Relaxation rate in ultra thin silicon membrane

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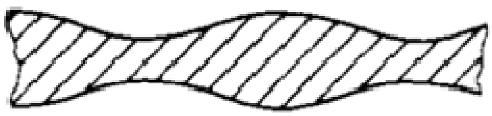
CREATING A DIMENSION OF INFINITE POSSIBILITIES

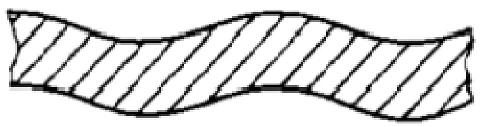
Motivation

Confined acoustics phonons

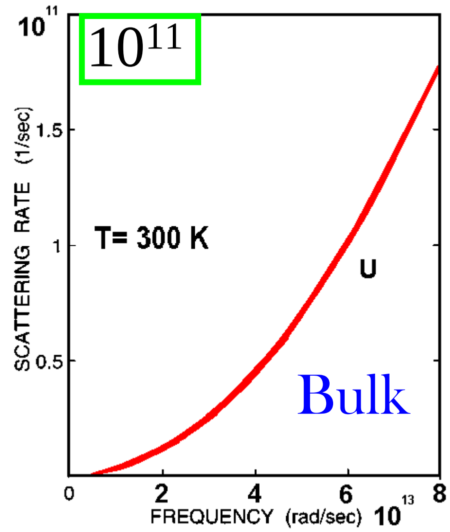
Symmetric

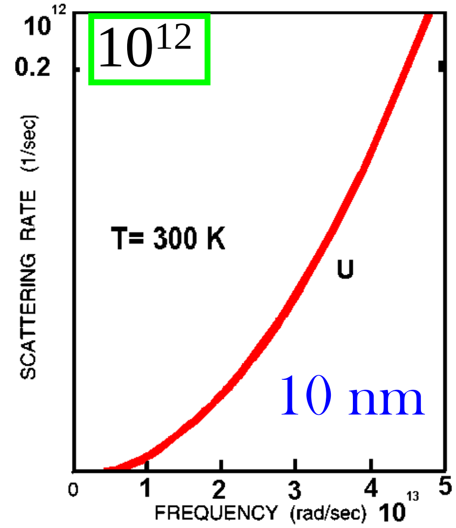


Antisymmetric



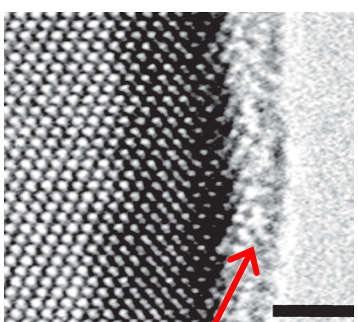
Modification of phonon lifetimes



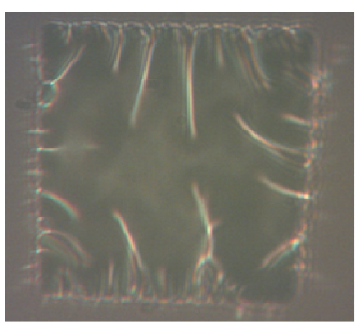


A. Balandin et al, PRB 58(1998) 1544

Effect of native oxide on dispersion relation

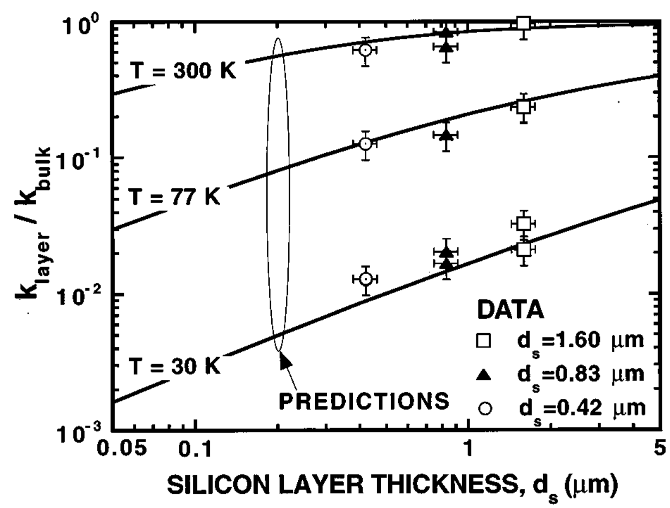


Native oxide



30 nm

Heat transport in nm scale



M. Asheghi APL, 71(1997), 1798

Motivation

Modification of dispersion relation (phonon engineering)

Modification of group velocity

Modification of relaxation rate

Thermal conductivity

Improve ZT

Outline

- ♣ **Theory:**
  - – Elastic continuum model
  - – Equation of motion
  - – Dispersion relation

- ♣ Relaxation rate & Thermal conductivity:
  - – Scattering mechanisms: Umklapp & Normal
  - – Relaxation rate for U-processes
  - – Thermal conductivity

- ♣ Numerical results: discussion

- ♣ Conclusions

Theory

Elastic continuum theory

- Stress-strain relationship
- "Macroscopic model" i.e. continuum-based and isotropic
- Well-suited for nanoscale confinement studies

Stress tensor   Elastics Tensor

$$T_{ij} = C_{ijkl} S_{kl}$$

Strain tensor

Isotropic media

$$T_{ij} = \lambda S_{kk} \delta_{ij} + 2\mu S_{ij}$$

Motion equation :

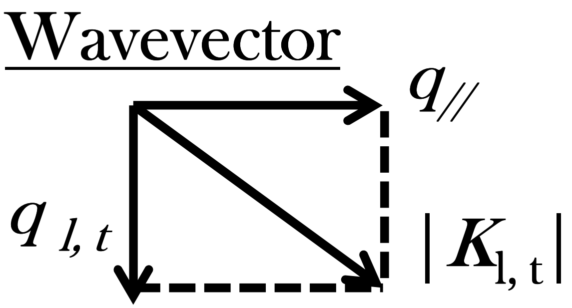
$$\partial^2 U / \partial t^2 = S_T^2 \nabla^2 U + (S_L^2 - S_T^2) \nabla (\nabla \cdot U)$$

$$S_T = \sqrt{(\lambda + 2\mu)/\rho}$$

$$S_L = \sqrt{\mu/\rho}$$

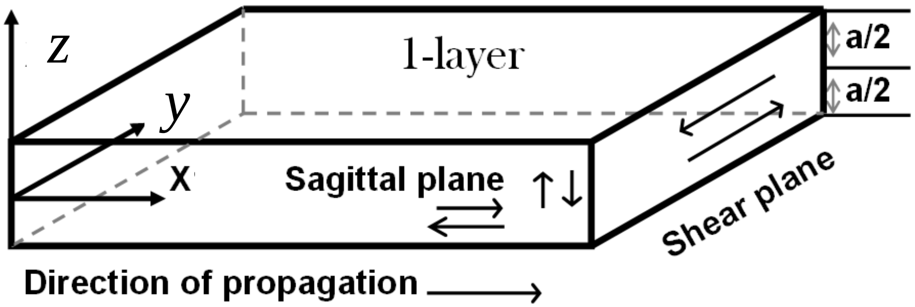
U = Vector amplitude of displacement
ρ = Density
λ, μ = Lamé constants
S_T, S_L = Transversal and longitudinal sound speed

Single Layer Solutions



$$\partial^2 U/\partial t^2 = S_T^2 \nabla^2 U + (S_L^2 - S_T^2)\nabla(\nabla \cdot U)$$

$$\omega = S_{L,T}\left|K_{l,t}\right| = S_{L,T}\sqrt{q_{//}^2 + q_{l,t}^2}$$



$$T_{iz}\Big|_{z=surface} = 0$$

$$i = x, y, z$$

Solutions

$U_y(z) = A\sin(q_z z)$ *or* $B\cos(q_z z)$ *Shear Waves*

$U_x(z) = iAq\cos(q_l z) + iBq_t\cos(q_t z)$ *Dilatational Waves*

$U_z(z) = -Aq_l\sin(q_l z) + Bq\sin(q_t z)$

Coupled solutions

$U_x(z) = iAq\sin(q_l z) + iBq_t\sin(q_t z)$ *Flexural Waves*

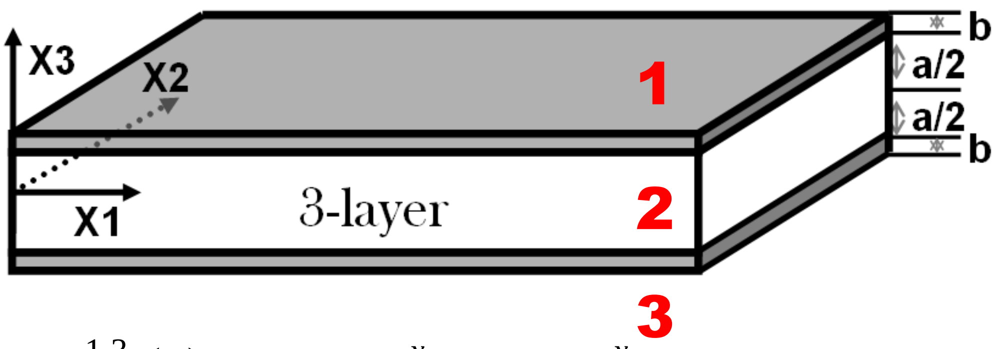
$U_z(z) = Aq_l\cos(q_l z) - Bq\cos(q_t z)$

Coupled solutions

J.L. Rose, *Ultrasonic waves in solid media*, Cambridge University press, UK, 2004

Three layer Solutions

$$T_{iz}\big|_{z=surface} = 0$$



$$T_{iz}^{1}\big|_{z=interface} = T_{iz}^{2}\big|_{z=interface}$$

$$U_{i}^{1}\big|_{z=interface} = U_{i}^{2}\big|_{z=interface}$$

$$i = x, y, z$$

$$U_x^{1,3}(z) = DW^x + FW^x$$

$$U_z^{1,3}(z) = DW^z + FW^z$$

$$U_x^{2}(z) = DW^x \text{ or } FW^x$$

$$U_z^{2}(z) = DW^z \text{ or } FW^x$$

$$+ \begin{matrix} B.C \\ C.C \end{matrix} + \omega = S_{T,L}^{1,2}\sqrt{q_{t,l}^{1,2\,2} + q_{//}^{2}} = \boxed{\begin{matrix}12\\ \text{equations}\end{matrix}}$$

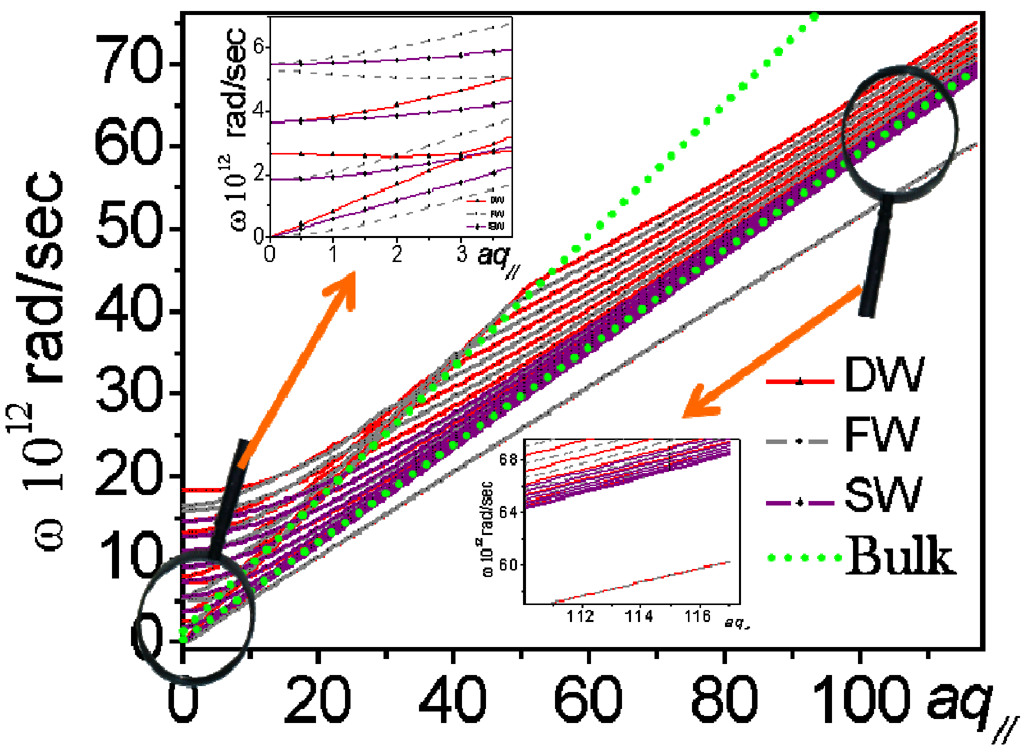
System symmetry → 6 linear equations, i.e., 6x6 matrix.

$DW^{x(z)}$: Dilatational Waves solutions en x (z) components .
$FW^{x(z)}$: Flexural Waves solutions en x (z) components.
B. C. : Boundary Conditions.
C. C. : Continuity Conditions.

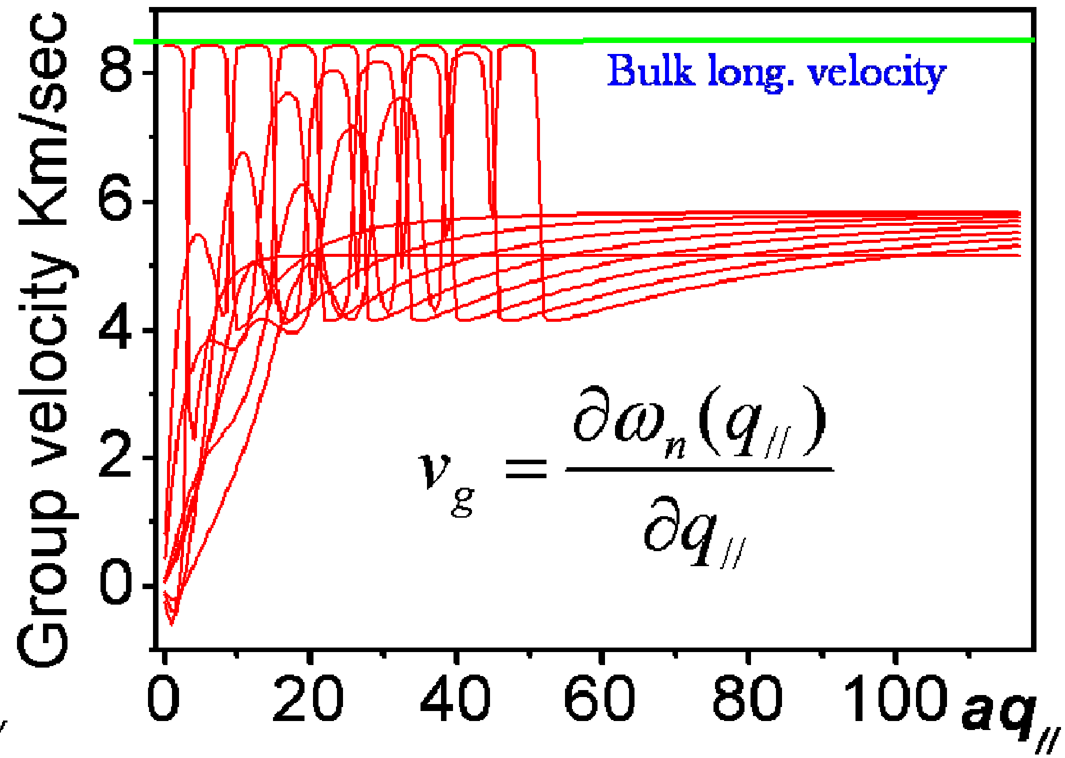
L. Donetti, F. Gámiz, J. B. Róldan and A. Godoy, J Appl. Phys. 100 (2006), 013701

Dispersion Relation & Group velocity

Sagittal & Shear Waves



Group Velocity: Dilatational Waves



Confinement → More modes, hybridization of sagittal waves !

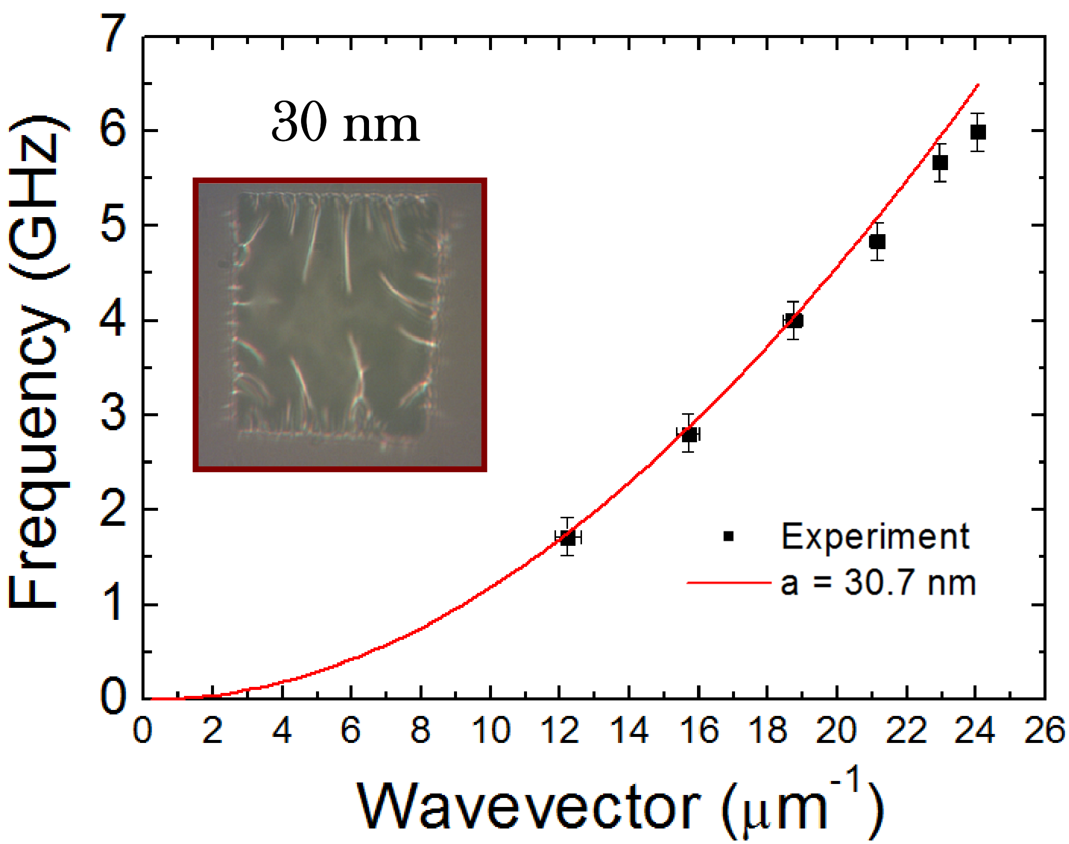
→ Group velocity (v_g) dependant on $q_{//}$

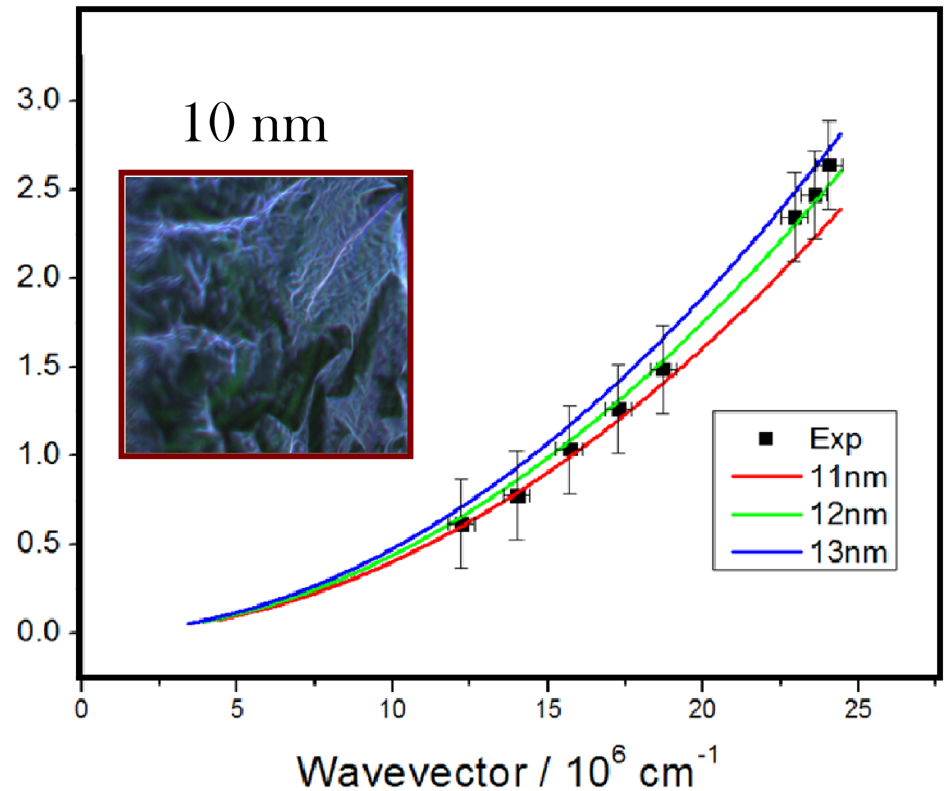
DW: Dilatational Waves
FW: Flexural Waves
SW: Shear Waves

S_L=8.440 kms^{-1}, S_T=5.845 kms^{-1}, a=10 nm

Experimental Results & Theory

Flexural Waves





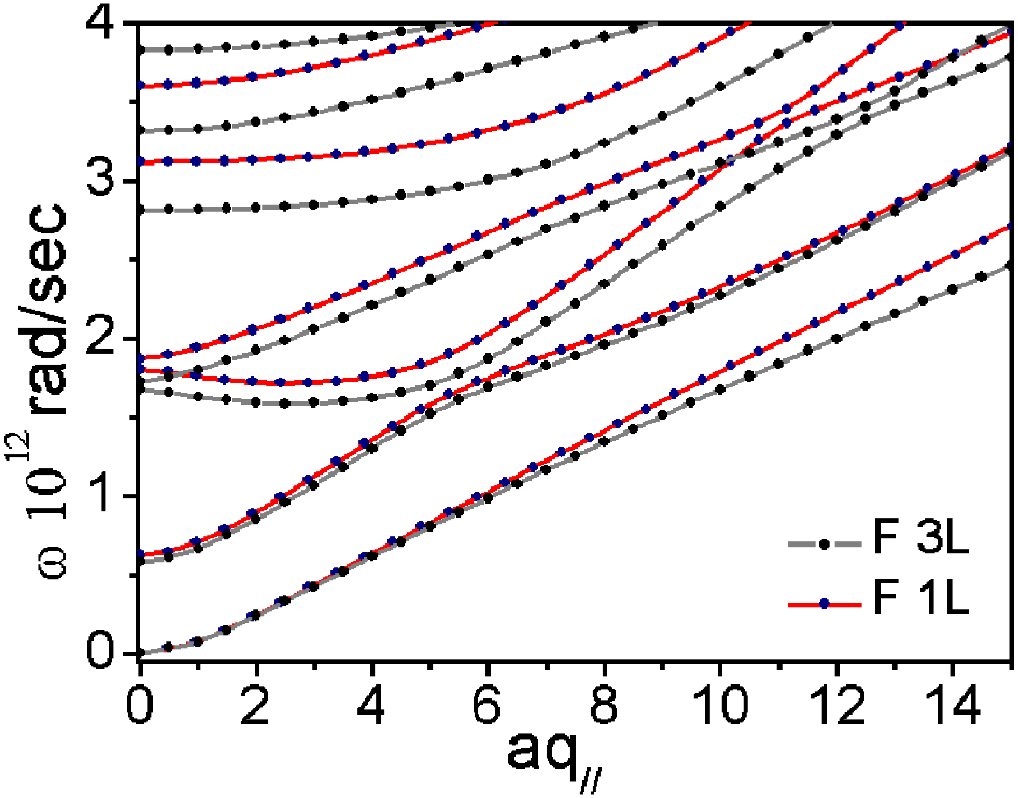
Good match between theoretical model and experiments

with VTT

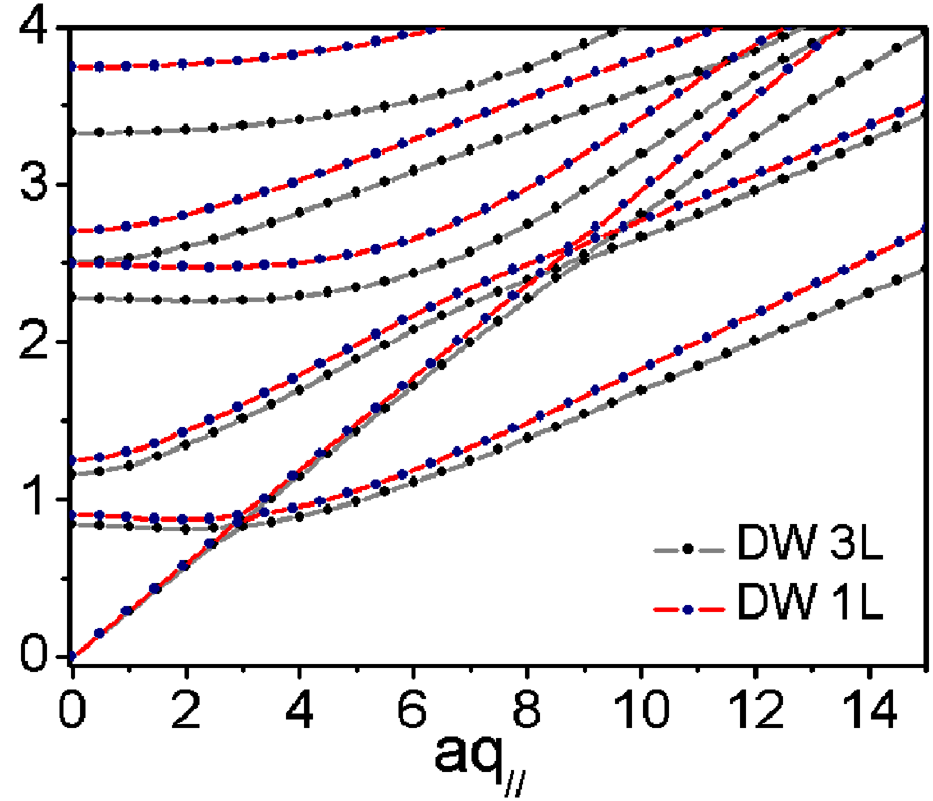
Dispersion of Confined Acoustic Phonons in Ultra-Thin Silicon Membranes, J. Cuffe *et al., in preparation*

Si v/s SiO_2-Si-SiO_2

Flexural Waves



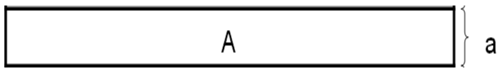
Dilatational Waves



Oxide effect: decrease of frequency for large $q_{//}$ & high order modes

a=28.5 nm

b=1.6 nm

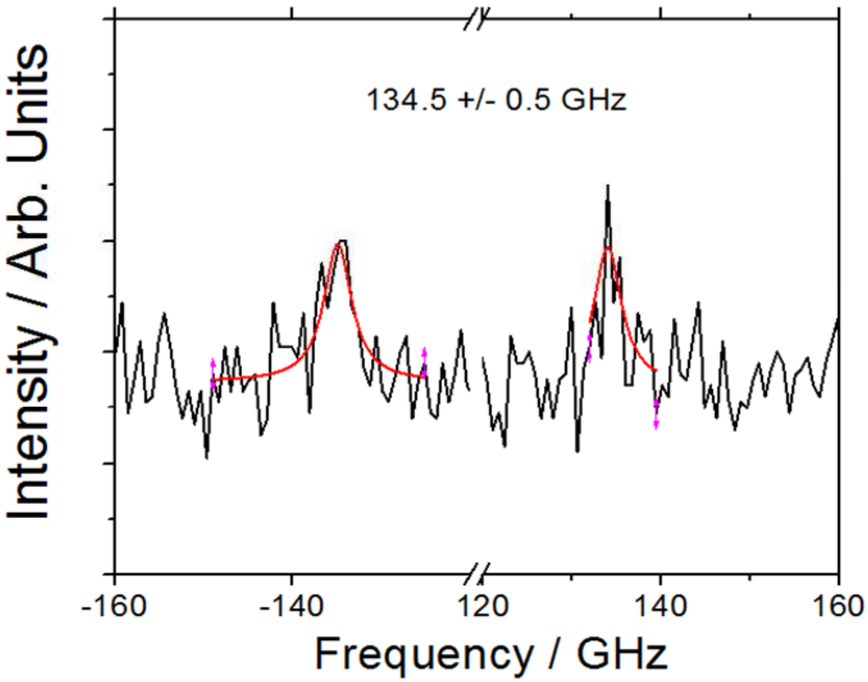


a=29.42 nm

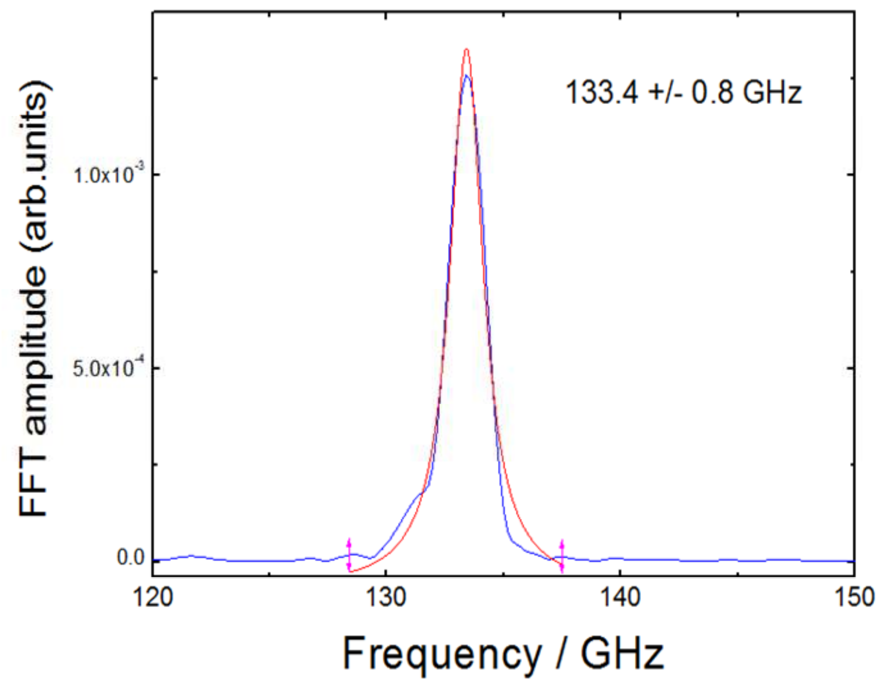
Experimental Results & Theory

30 nm Si membrane

Brillouin Scattering Spectroscopy



ASOPS technique

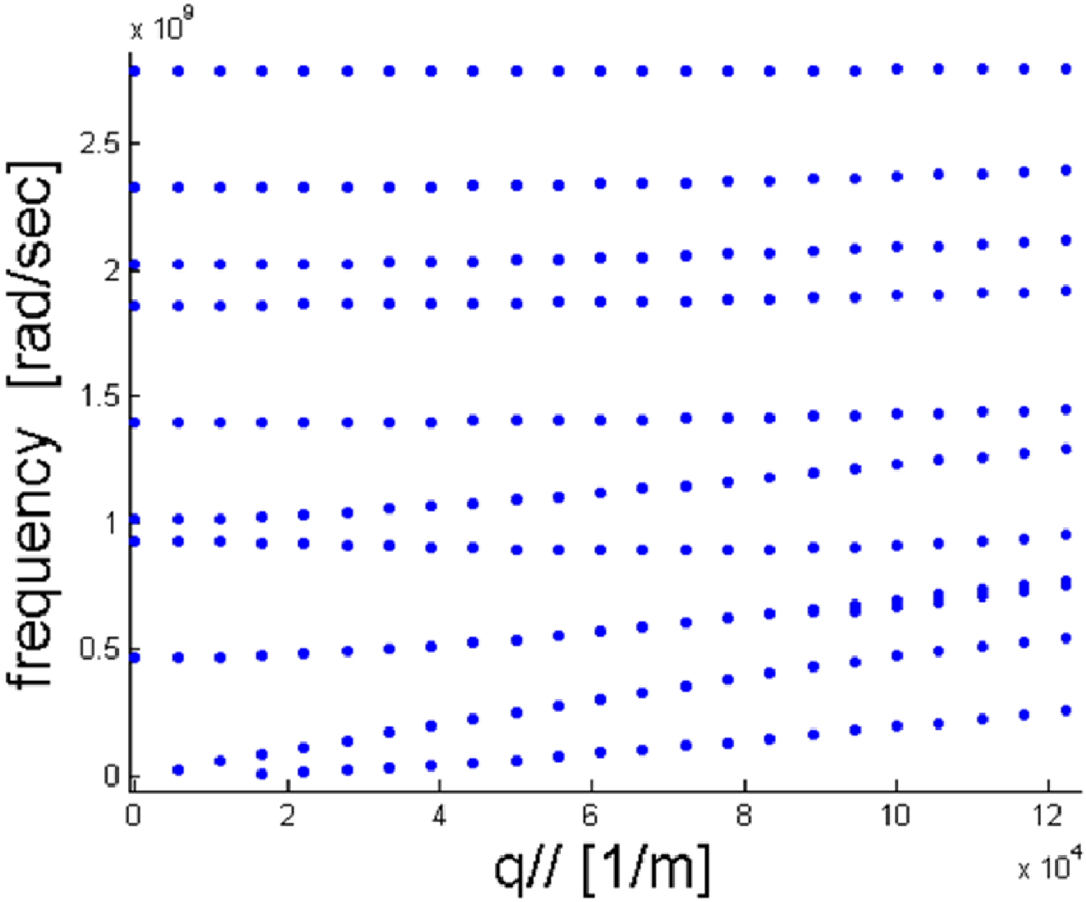


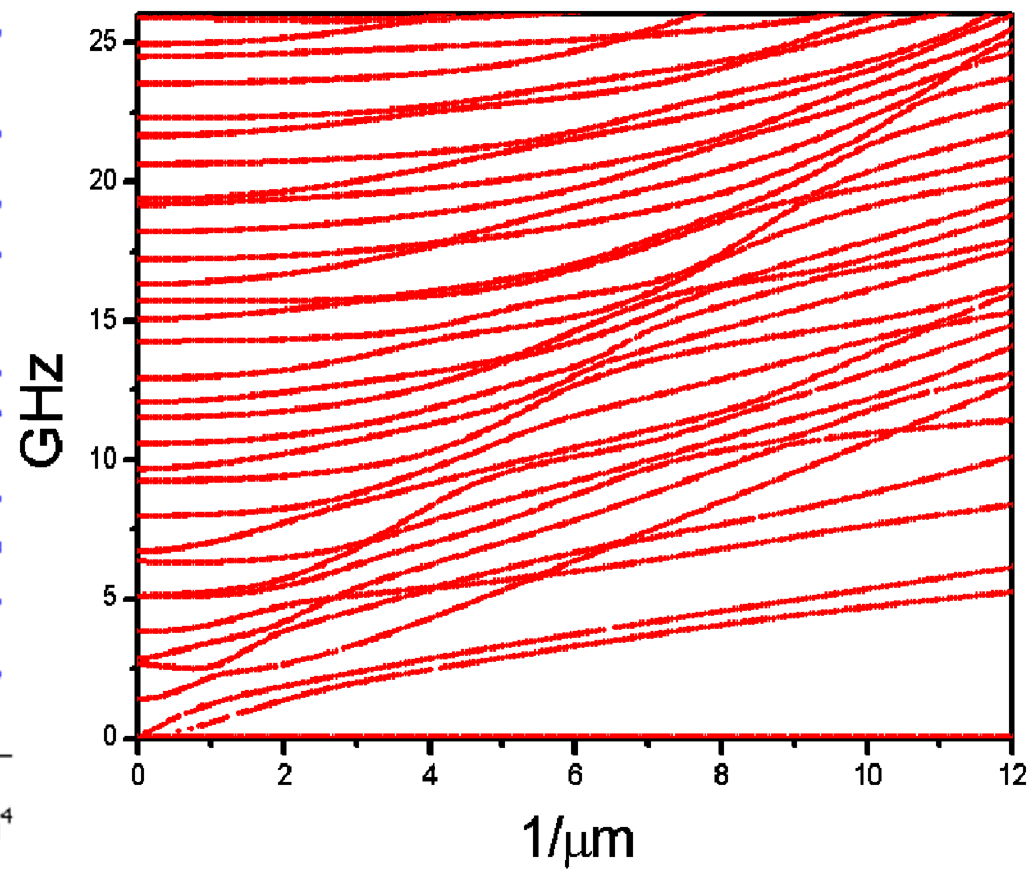
1-L Prediction: 143.5 GHz

3-L Prediction: 133.8 GHz

With: Universität Konstanz

Other systems





Sagittal Modes

Outline

- ♣ **Theory:**
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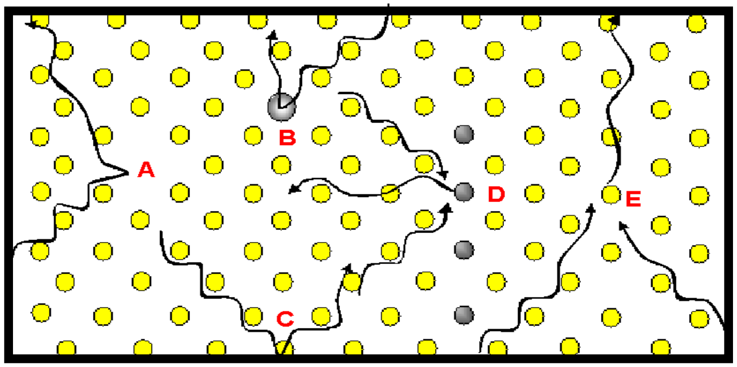
- ♣ Relaxation Rate & Thermal Conductivity:
  - – Scattering mechanisms: Umklapp & Normal
  - – Relaxation rate for U-processes
  - – Thermal Conductivity

- ♣ Numerical results: discussion

- ♣ Conclusions

Scattering Mechanisms

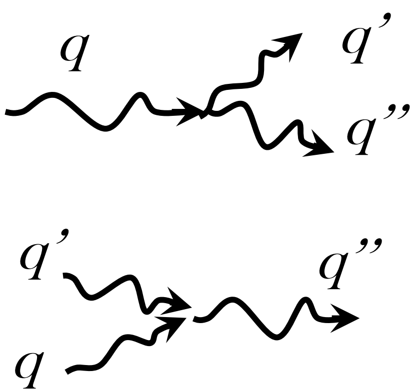


A: Lattice vacancy
B: Point defect
C: Crystal boundary
D: Umklapp
E: Normal

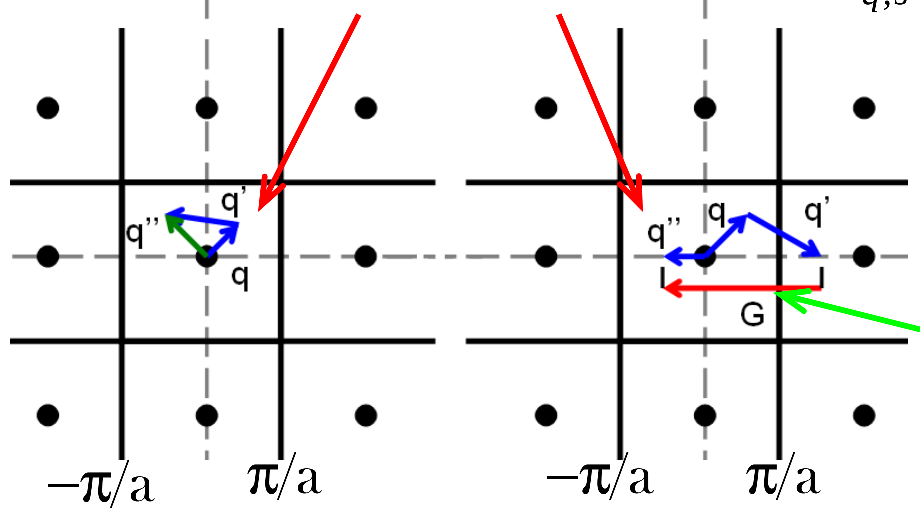
Matthiessen's rule & Thermal Conductivity

$$\frac{1}{\tau_{eff}} = \sum_j \frac{1}{\tau_j} = \frac{1}{\tau_U} + \frac{1}{\tau_b} + \frac{1}{\tau_i} + \dots$$

$$\kappa = \frac{1}{3} \sum_{q,s} v_{q,s}^2 \tau_{eff} C_V$$



1st Brillouin Zone



Lattice Vector

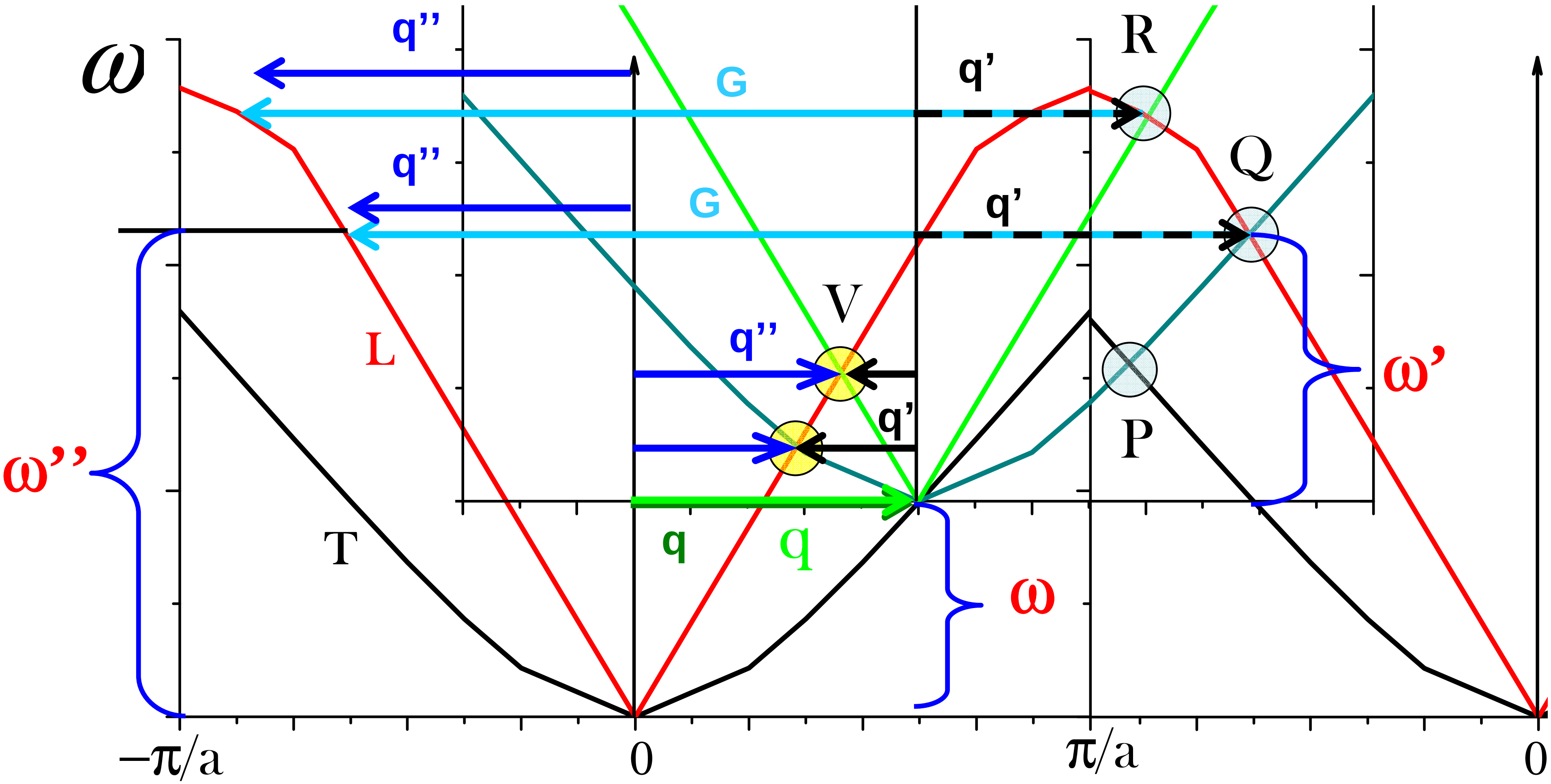
N-process U-process

Consequence of anharmonicity → Phonon-phonon interaction → Finite phonon lifetime

Possibilities:

1. Annihilation of two phonons and creation of a third phonon.
2. Annihilation of one phonon and creation of two phonons

Selection Rules: U & N-Process



U-process $\vec{q}+\vec{q}\,'=\vec{G}+\vec{q}\,''$

$\omega + \omega' = \omega''$

$\vec{q}+\vec{q}\,'=\vec{q}\,''$ N-process

$P: \; T_1 + T_2 \rightarrow T_2$ If T is degenerate

$Q: \; T_1 + T_2 \rightarrow L$ If T is degenerate

$R: \; T + L \rightarrow L$

$S: \; T_1 + T_2 \rightarrow L$ If T is degenerate

$V: \; T + L \rightarrow L$

Relaxation Rate & Thermal conductivity

$$\frac{1}{\tau_{U;q,s}} = \frac{\pi\gamma^2\hbar}{\rho N_0 \Omega \bar{v}^2} \sum_{q's',q''s'',G} \omega_{q,s}\omega_{q',s'}\omega_{q'',s''}(n_{q's'} - n_{q''s''})\delta(\omega_{qs} + \omega_{q's'} - \omega_{q''s''})\delta_{q+q',q''+G}$$

Phonon average group velocity

$$\bar{v}_s = \sum_q v_{qs} n_{qs} \Big/ \sum_q n_{qs}$$

Kinetic theory

$$\kappa = \frac{1}{3}\sum_{q,s} v_{q,s}^2 \tau_{eff} C_V$$

$$\kappa = \frac{\hbar\rho\bar{v}^2}{3\pi\gamma^2 k_B T^2} \sum_{qs} v_{qs}^2 \omega_{qs}^2 n_{qs}(n_{qs}+1) \left\{ \sum_{q's';q''s'';G} (n_{q's'} - n_{q''s''})\omega_{qs}\omega_{q's'}\omega_{q''s''}\delta(\Delta\omega)\delta_{q+q'-q'',G} \right\}^{-1}$$

More Branches → More interactions → Decrease thermal conductivity.

Change of group velocity (v_{qs}) → Change in thermal conductivity

A. AlShaikhi and G.P. Srivastava, *Phys. Rev. B,* 76 (2007), pp. 195205-1.

B. G. P. Srivastava, "*The Physics of Phonons*" , Taylor & Francis Group, NY, 1990.

Outline

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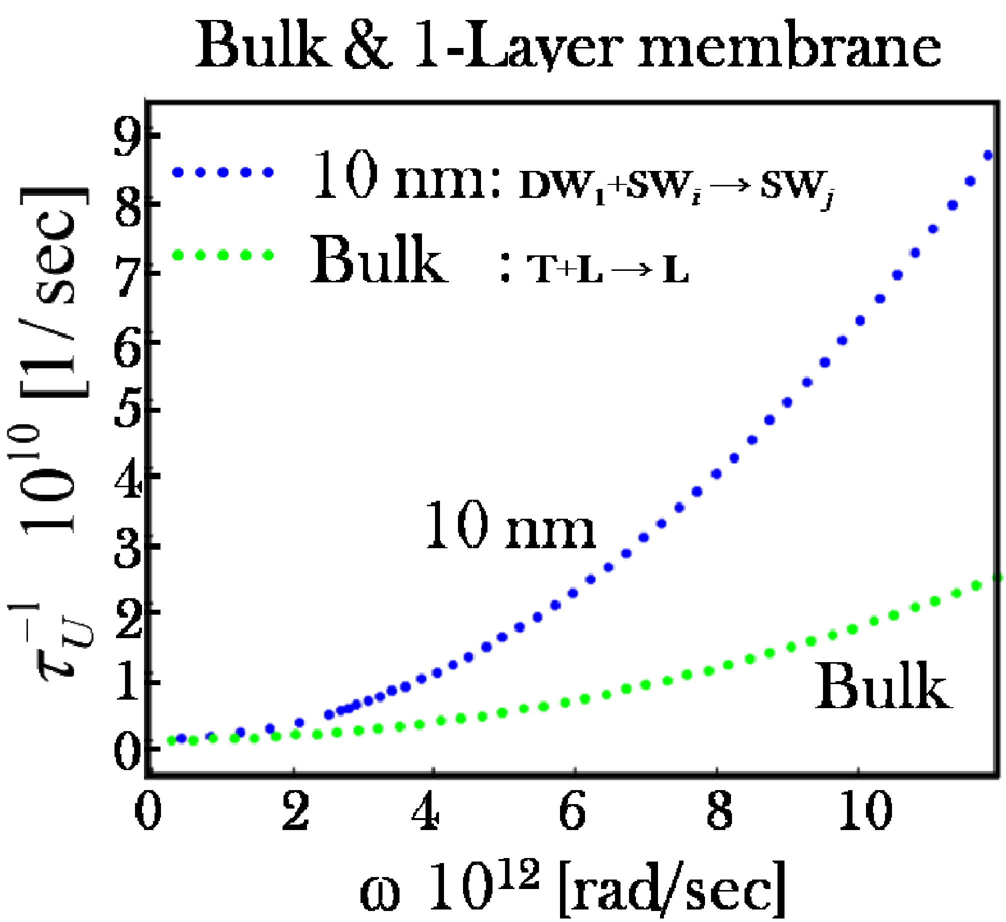
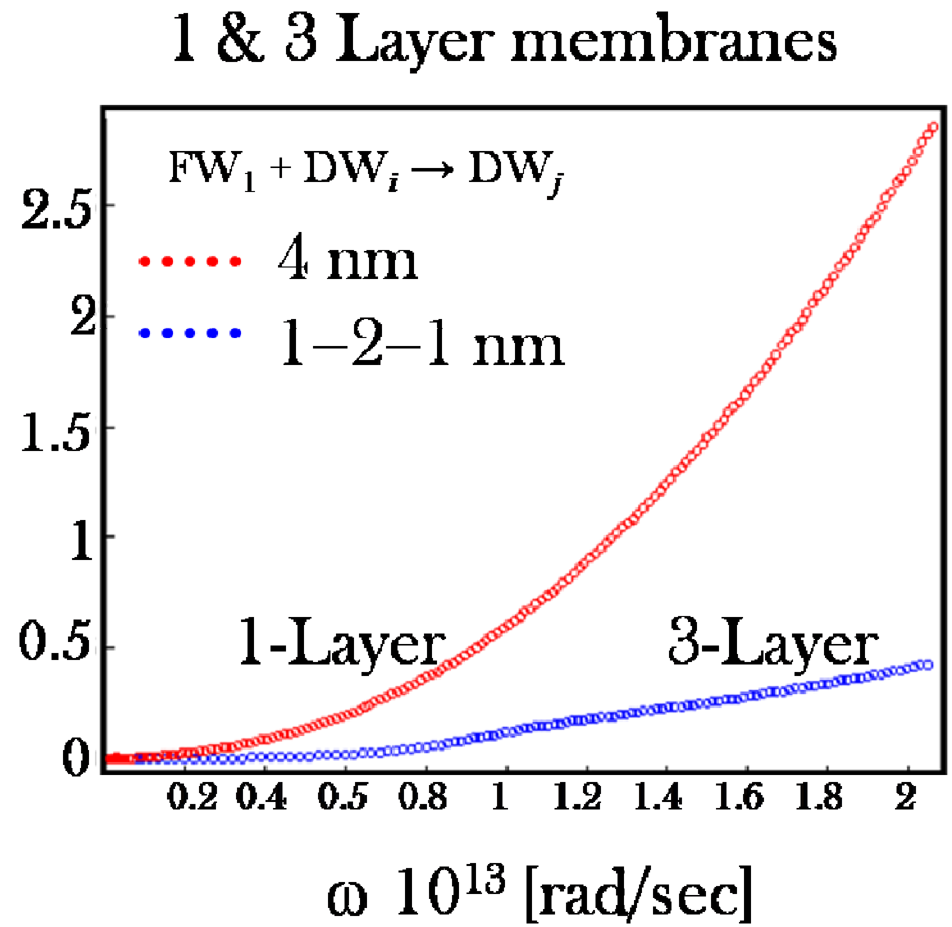
Results: Relaxation Rates

T= 300 K



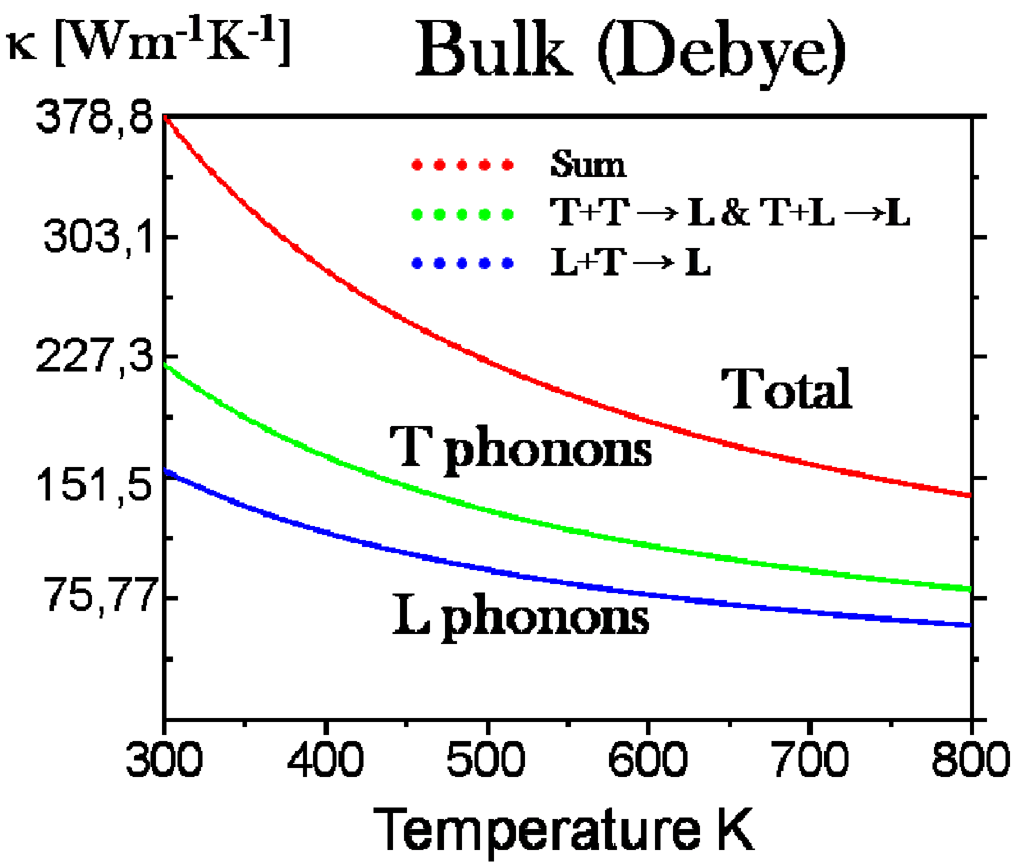


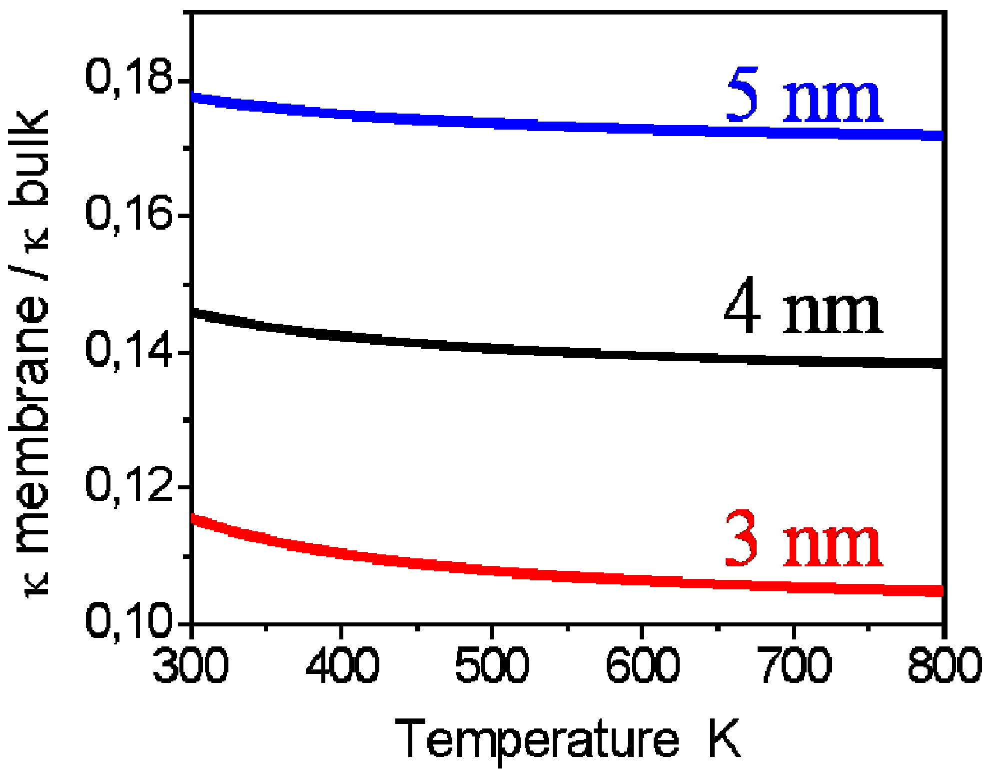
The modification of dispersion and group velocity lead to increase of relaxation rate compared with the bulk (left).

The decrease in frequency of 3-layer membrane lead to decrease on relaxation rate compared with 1-layer membrane (right).

Results: Thermal Conductivity

Intrinsic thermal conductivity

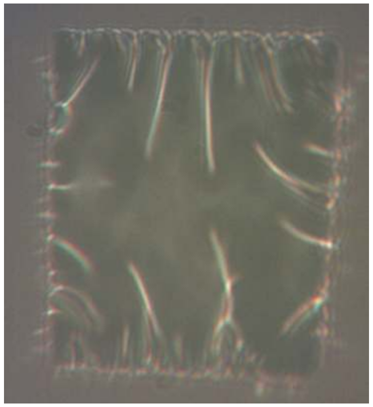




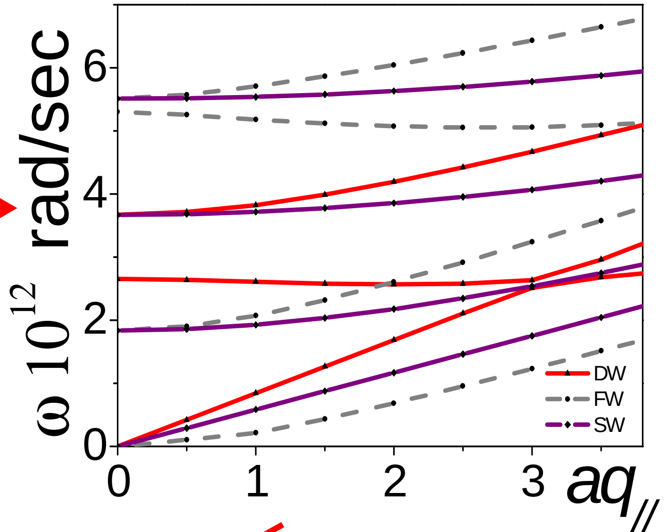
The numerical calculations predict a strong decrease of the thermal conductivity of a 1-layer membranes.

Summary

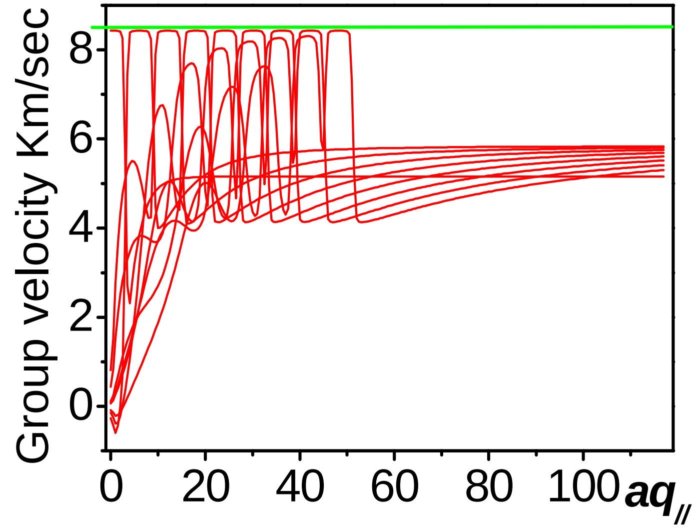
Spatial confinement



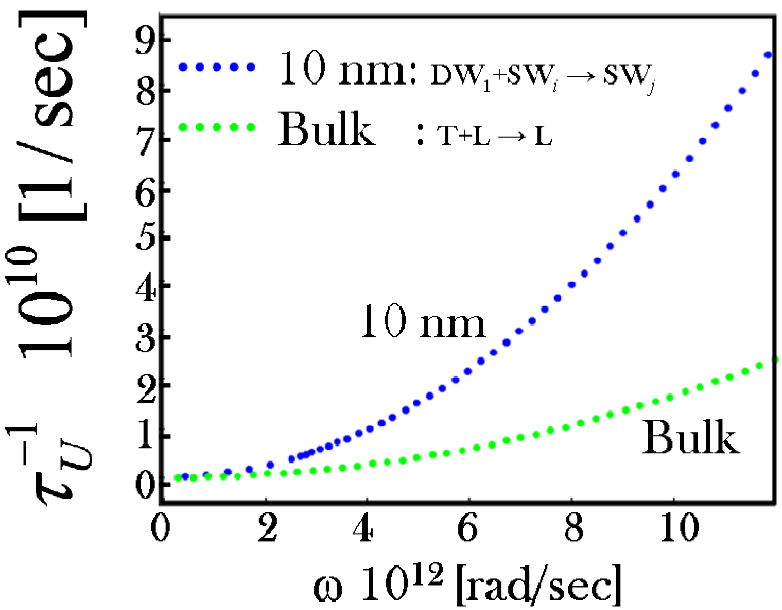
Modification of dispersion relation



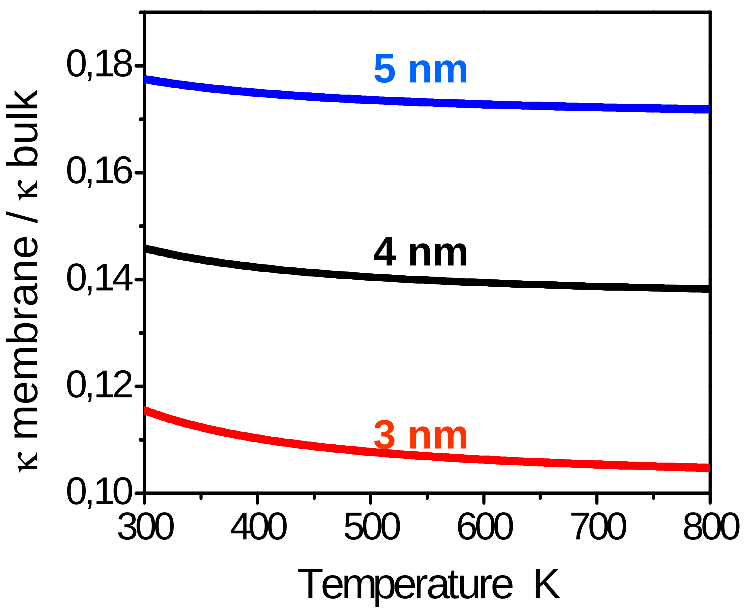
Modification of group velocity



Increase of relaxation rate



Decrease of thermal conductivity



Conclusions

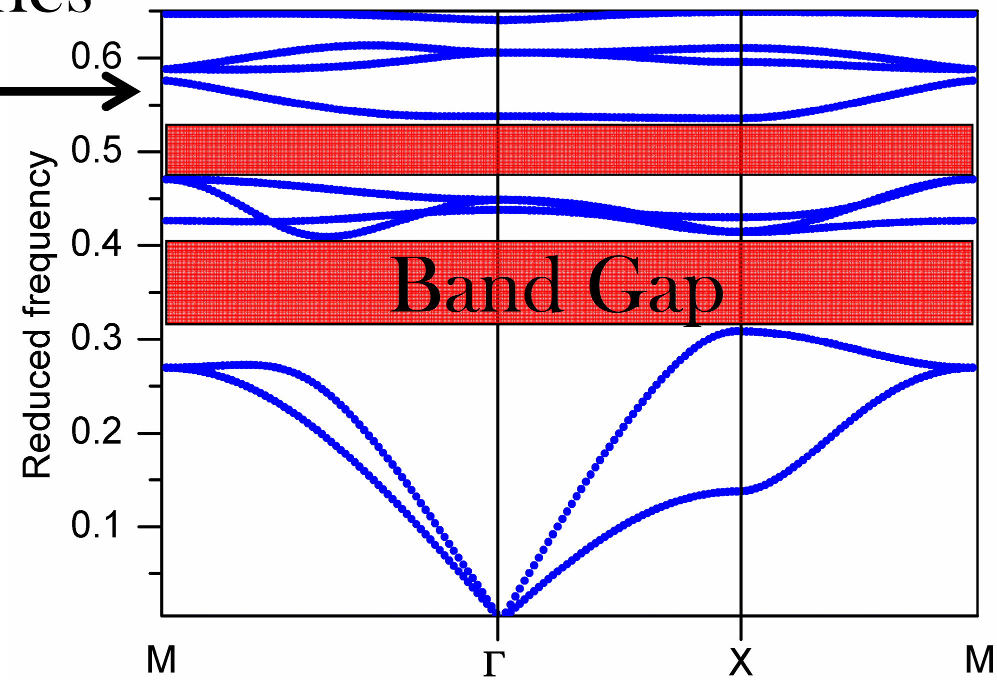
- ♣ Hybridization of sagittal waves.
- ♣ Group velocity dependence on $q_{//}$: $v_g(q_{//})$.
- ♣ Oxide effect: decrease of frequency for large $q_{//}$
  $\rightarrow$ Decrease in relaxation rate.
- ♣ The change in dispersion relation and the emergence of more branches implies an increase of phonon-phonon interactions. This causes an increase in relaxation rates and a corresponding decrease in the thermal conductivity.

Future Work

Phononic structures

PWE solutions

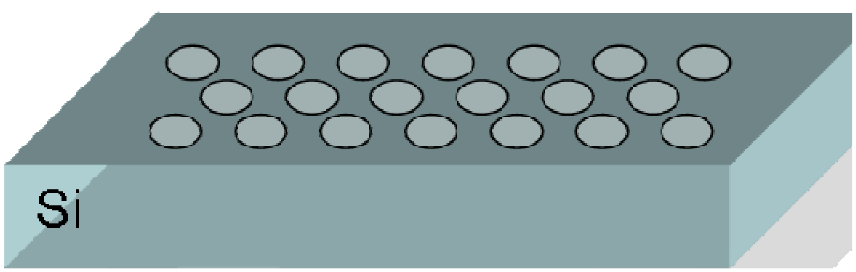
Flat Branches



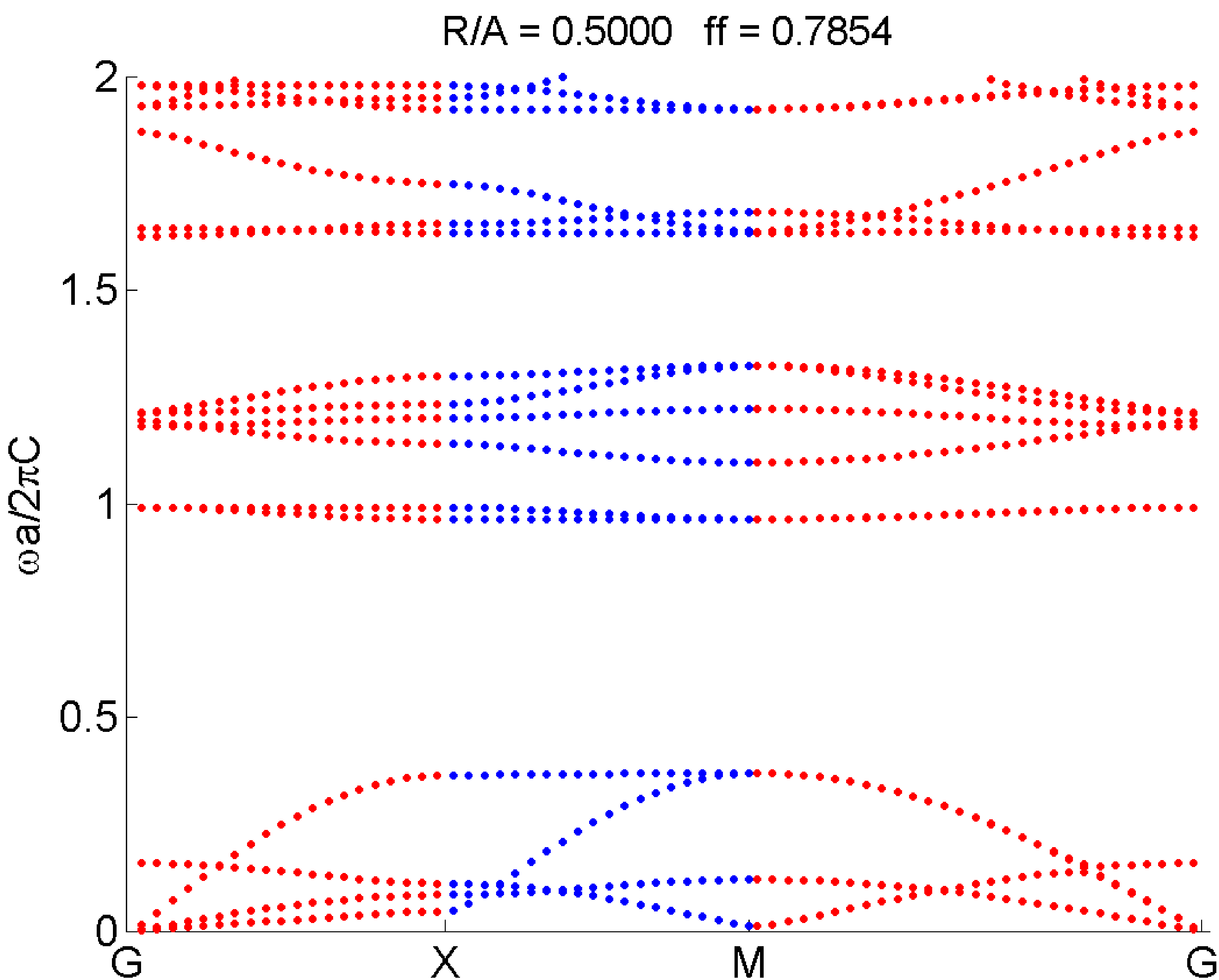
Theoretical 2D dispersion relation for carbon cylinder in an epoxy matrix (sagittal waves)

With:

iemn
UMR CNRS 8520



Y. Pennec et al, surface science reports 65(2010), pp 229-291


R/A = 0.5000   ff = 0.7854
ωa/2πC
0
0.5
1
1.5
2
G
X
M
G

Thanks you