g(\omega)t_{12}(\omega)d\omega$$

Energy transmission coefficient

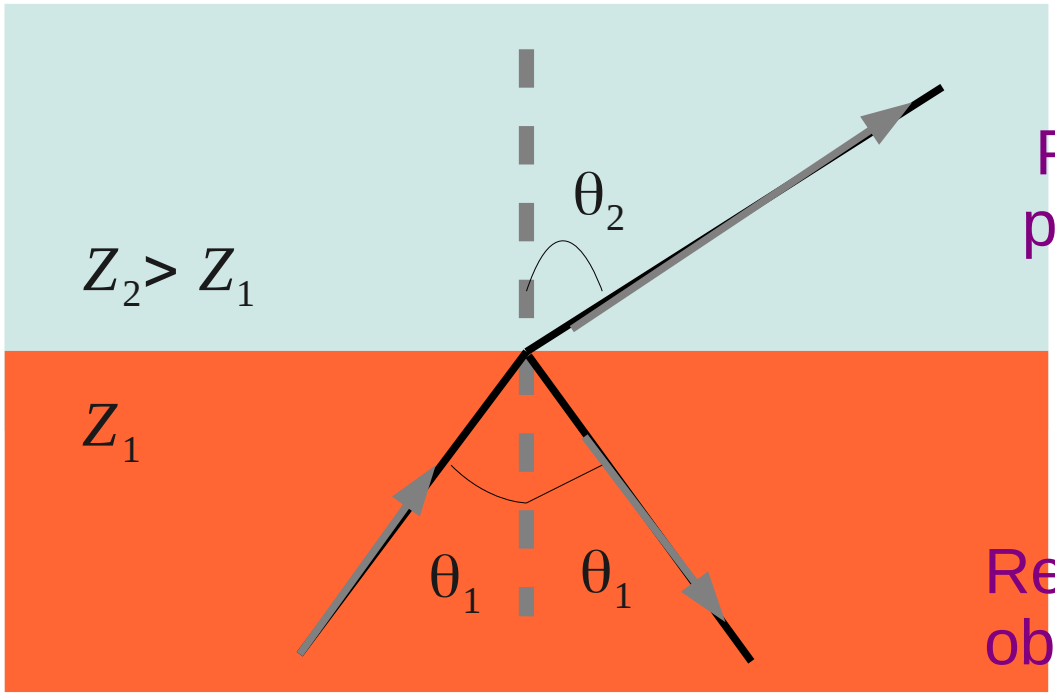
$G\simeq 1-1000\,MW/m^2/K$

Equivalent thickness : $l=\lambda/G=1-1000\,nm$



Hopkins 2013

Acoustic mismatch model (AMM)



W.A. Little (1959)

Phonons treated as plane waves propagating in continuous media

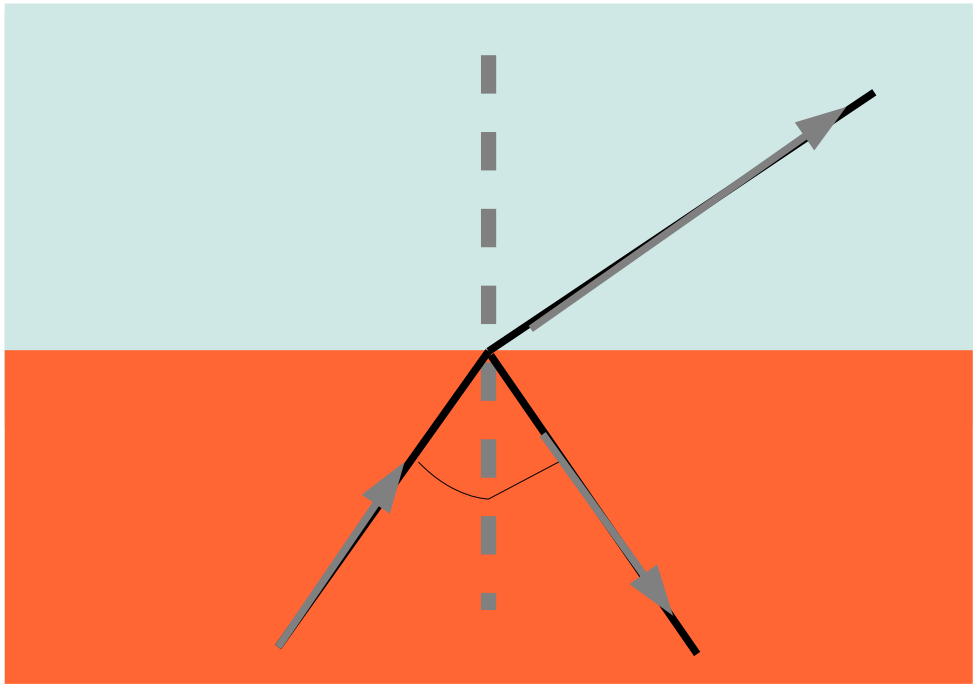
acoustic impendance $Z_i = \rho_i c_i$

Reflection/refraction at the interface obey laws analogous to Snell's laws

$$\frac{\sin\theta_1}{c_1} = \frac{\sin\theta_2}{c_2}$$

Transmission coefficient : $$t_{12} = \frac{4 Z_1 Z_2 \cos\theta_1 \cos\theta_2}{(Z_1 \cos\theta_1 + Z_2 \cos\theta_2)^2}$$

Diffuse mismatch model (DMM)



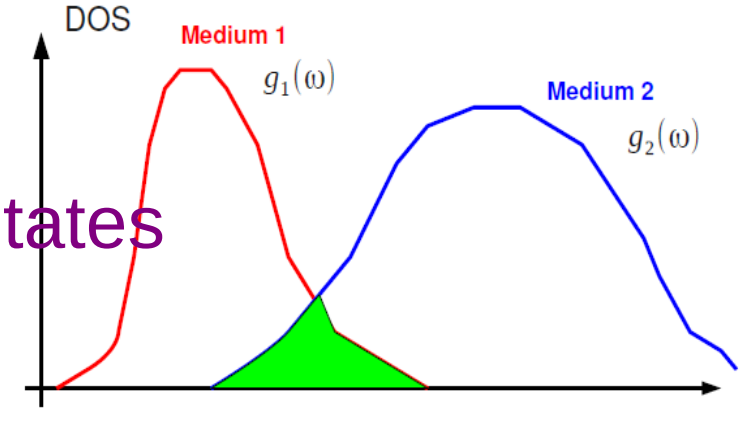
(Swartz 1989)

All the phonons are diffusively scattered by the interface

The transmission coefficient is given by detailed balance

$$\alpha_{12}(\omega) = \frac{c_2 g_2(\omega)}{c_2 g_2(\omega) + c_1 g_1(\omega)}$$

The conductance is related to the overlap between the density of states characterizing the two media

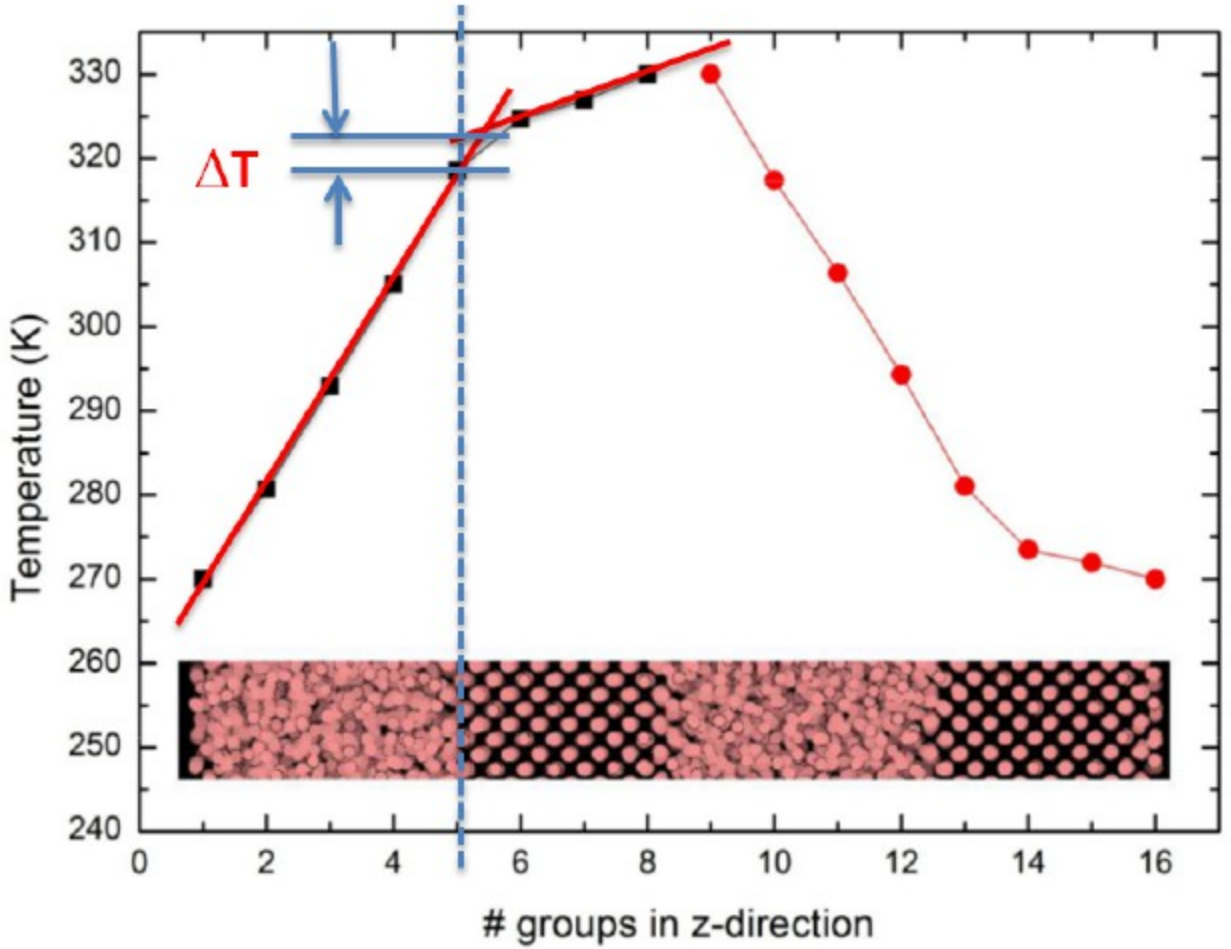


Factors affecting the conductance : (a non exhaustive list)

- « Bonding strength» between the two solids
- Lattice parameters mismatch
- Interfacial roughness
- Defects at the interface (vacancies)
- Intermixing
- Electron-phonon coupling

Non-equilibrium simulations

Amorphous Si/
Crystalline Si



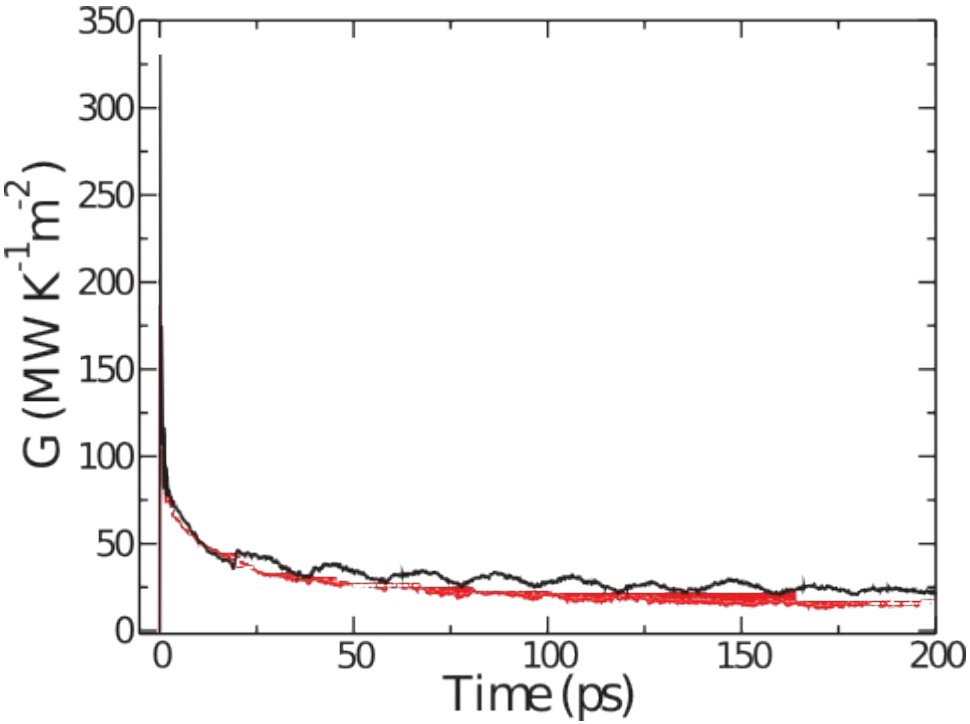
Fourier law : $J = -\lambda \frac{\partial T}{\partial z}$

Thermal boundary resistance : $R = \Delta T / J$

Equilibrium simulations

Puech formula

$$G = \frac{1}{A\,k_B T^2} \int_0^{+\infty} \langle q(t) \cdot q(0) \rangle \, dt$$



A interfacial area

Analogous to the Green-Kubo formula for the thermal conductivity

Interfacial flux :

$$q = \Sigma_{i \in 1,\, j \in 2} \vec{F}_{ij} \frac{\left(\vec{v}_i + \vec{v}_j\right)}{2}$$

Barrat and Chiaruttini, *Mol. Phys.* 2003
SM and Termentzidis, *PRB* 2012

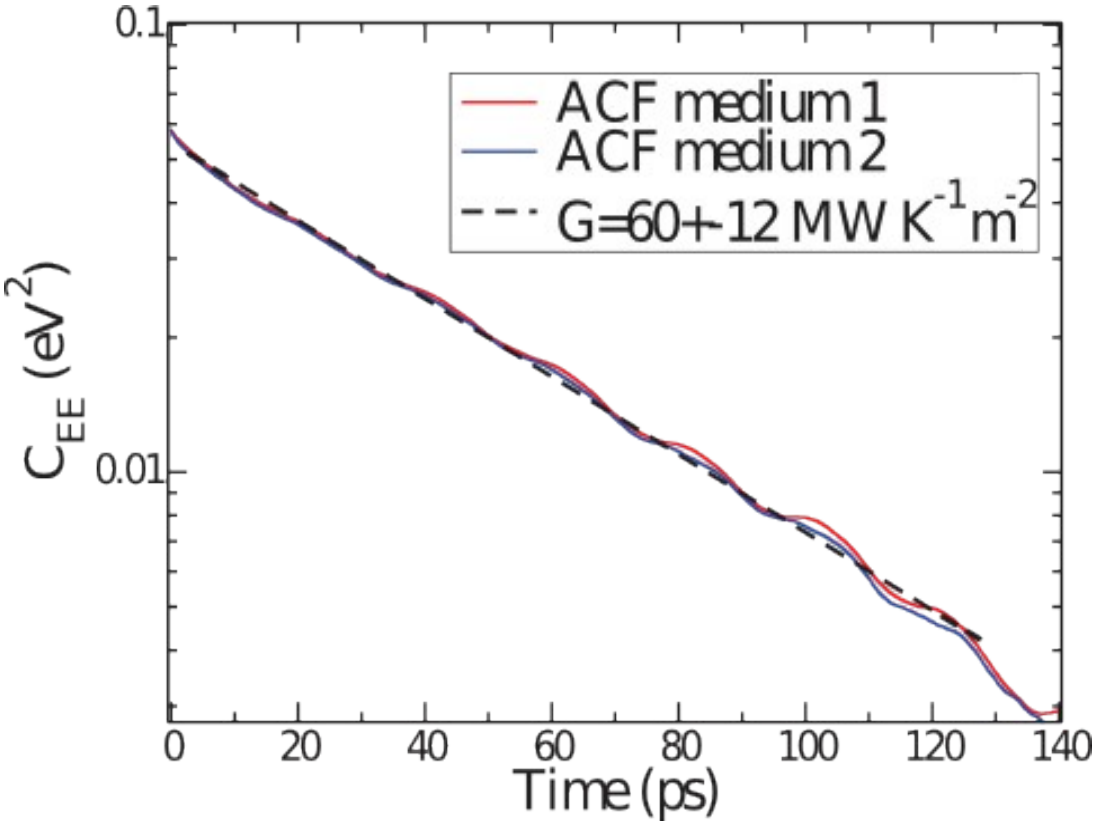
Equivalent formula

$$G = \frac{-1}{A\,k_B T^2}\left(\frac{dC_{EE}}{dt}\right)_{t=0}$$

$$C_{EE}(t) = \langle \delta E(t)\,\delta E(0)\rangle$$

$$C_{EE}(t) \sim C_{EE}(0)\exp(-t/\tau)$$

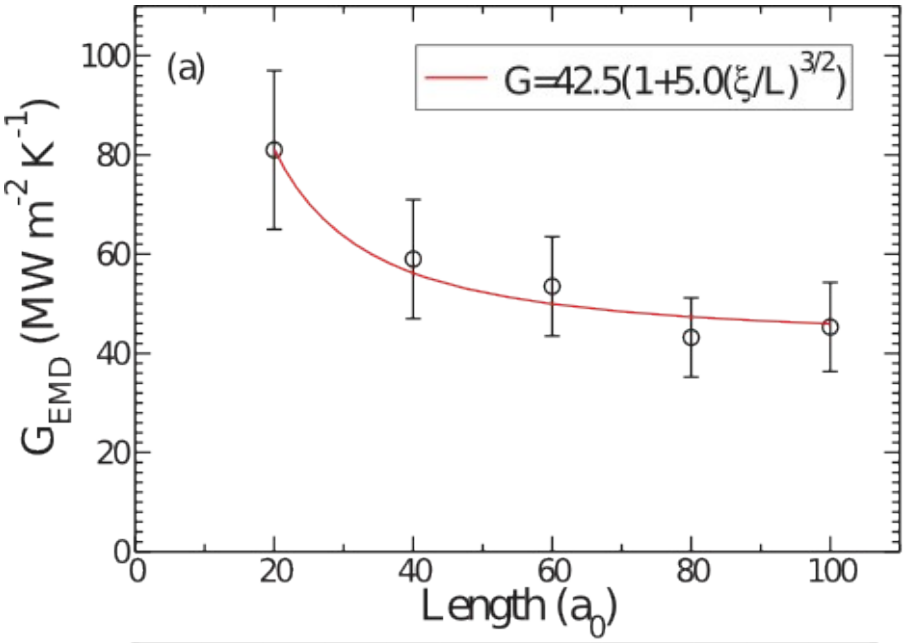
$$G = \frac{1}{Ak_B T^2}\frac{C_{EE}(0)}{\tau}$$

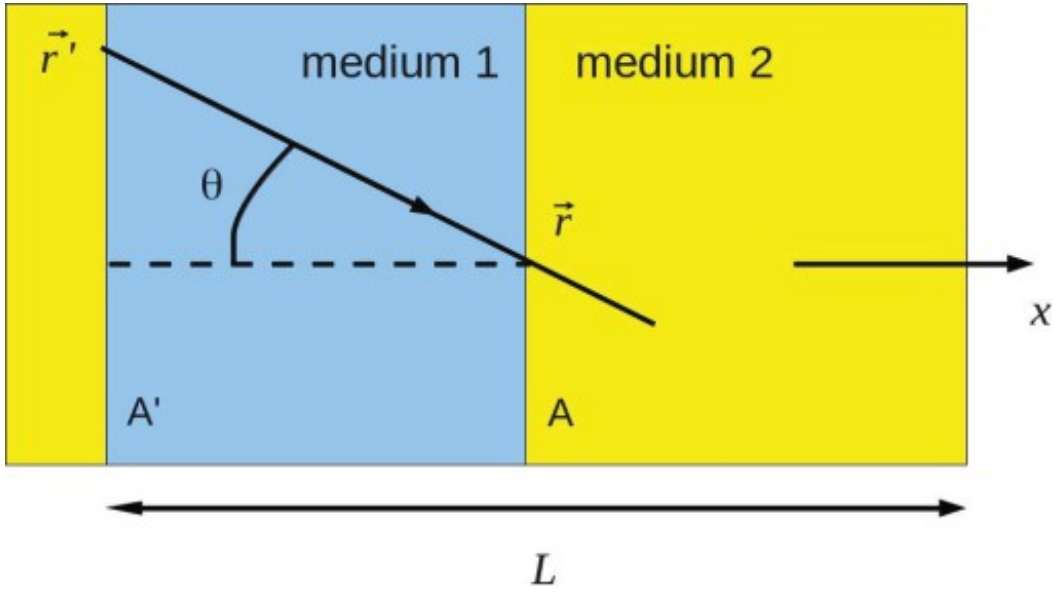


SM and Termentzidis, PRB 2012

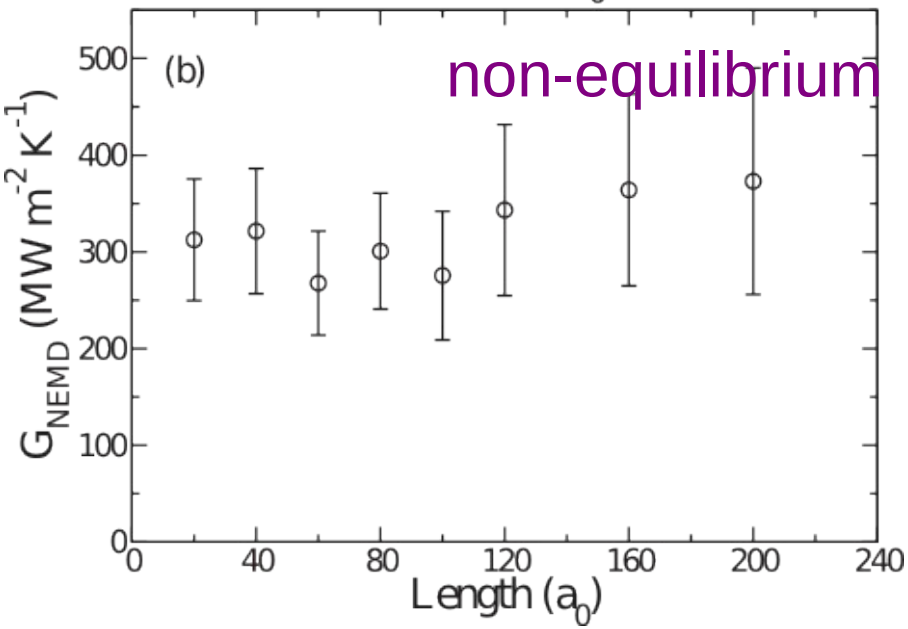
Finite size effects

equilibrium

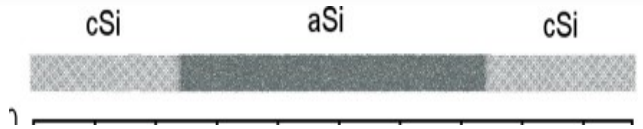




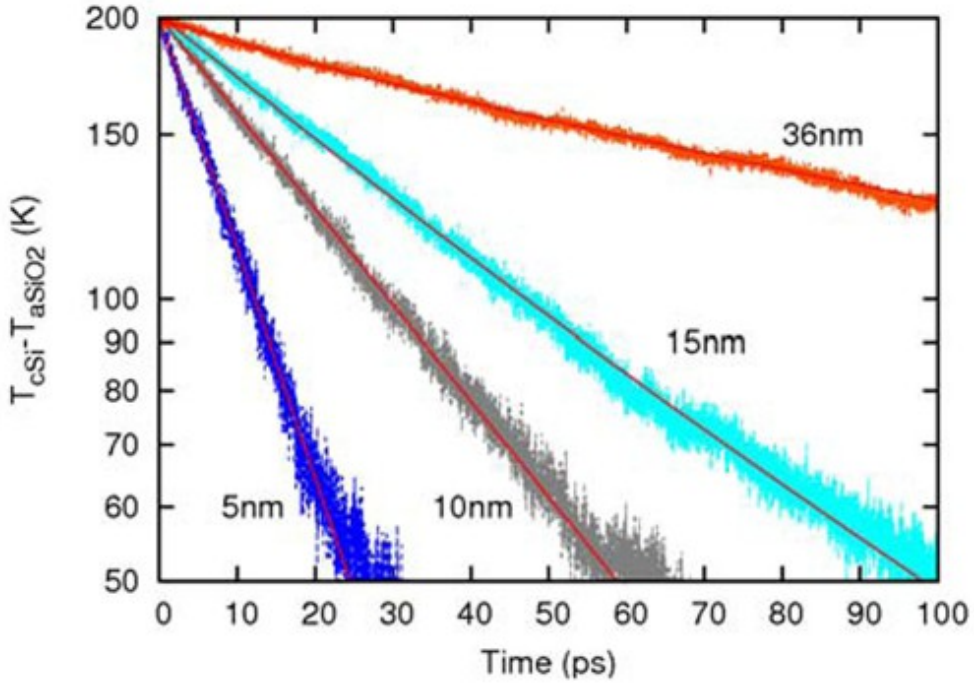
non-equilibrium



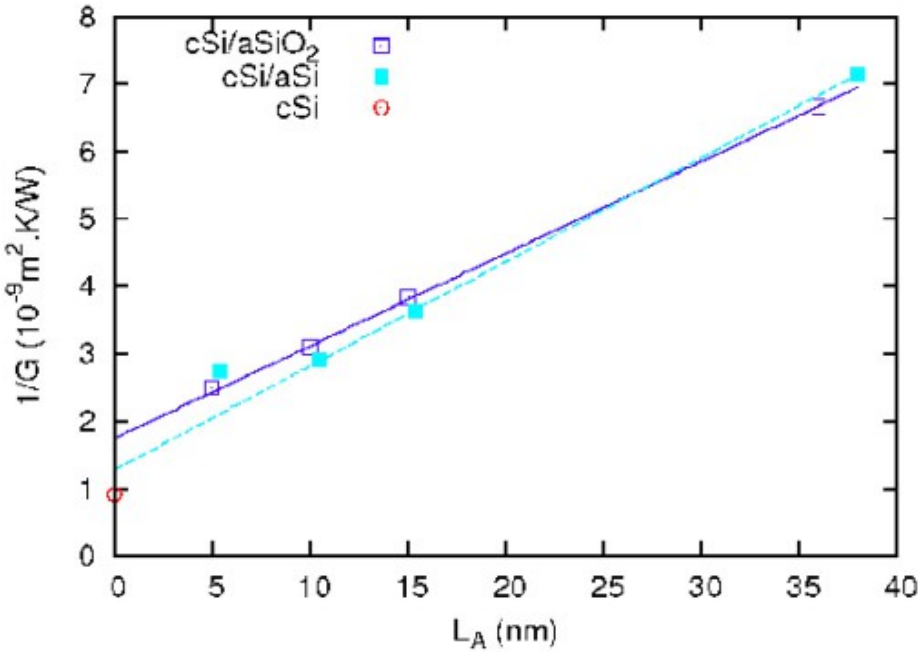
« Approach to equilibrium »



Temperature relaxation



Finite size effects

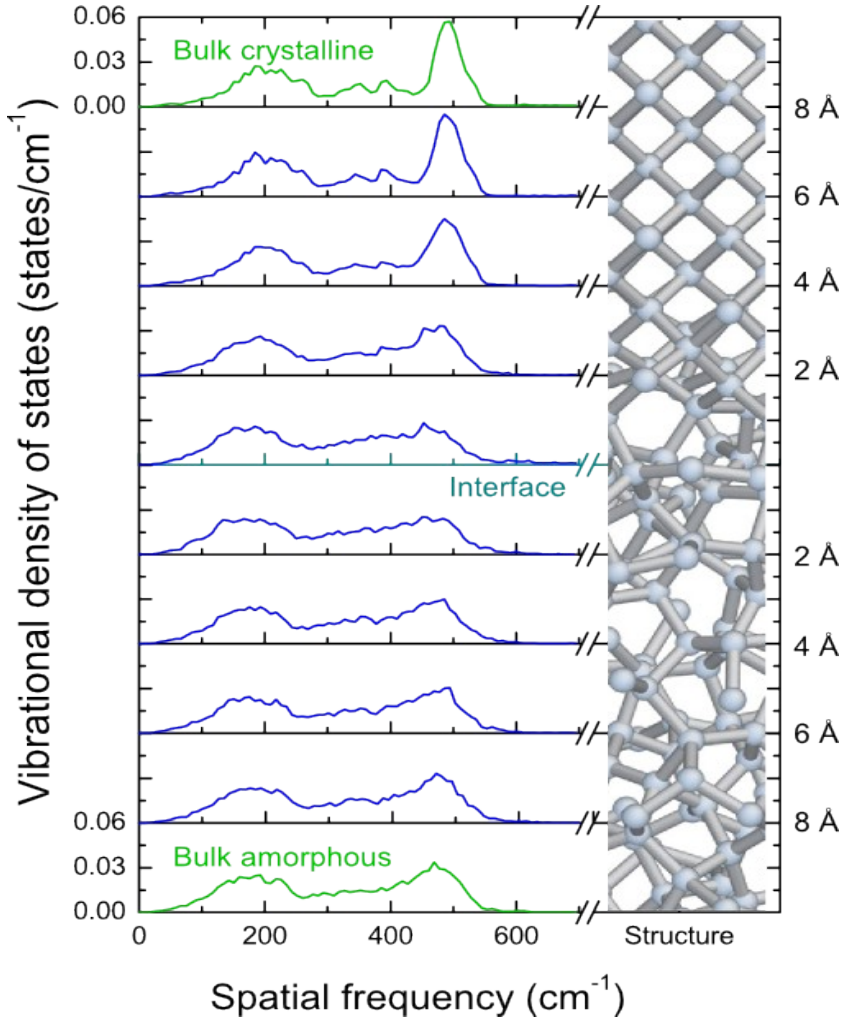


$$\Delta T(t) \propto \exp(-t/\tau)$$

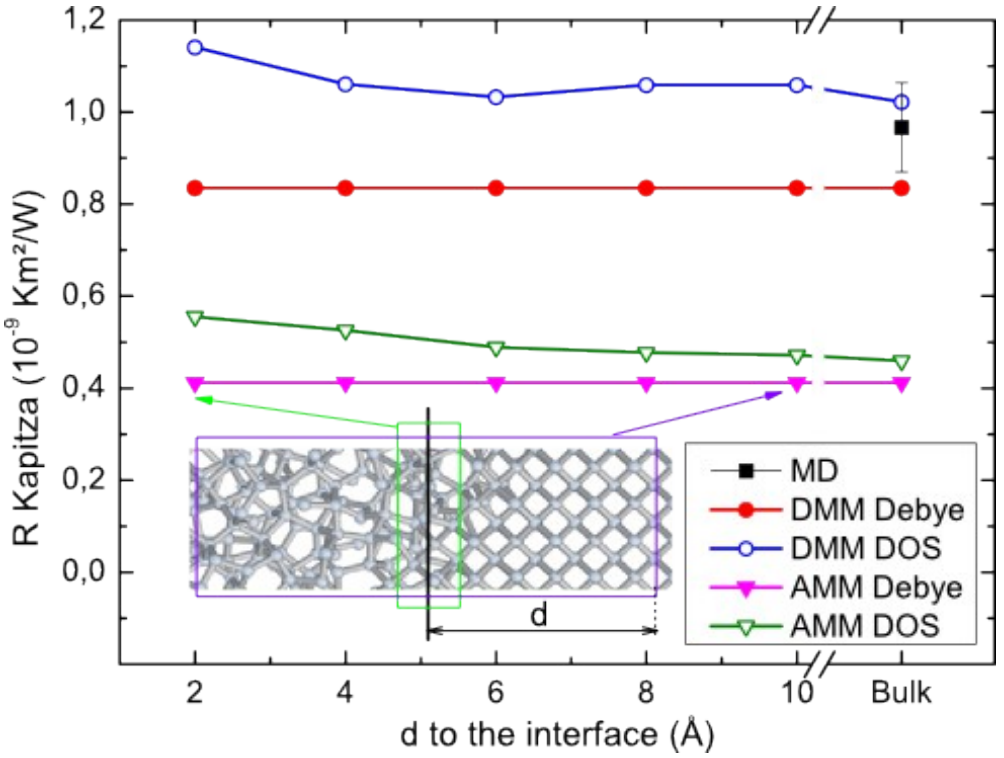
$$G = C_v/(A\tau)$$

E. Lampin et al., *APL* 2012

Comparison with the models



Thermal boundary resistance



$$G = 1/R = \int g(\omega) C_v(\omega) v_g(\omega) t_{12}(\omega) d\omega$$

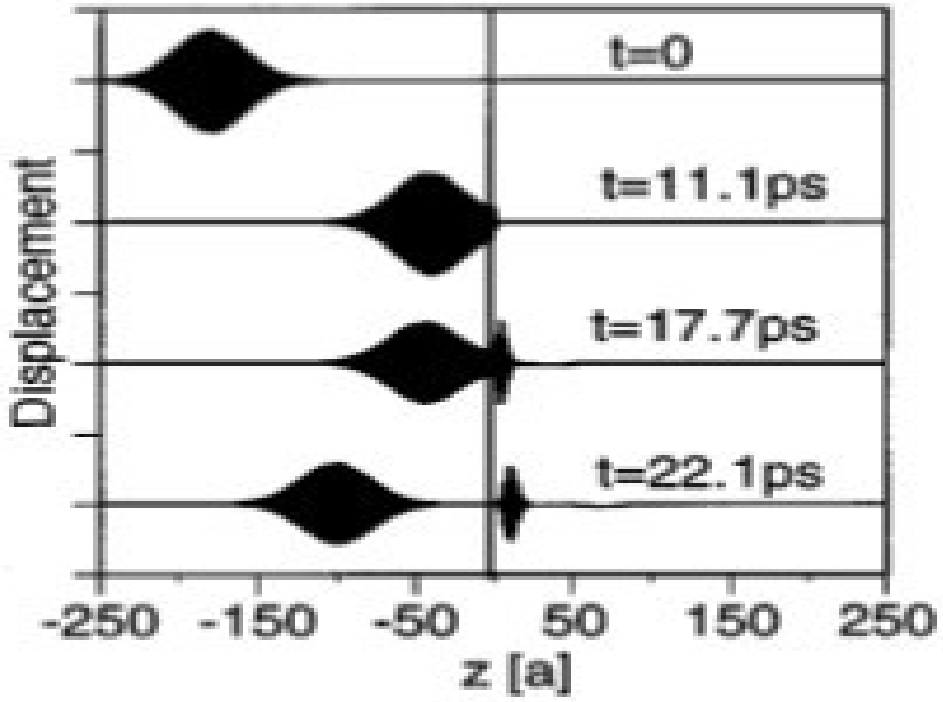
AMM $$t_{12} = \frac{4 Z_1 Z_2 \cos\theta_1 \cos\theta_2}{(Z_1 \cos\theta_1 + Z_2 \cos\theta_2)^2}$$

DMM $$t_{12}(\omega) = \frac{c_2 g_2(\omega)}{c_2 g_2(\omega) + c_1 g_1(\omega)}$$

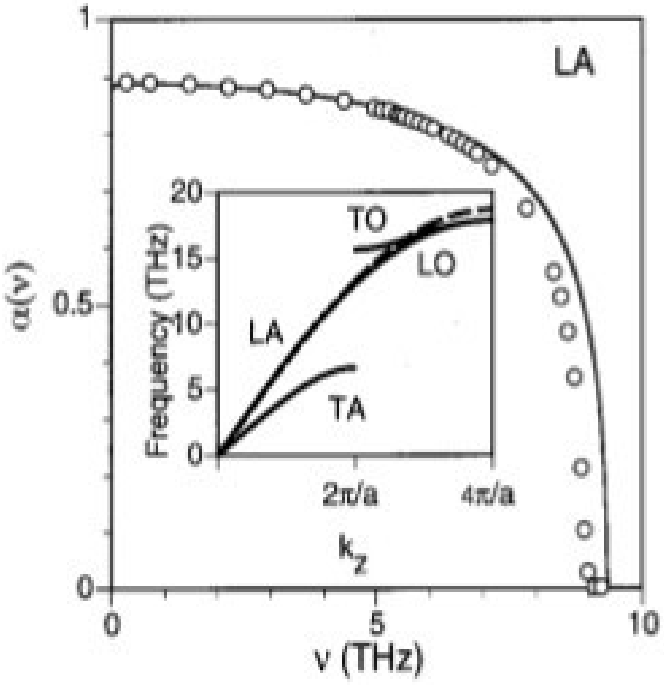
A. France Lanord et al., *J. Phys. Cond. Mat.*, 2014

Phonon transmission coefficient

crystalline Si/heavy Si interface



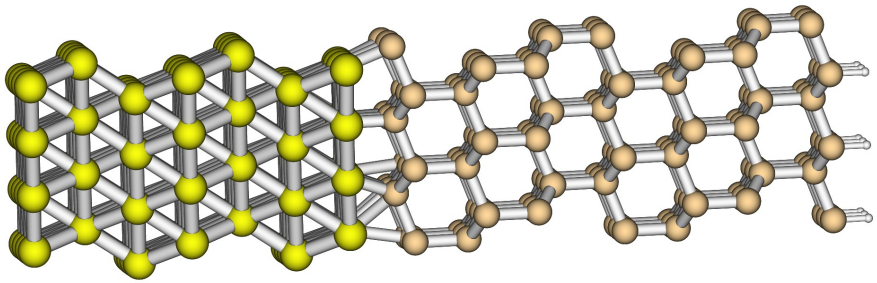
Transmission coefficient



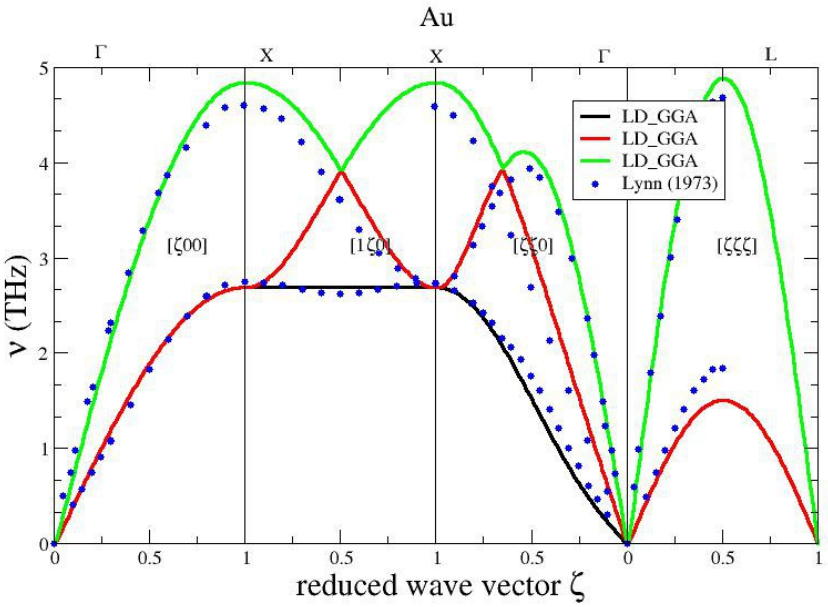
First paper : Shelling,Keblinski *APL* 2002

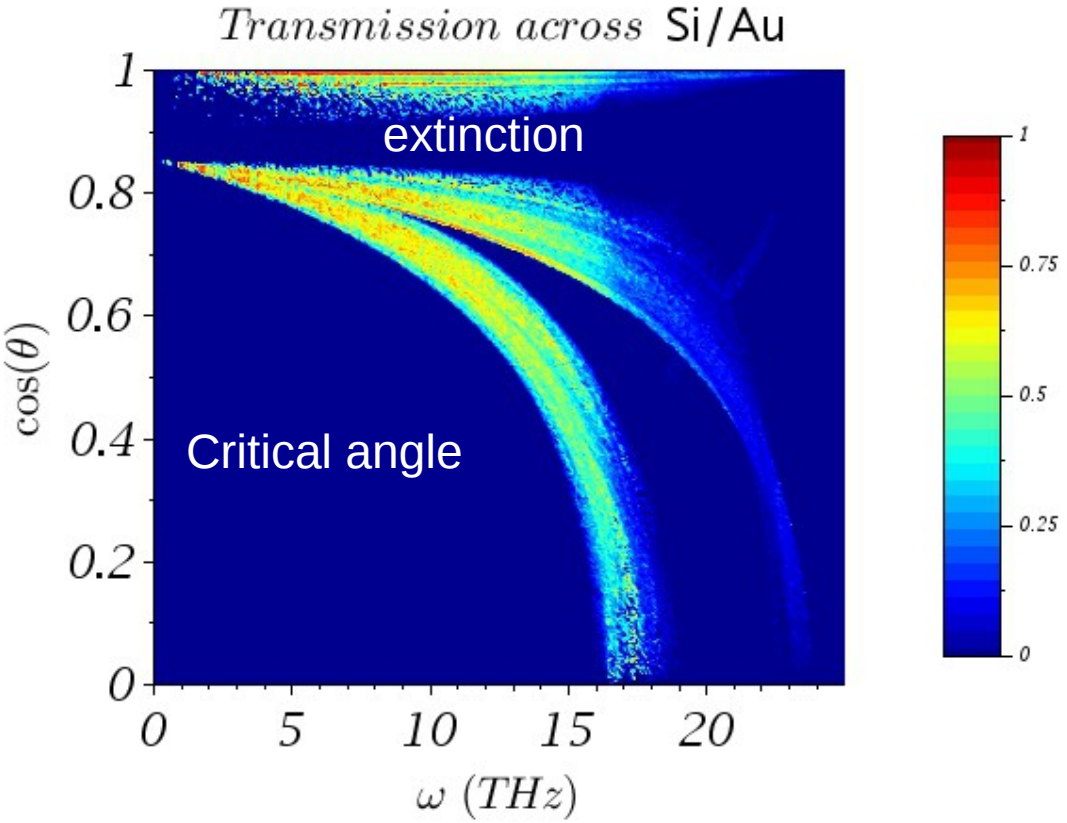
Phonon transmission coefficient

Au/ Si interface



$$t_{1\to 2} = \frac{\rho_{m,2}}{\rho_{m,1}} \sum_{q=4}^{6} \frac{v_{g,q}^{z} . |A_q|^2}{v_{g,0}^{z} . |A_0|^2}$$





Electron-phonon couplings

Two temperature model

$$c_e\,\partial_t T_e = k_e\,\partial^2_{xx} T_e - G(T_e - T_p),$$

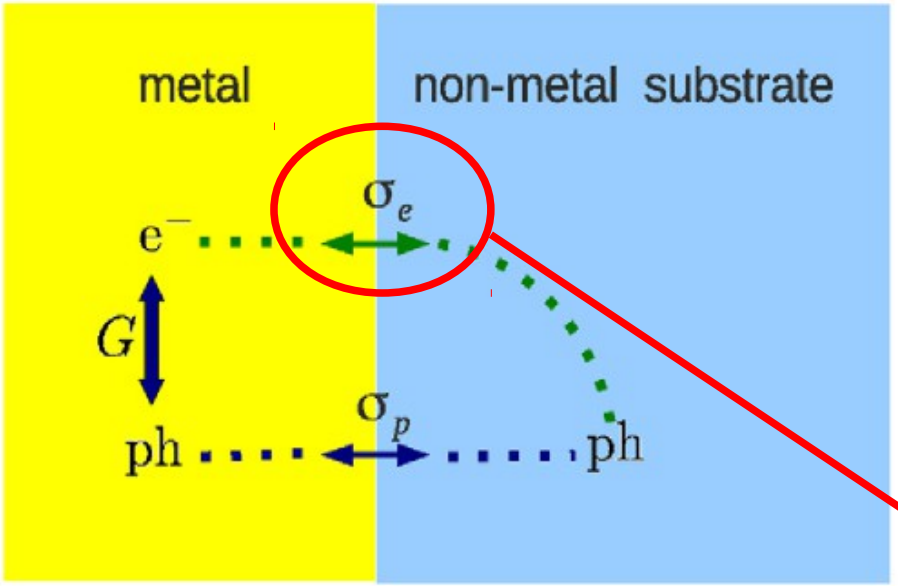
$$c_p\,\partial_t T_p = k_p\,\partial^2_{xx} T_p + G(T_e - T_p),$$

$$c_s\,\partial_t T_s = k_s\,\partial^2_{xx} T_s.$$

+ boundary conditions

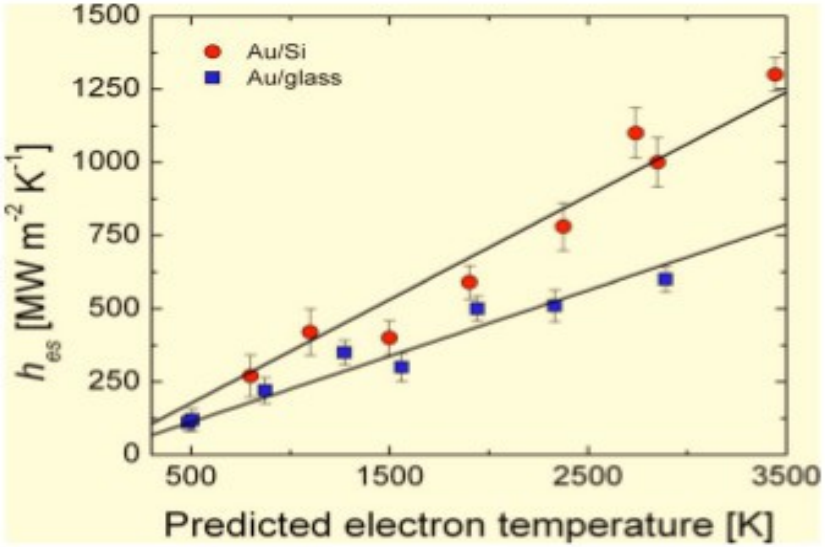
$$-k_s\,\partial_x T_s = \sigma_e(T_e - T_s) + \sigma_p(T_p - T_s),$$

$$= -k_e\,\partial_x T_e - k_p\,\partial_x T_p.$$



Measurements :

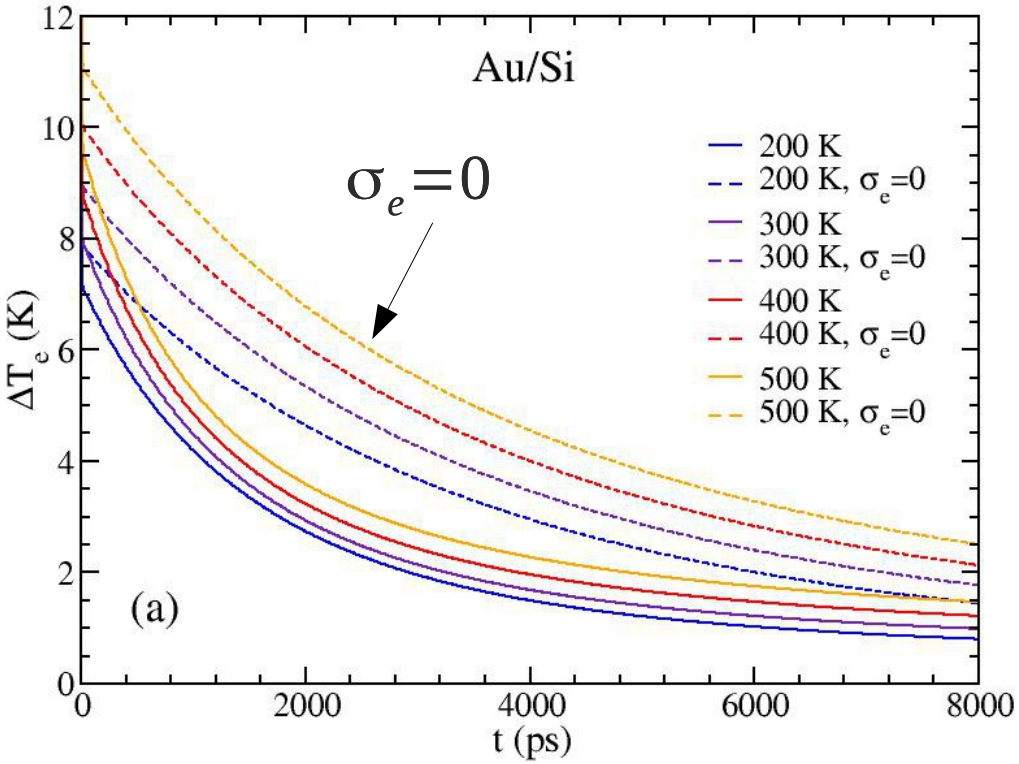
Hopkins et *al. JAP* 2009

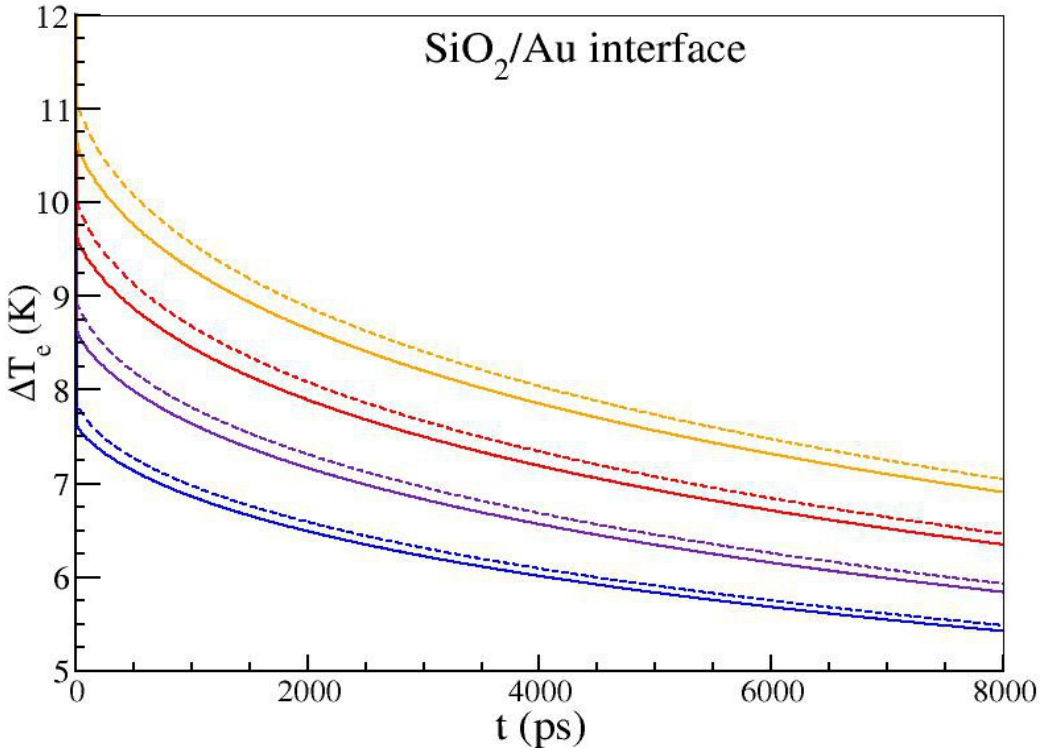


Theory :

Sergeev, *PRB* 1998
Mahan, *PRB* 2009

Two temperature model





Two temperature model

$$c_e \frac{\partial T_e}{\partial t} = k_e \partial^2_{xx} T_e - G(T_e - T_p)$$

$$c_p \frac{\partial T_p}{\partial t} = k_p \partial^2_{xx} T_p + G(T_e - T_p)$$

$$c_s \frac{\partial T_s}{\partial t} = k_s \partial^2_{xx} T_s$$

Boundary conditions

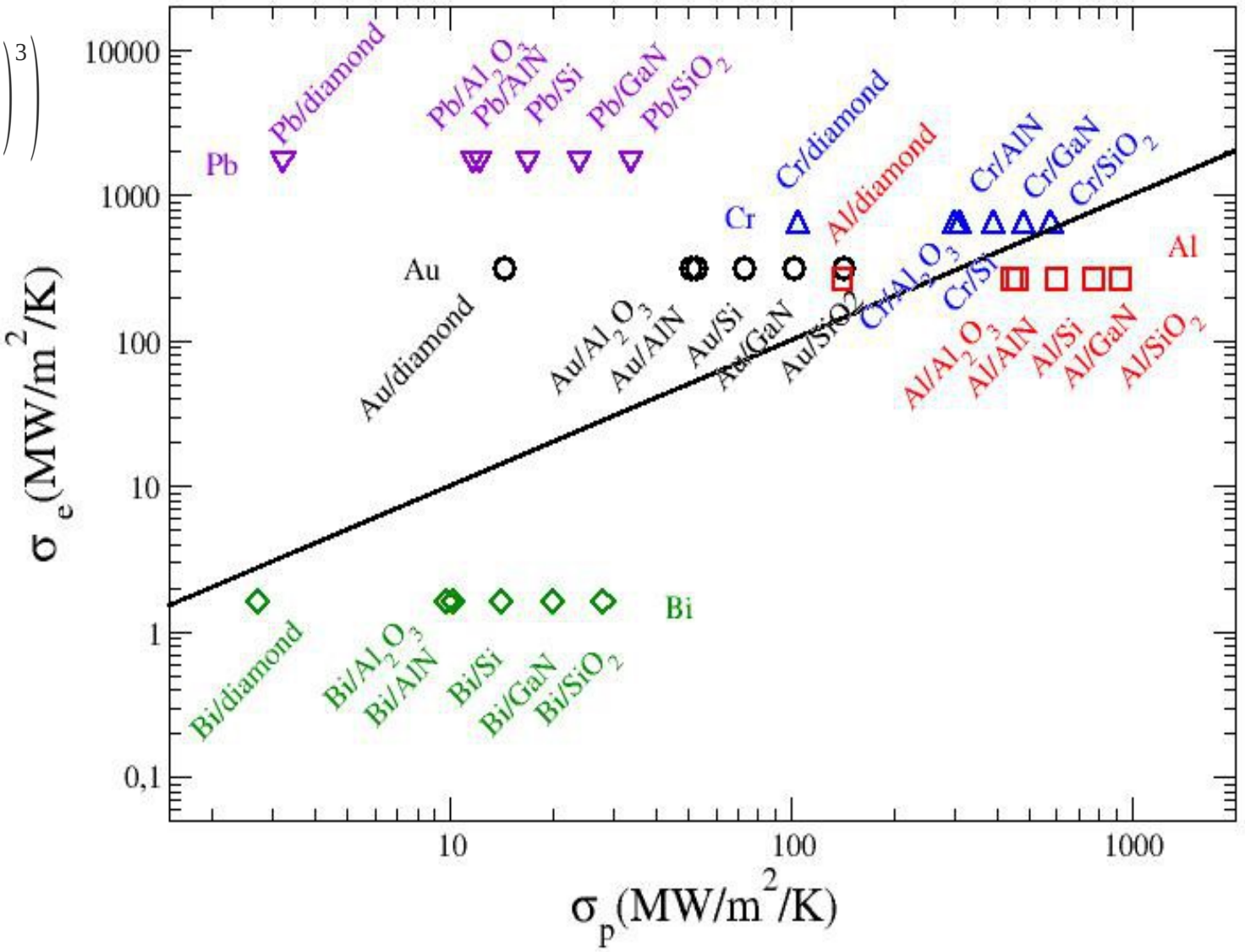
$$x = h$$

$$J = -k_s \partial_x T_s = \sigma_e (T_e - T_s) + \sigma_p (T_p - T_s)$$
$$= -k_e \partial_x T_e - k_p \partial_x T_p$$

J. Lombard et al. *J. Phys. Cond. Mat*. 2015

Two temperature model

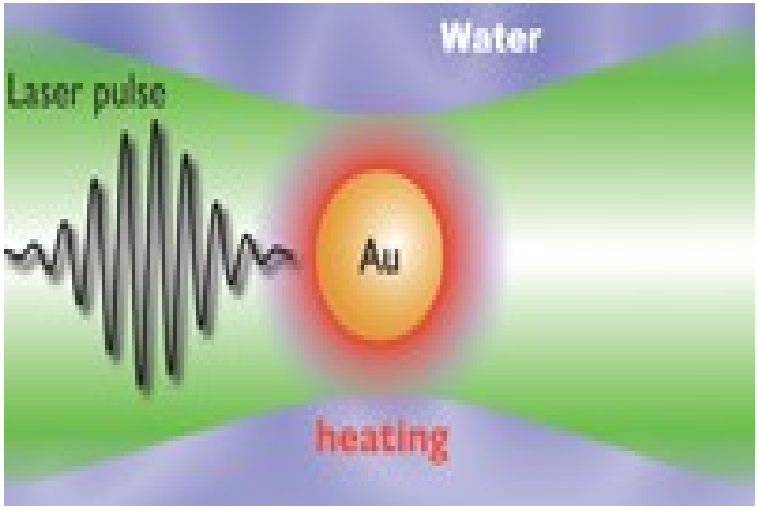
$$\sigma_e \propto \frac{\bar{h}}{k_B} \frac{\gamma u_L}{\tau_{e-ph}} \left(1+2\left(\frac{u_L}{u_T}\right)^3\right)$$



J. Lombard et al. *J. Phys. Cond. Mat*. 2015

Heat transport at solid/liquid interfaces

Heat transfer at solid/liquid interfaces

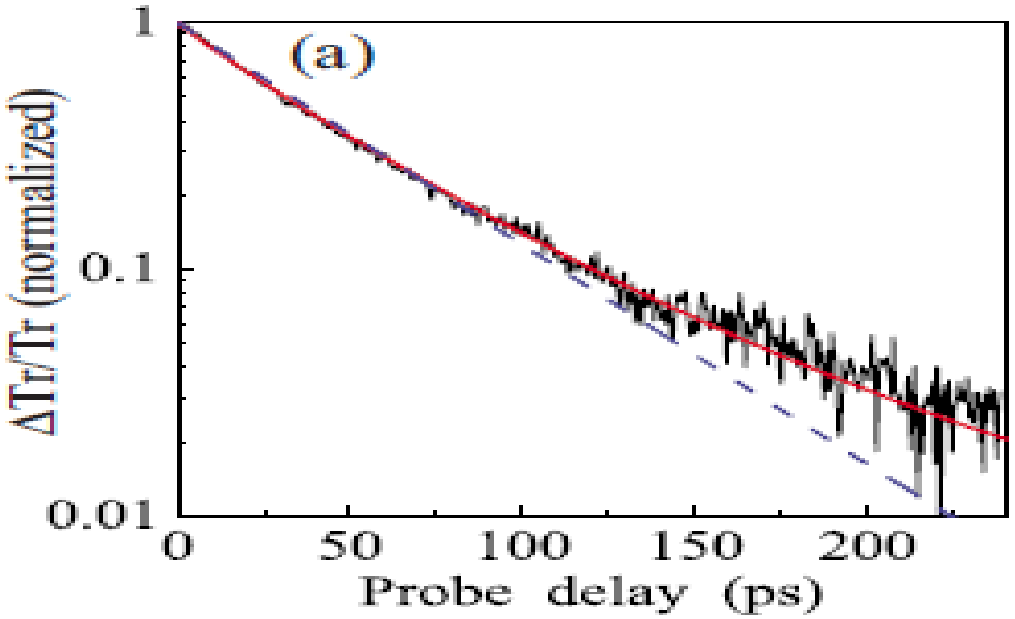


	<100 fs	100 fs	1 ps	10 ps	100 ps	1 ns	>1 ns
Electron heating	Energy absorption by electrons						
Electron-phonon coupling		Lattice heating and increase of particle temperature					
Phonon-phonon coupling			Heat transfer from particles to its surroundings				

Wen, *Int. J. Hyperthermia*, 2009

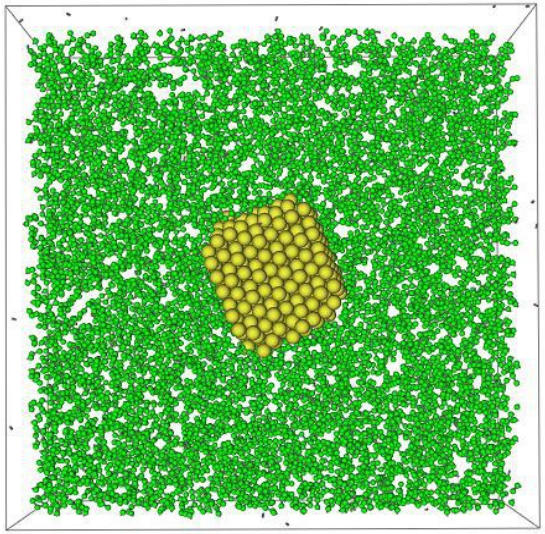
$$\frac{\partial T_p(t)}{\partial t} = -\frac{3G}{Rc_p}[T_p(t) - T_m(R,t)],$$

$$c_m \frac{\partial T_m(r,t)}{\partial t} = \Lambda_m \frac{1}{r}\frac{\partial^2}{\partial r^2}[rT_m(r,t)],$$

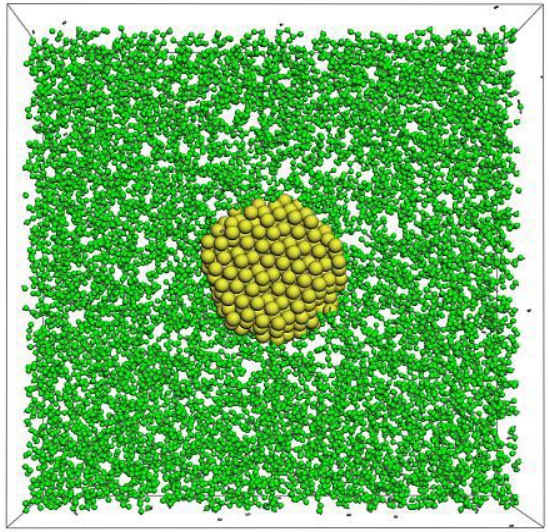


Molecular dynamics results

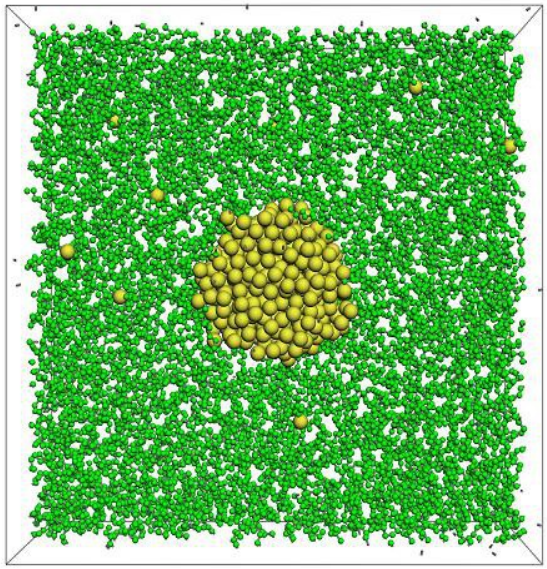
$300\,K$
$0\,nW$



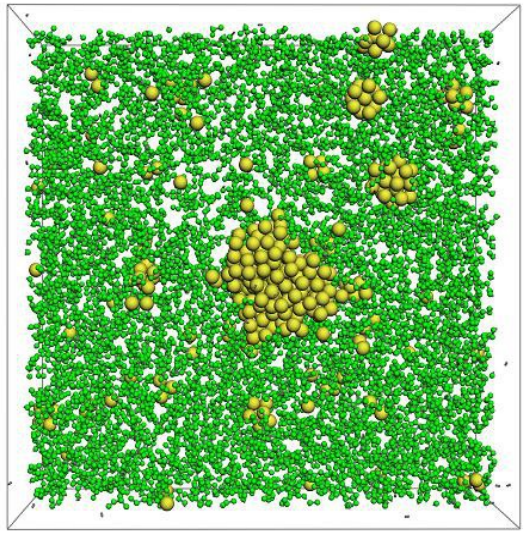
$800\,K$
$400\,nW$



$1200\,K$
$600\,nW$



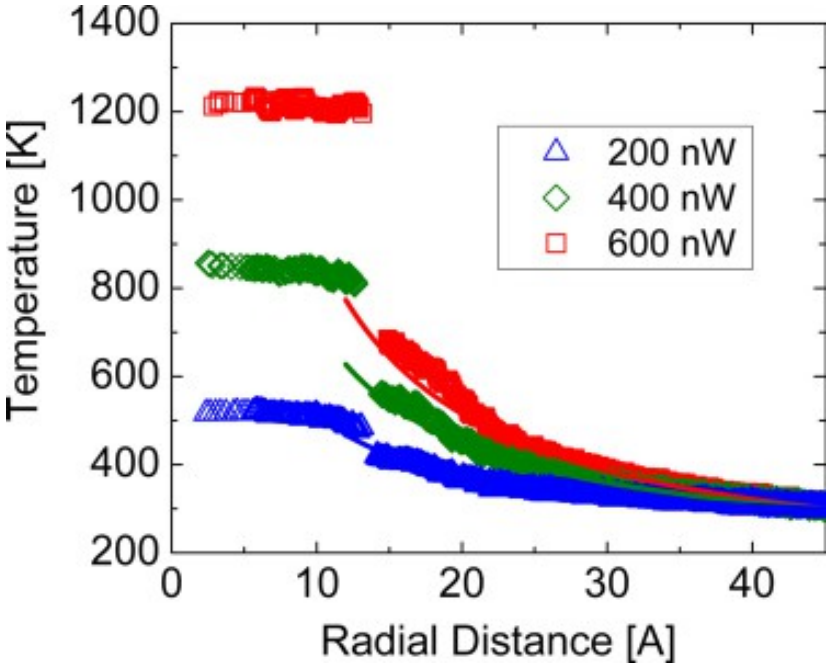
$1000\,nW$

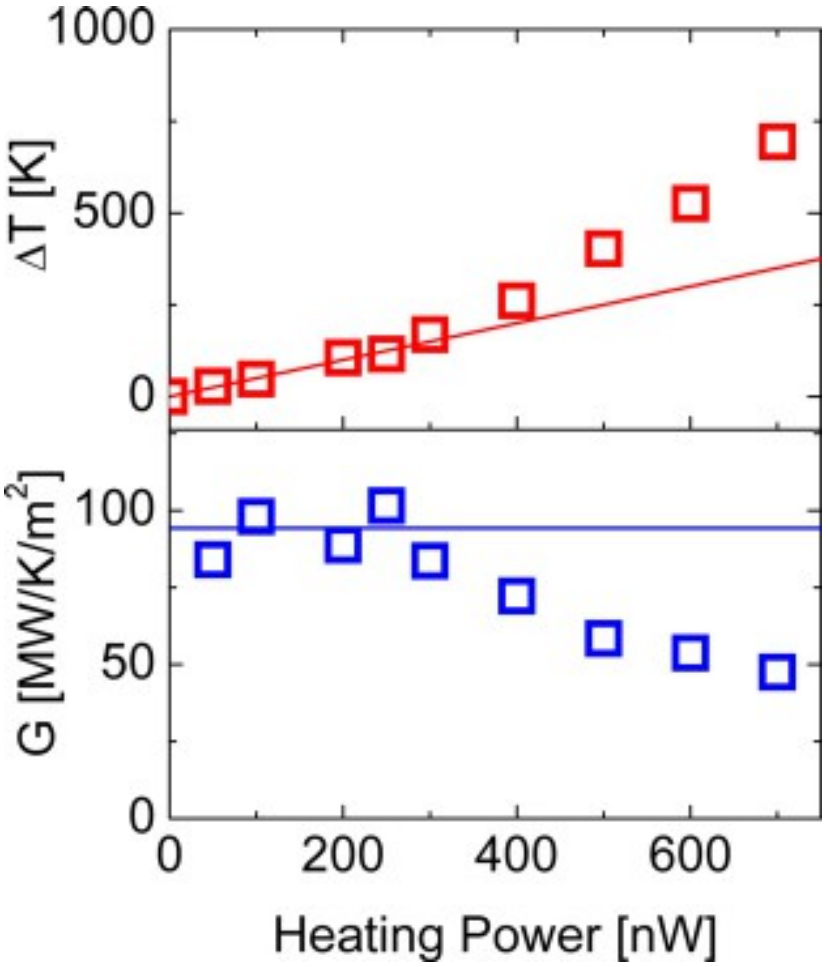


Gold Np in octane

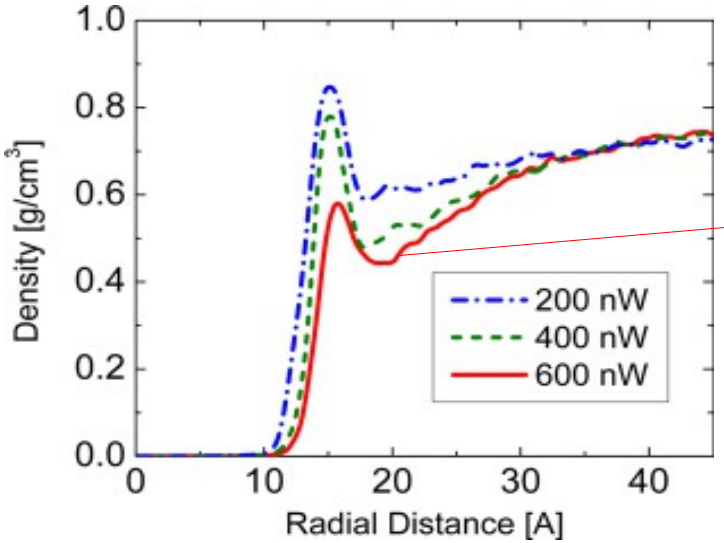
SM et al., PNAS 2009

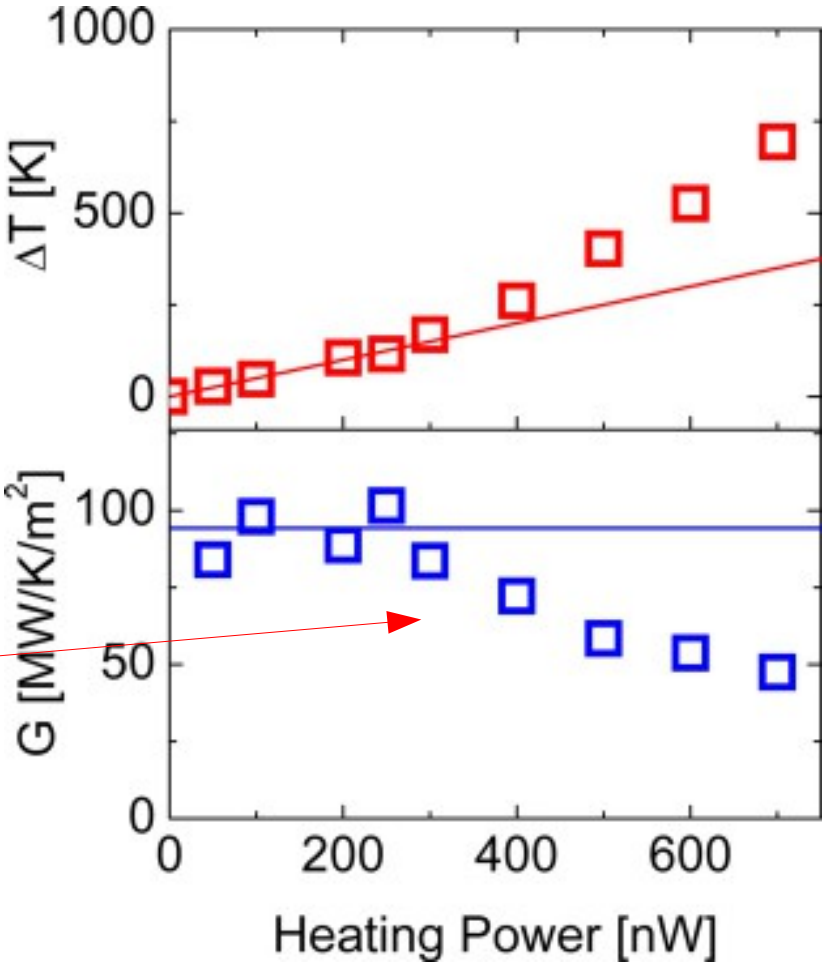
Gold nanoparticles in liquid octane



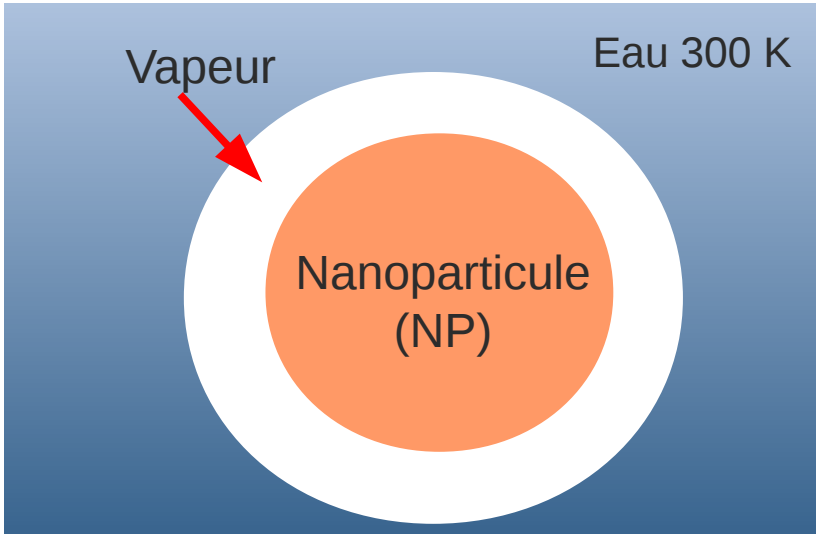


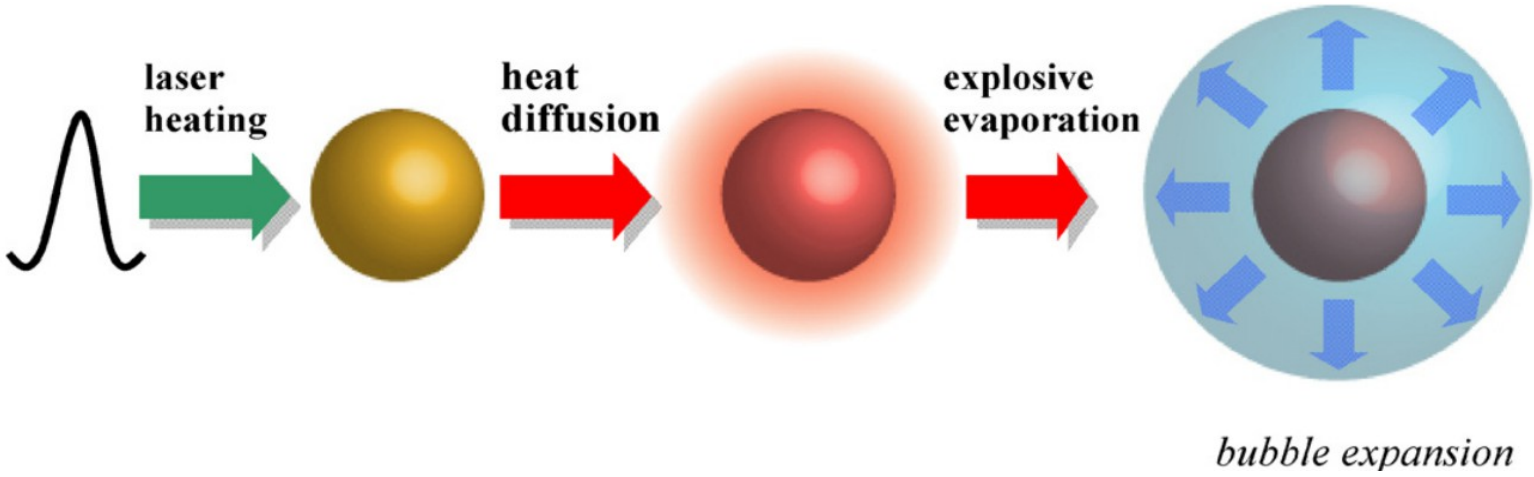
Gold nanoparticles in liquid octane





Nanobubbles

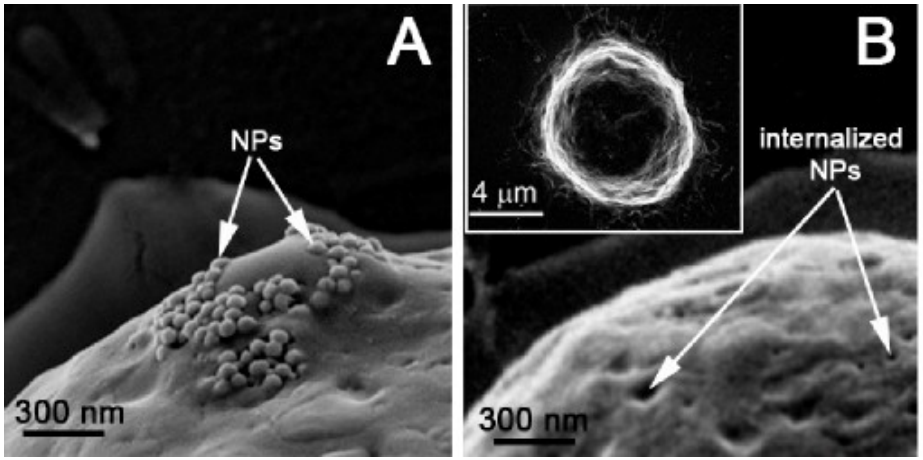


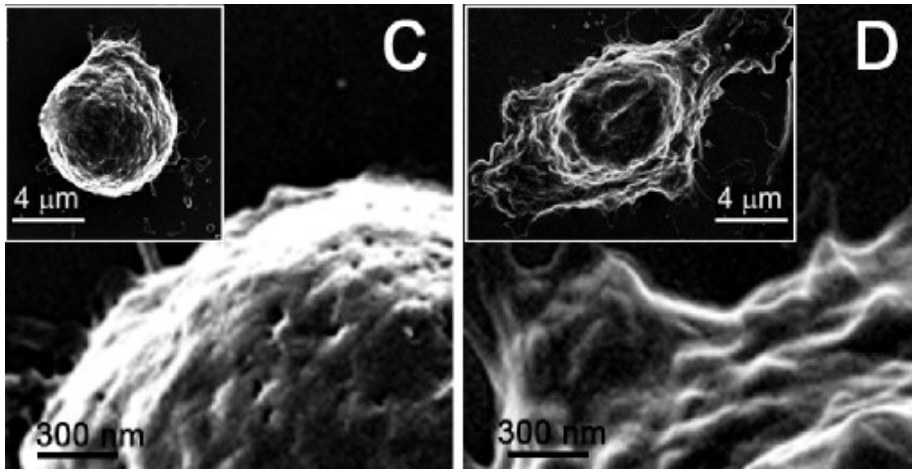


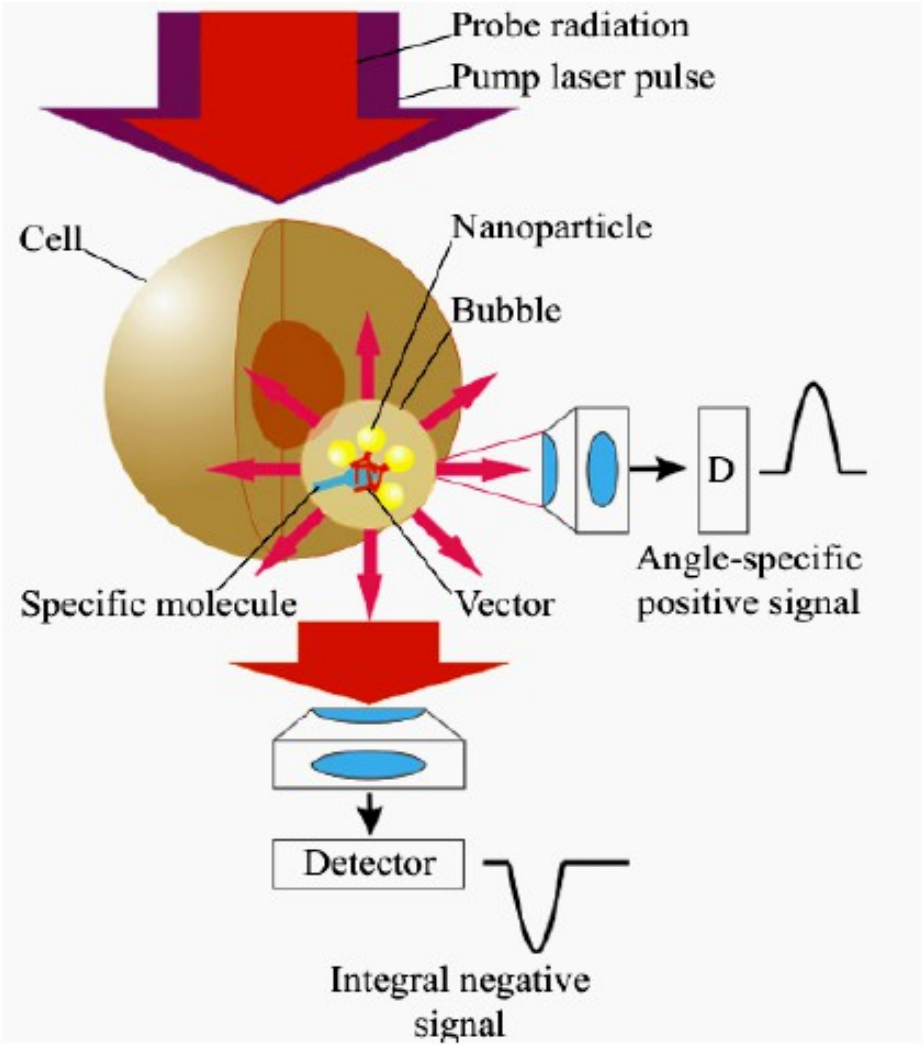
Hashimoto et *al.*, *J. of Photochemistry and Photobiology C: Photochemistry Reviews* (2012)

Biomedical applications

Diagnostic and tumor therapy



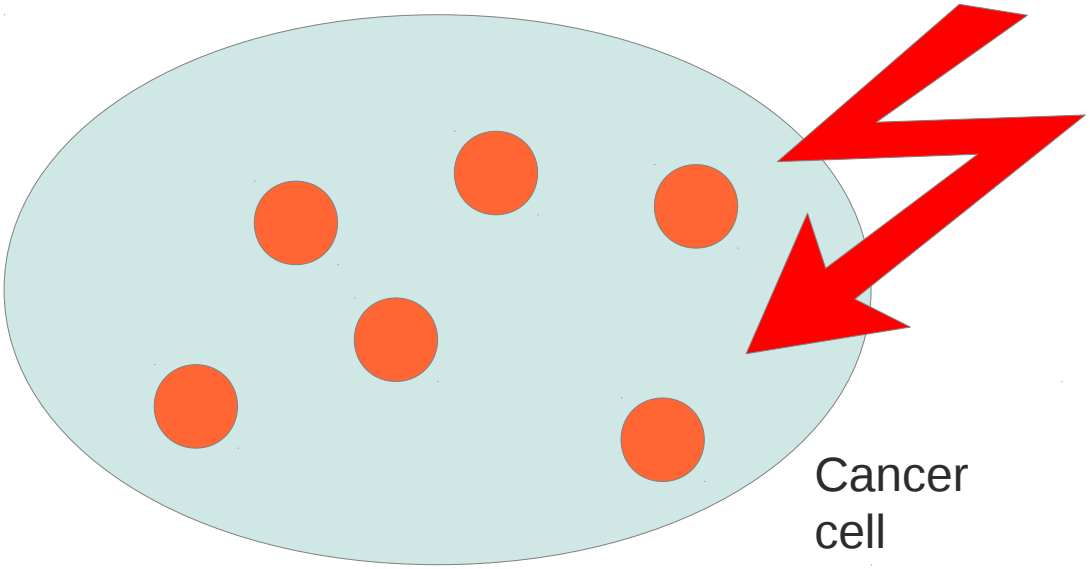




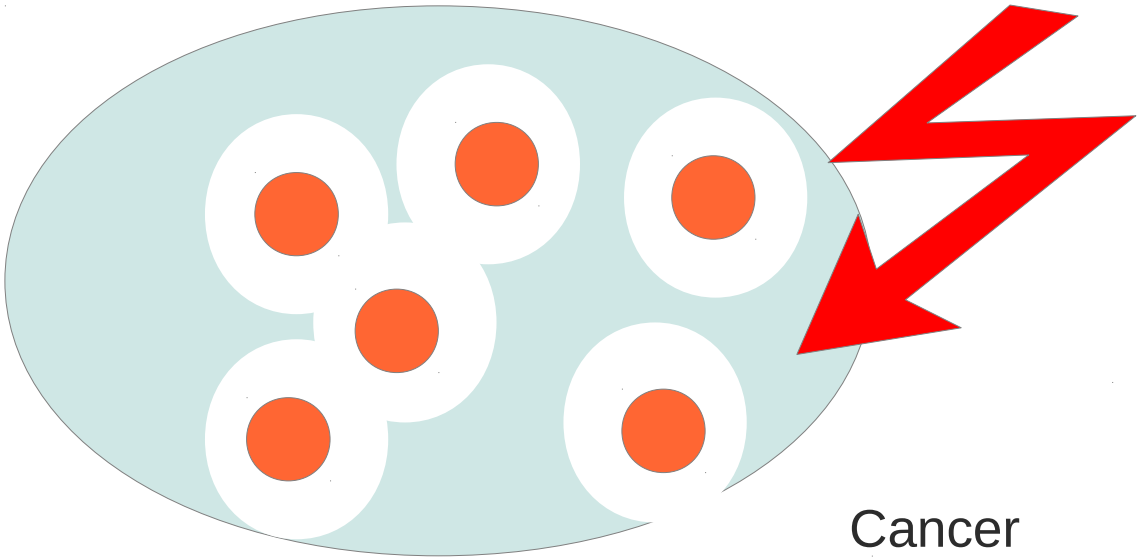
Lapotko et al., *ACS Nano* (2010)
Lapotko, Cancer (2011)

Questions

Threshold energy to drive nanobubble generation ?



What does control nanobubbles size ?



- => hydrodynamic models (phase field)

Fluid modeling

Ø Conservation equations : mass, momentum and energy

$$\frac{\partial \rho}{\partial t} = -\nabla(\rho \mathbf{v})$$

$$\frac{\partial(\rho_m \mathbf{v})}{\partial t} = -\nabla(\rho_m \mathbf{v}.\mathbf{v} + \overline{\Pi} - \overline{\sigma})$$

$$\rho_m \, C_v[\frac{\partial T}{\partial t} + (\mathbf{v}.\nabla)T] = -l \, \nabla.\mathbf{v} + \nabla(\lambda \nabla T) + \eta(\nabla \mathbf{v})^2$$

Ø Capillary effects : density functional theory

$$f(\rho, T) = f_{VdW}(\rho, T) + \frac{1}{2} w |\nabla \rho|^2 + f_{surface}$$

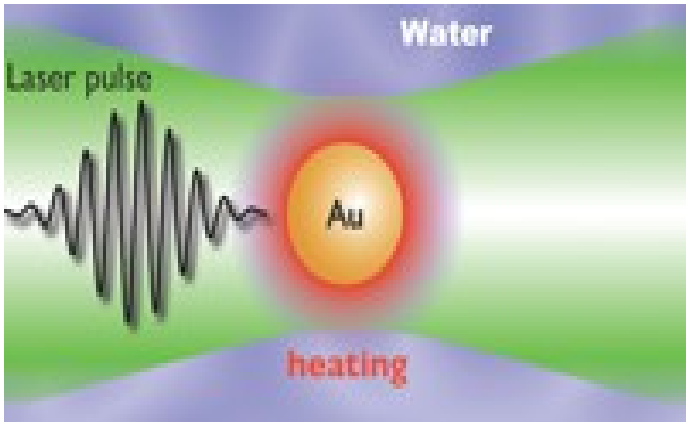
Pressure tensor : $\Pi_{\alpha\beta} = \left(\rho \frac{\partial f}{\partial \rho} - f \right) \delta_{\alpha,\beta} + w \partial_\alpha \rho \partial_\beta \rho$

Nanoparticle modeling

$$\frac{4}{3}\pi R_{np}^3 \; C_p^{np} \; \frac{dT_{np}}{dt} = P_{pulse} H(t_{pulse} - t) - 4\pi R_{np}^2 \; \Phi_{th}$$

LASER

Liquid/nanoparticle interface : interfacial conductance

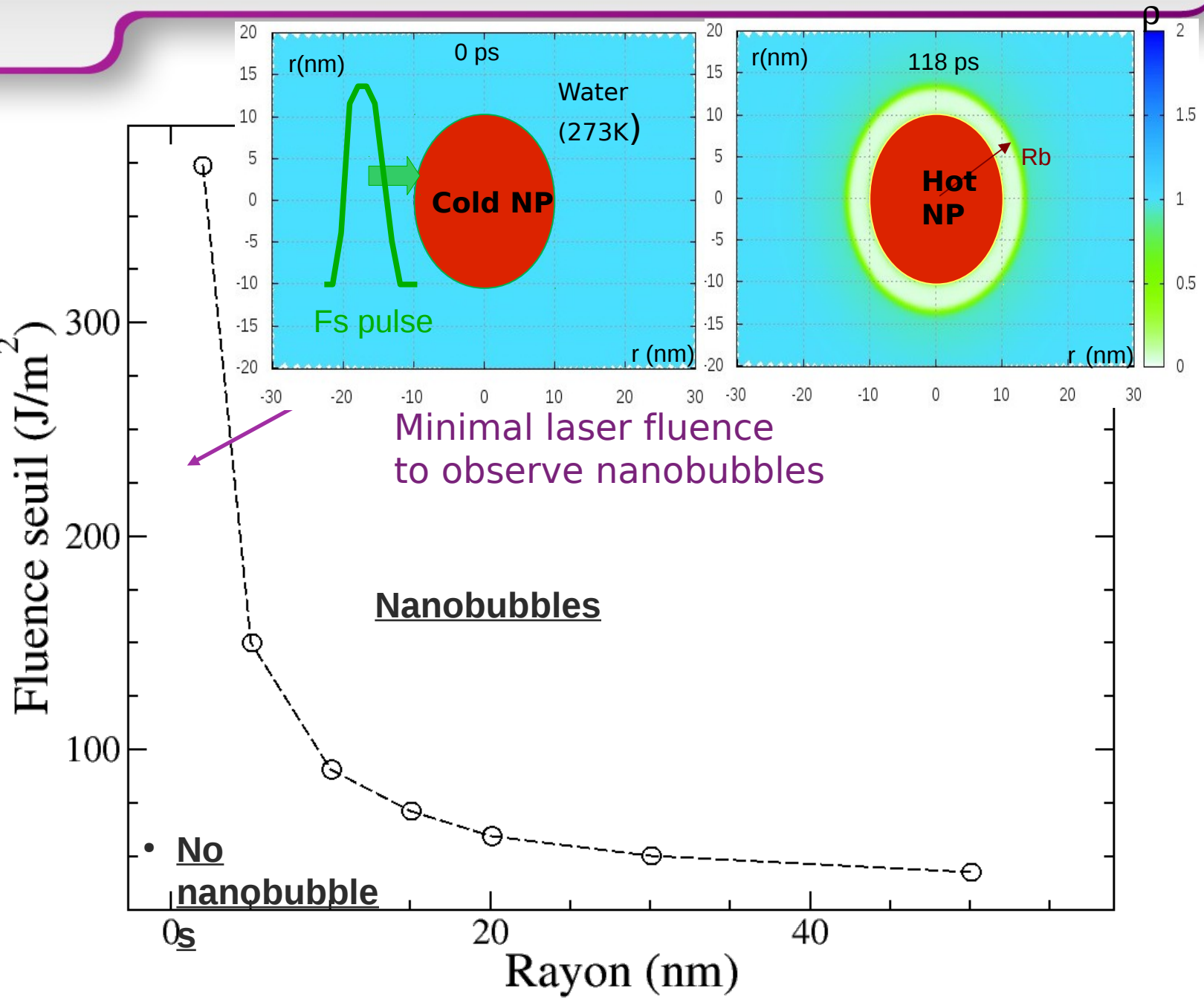


$$\Phi_{conductance} = G_0(1 + cos\theta)\,(T_{np} - T_{surface})$$

Vapor/nanoparticle interface : ballistic thermal transport

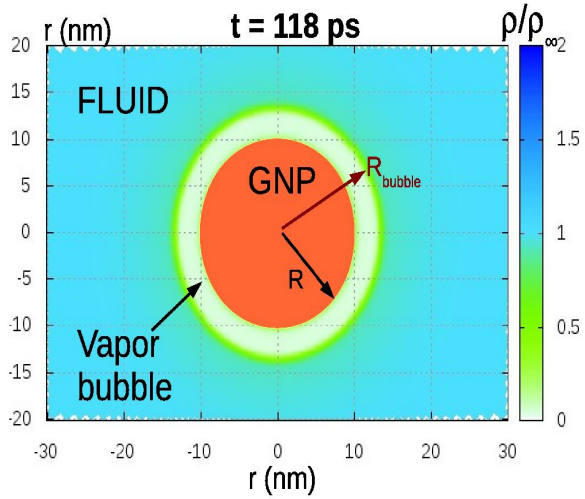
$$\Phi_{bal} = \rho_{vap}\sqrt{\frac{2}{m}}\left((k_B T_{np})^{\frac{3}{2}} - (k_B T_{r=R_{bulle}})^{\frac{3}{2}}\right)$$

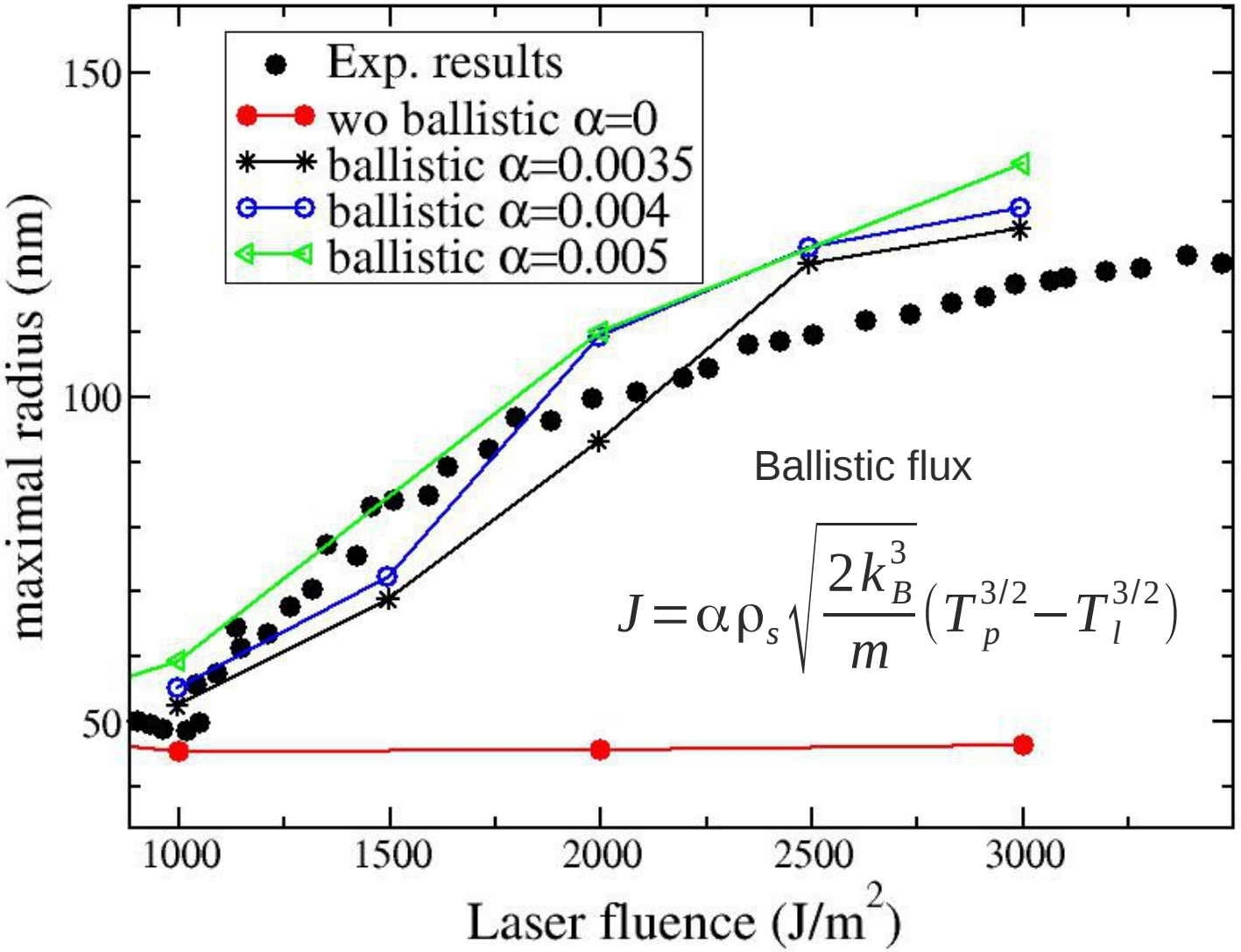
Threshold for explosive boiling



J.Lombard, T. Biben, SM, PRL (2014)

Maximal size of the nanobubbles





Experimental results : A. Siems et al., *New J. Phys.* 2011

Thank you for your attention !