

# PHONON ENGINEERING & CONFINED ACOUSTIC PHONONS IN SILICON MEMBRANES

CREATING A DIMENSION OF INFINITE POSSIBILITIES

Clivia M Sotomayor Torres



# COLLABORATORS



J Cuffe (UCC-IRCSET, IE), E Chavez (CONICYT, Chile), P-O. Chapuis, F Alzina, N Kehagias, L Schneider, T Kehoe, C Ribéreau-Gayon, (ECP, FR) ... the ICN team

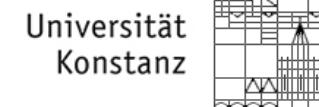


A Shchepetov, M Prunnila, S Laakso, J Ahopelto

J Johnson, A A. Maznev J Eliason, A Minnich, K Collins,  
G Chen, K A Nelson,



A Bruchhausen, M Hettich, O Ristow and T Dekorsy.

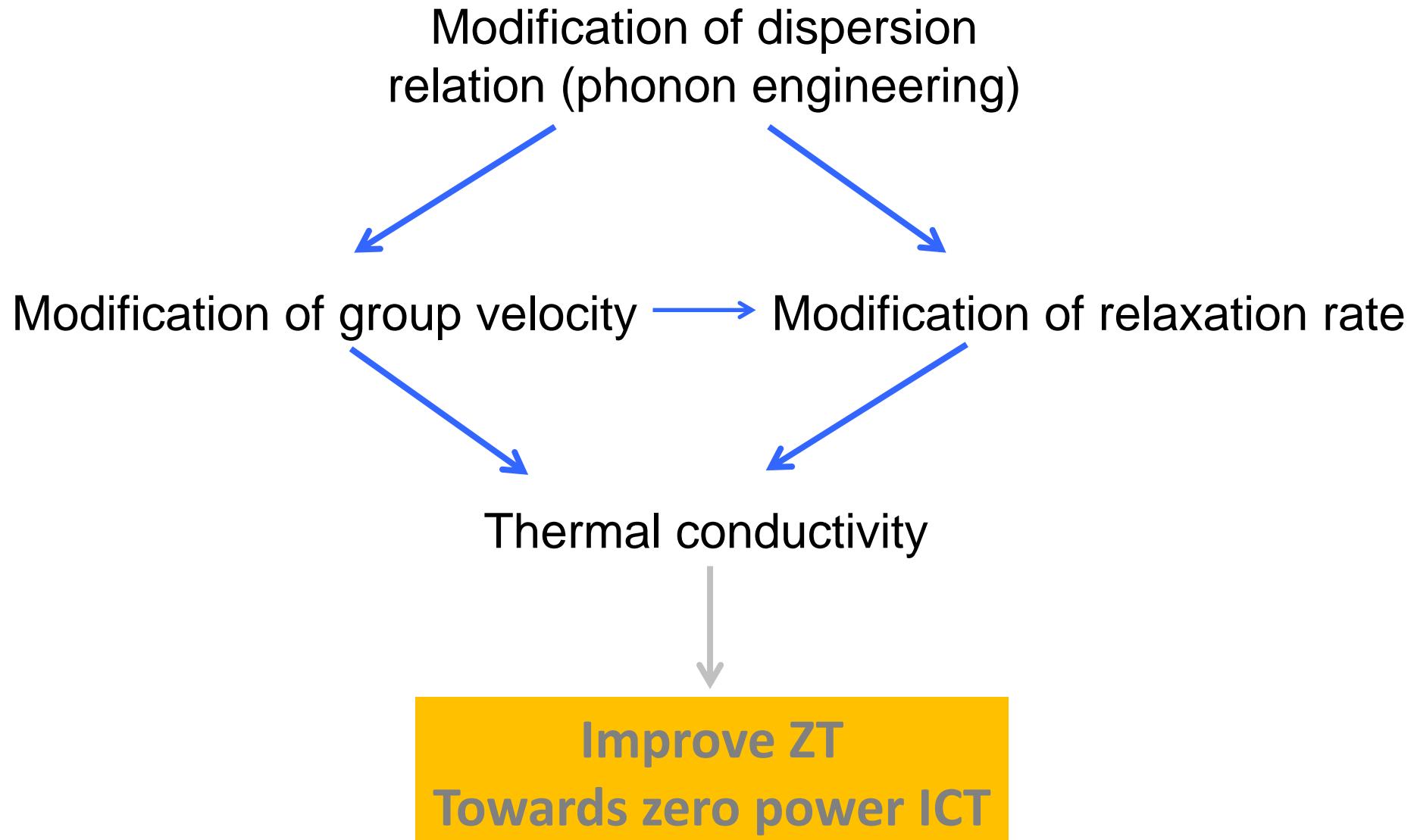


El-Houssain,(U Oujda), Y Pennec, B Djafari-Rouhani

A Mlayah, J Groenen, A Zwick  
and F Poinsotte, U P Sabatier, Toulouse



- Motivation
- Methods
  - Membranes
  - Inelastic light scattering
- Dispersion relations
- Impact on heat transfer
- Perspectives and Conclusions



## Phonon MFP

in bulk Si = 41 nm @ RT Debye model

260 nm considering dispersion

300 nm (Ju & Goodson, APL 1999)

(cf Electron MFP = 7.6 nm)

## Dominant phonon wavelength

$$\lambda_d = v_s / f_d$$

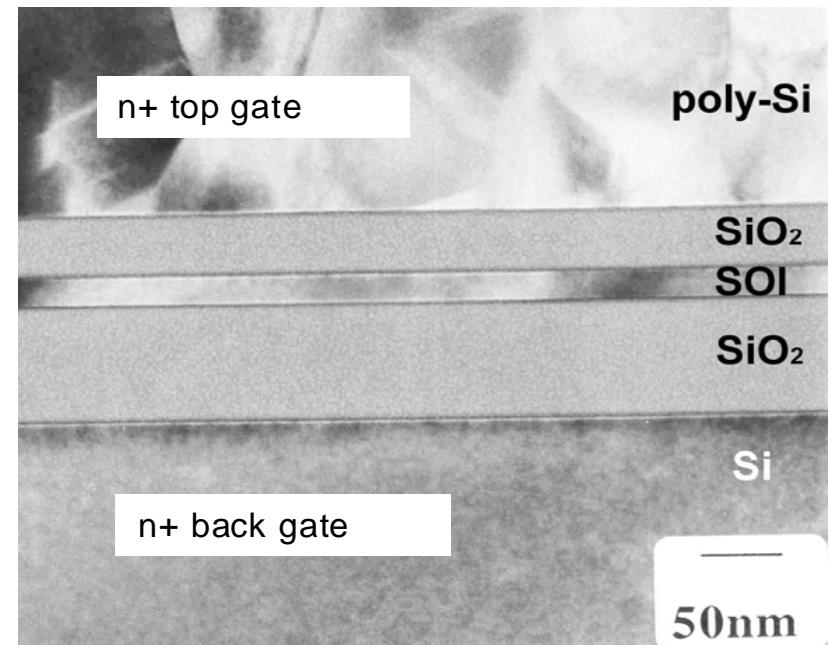
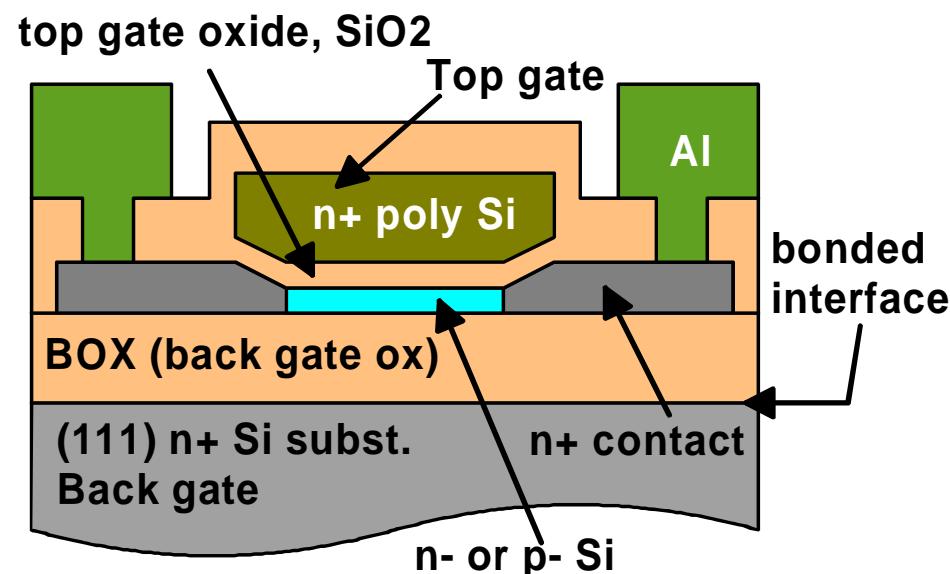
velocity of sound       $1.48 \frac{\hbar}{k_B T}$

in Si  $\lambda_d = 1.4 \text{ nm} @ \text{RT}$   
 $= 4000 \text{ nm} @ 0.1 \text{ K}$

*To confine phonons in the strong regime  
at RT need structures with  $\sim 1\text{-}10 \text{ nm}$   
lateral dimensions*

From A Balandin, UC Riverside

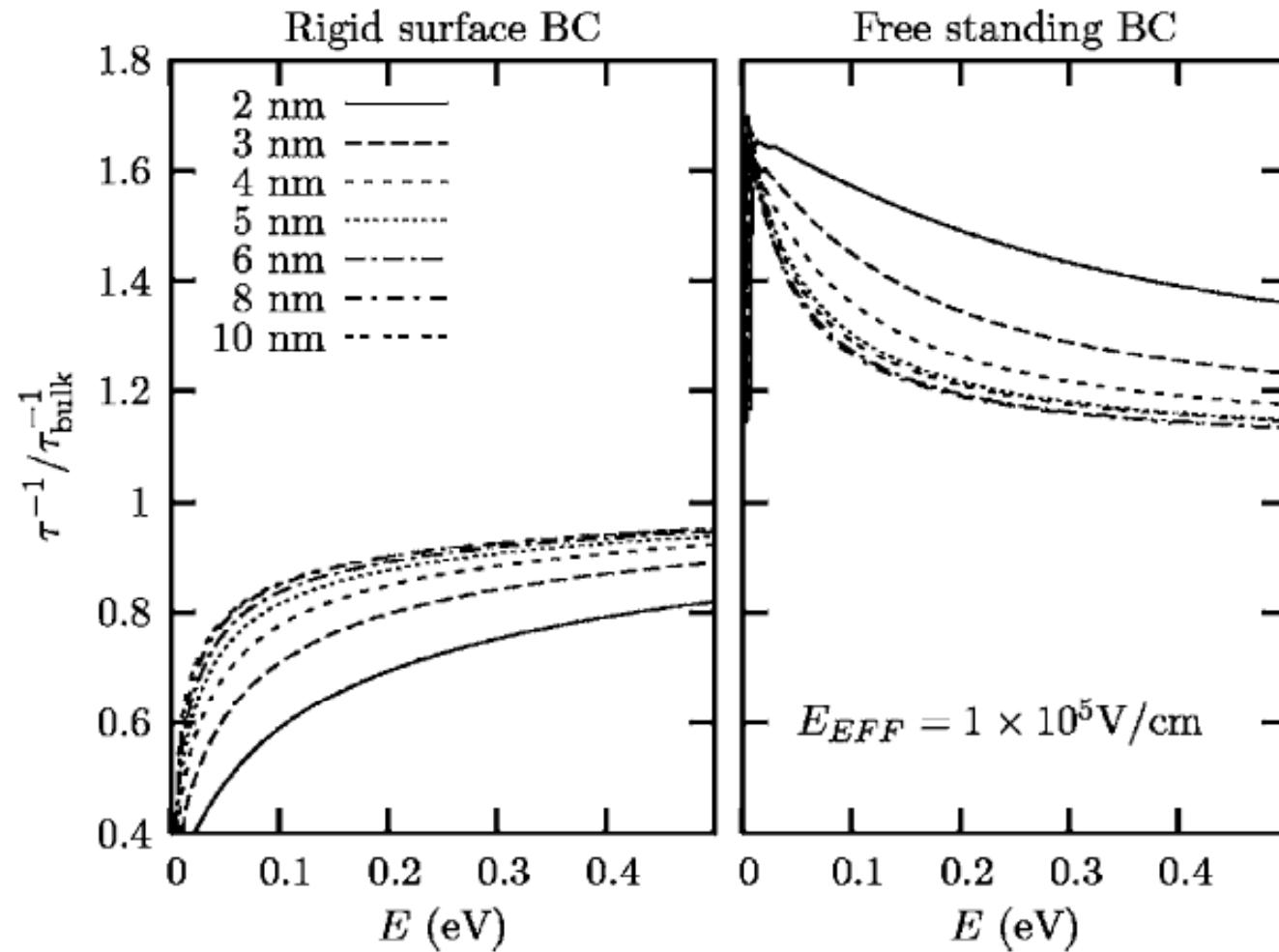
## Double-gate SOI transistors



Cross-sectional bright field TEM image of a DG-SOI FET with a 18 nm-thick channel

M Prunnila, J Ahopelto, K Henttinen and F Gamiz  
APL 85, 5442 (2004)

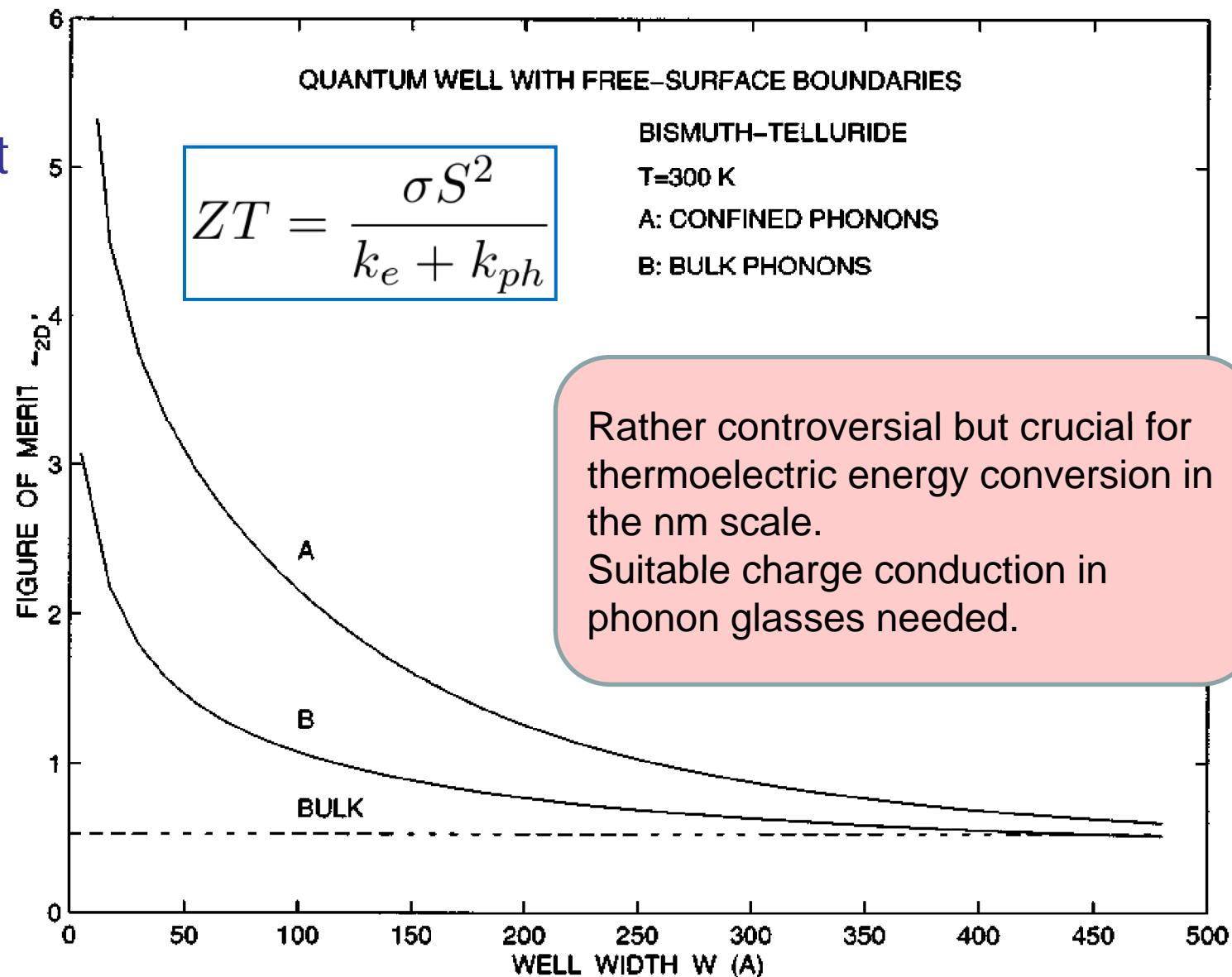
- Effect on charge carrier mobility



Effect of phonon confinement on ZT of quantum wells

Hicks & Dresselhaus 1993;  
A Balandin and K L Wang 1998

See also, M.S. Dresselhaus et al, Adv Mat 19, 1043 (2007).



# Phononic crystals

- Acoustic and elastic analogues of photonic crystals
- ‘stop bands’ in phonon spectrum (phonon mirrors);
- ‘negative refraction’ of phonons (phonon caustics)
- Good theory available: Multiple scattering theory for elastic and acoustic waves. See, for example:

Kafesaki & Economou PRB 60, 11993 (1999),

Liu et al PRB 62, 2446 (2000)

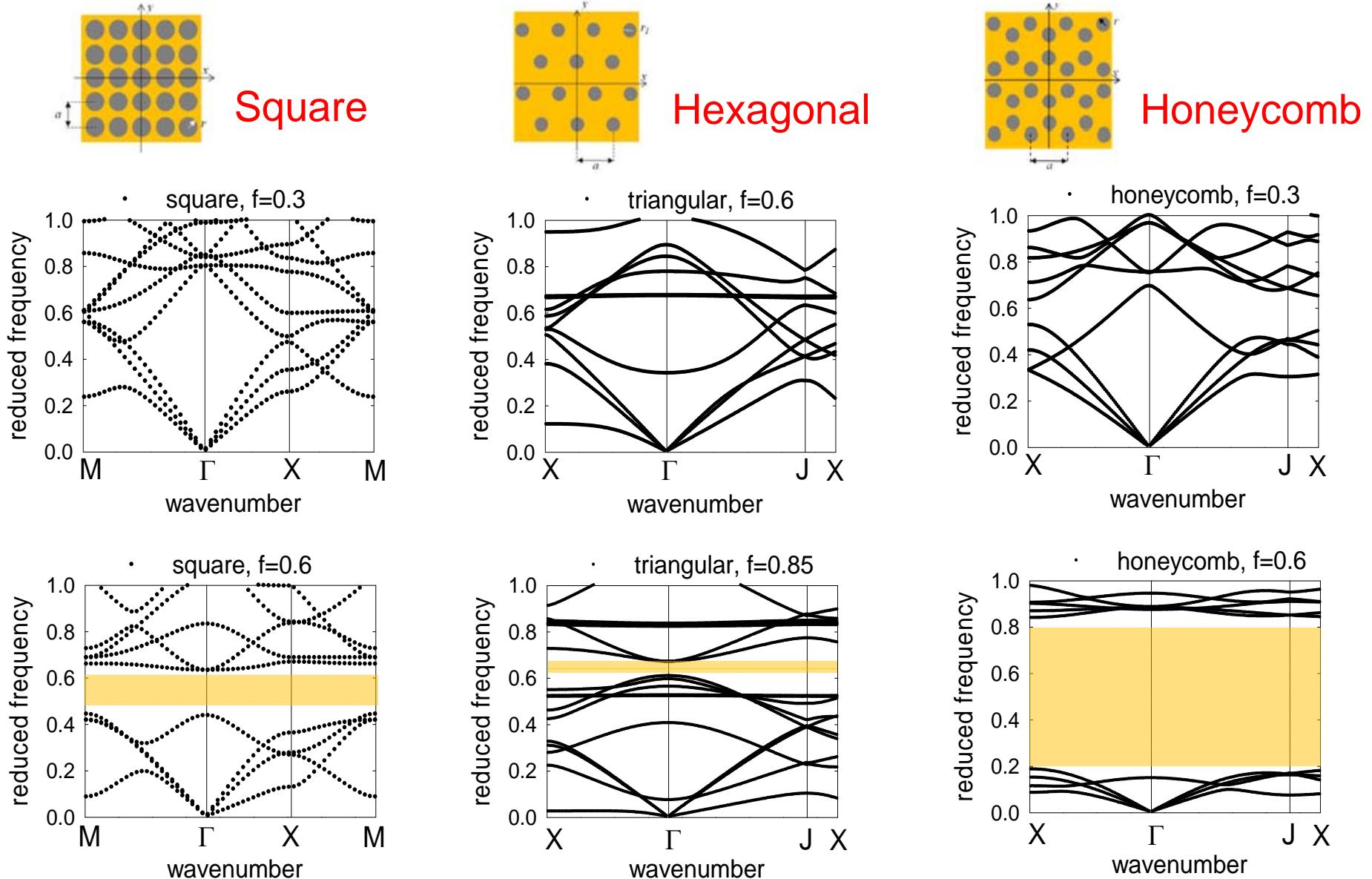
Psaroba et al PRB 62, 278 (2000).

And for a database 2006-2008:

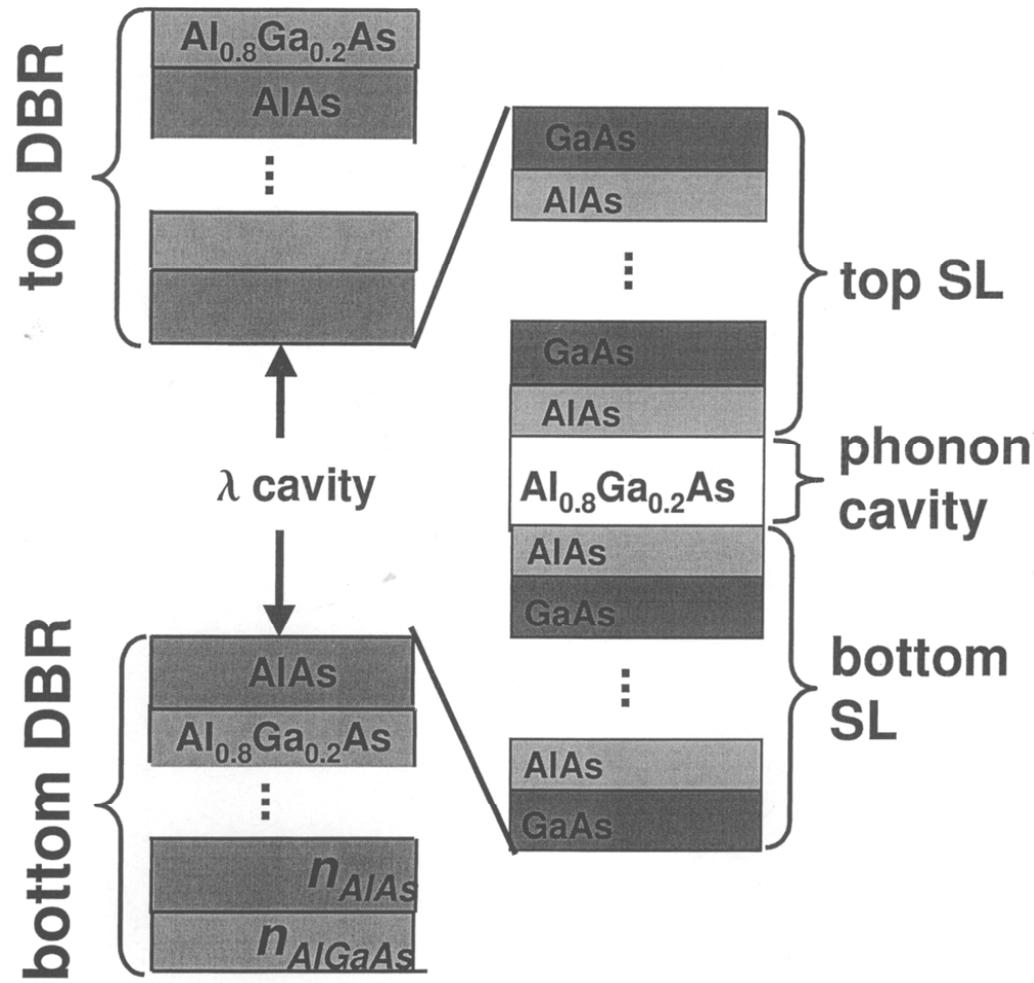
<http://www.phys.uoa.gr/phononics/PhononicDatabase.html>

*... cell phones have phononic crystal-like BAW filters*

# 2D infinite phononic crystal: air holes in silicon matrix (B Djafari-Rouhani, Y Pennec, IEMN, U Lille)



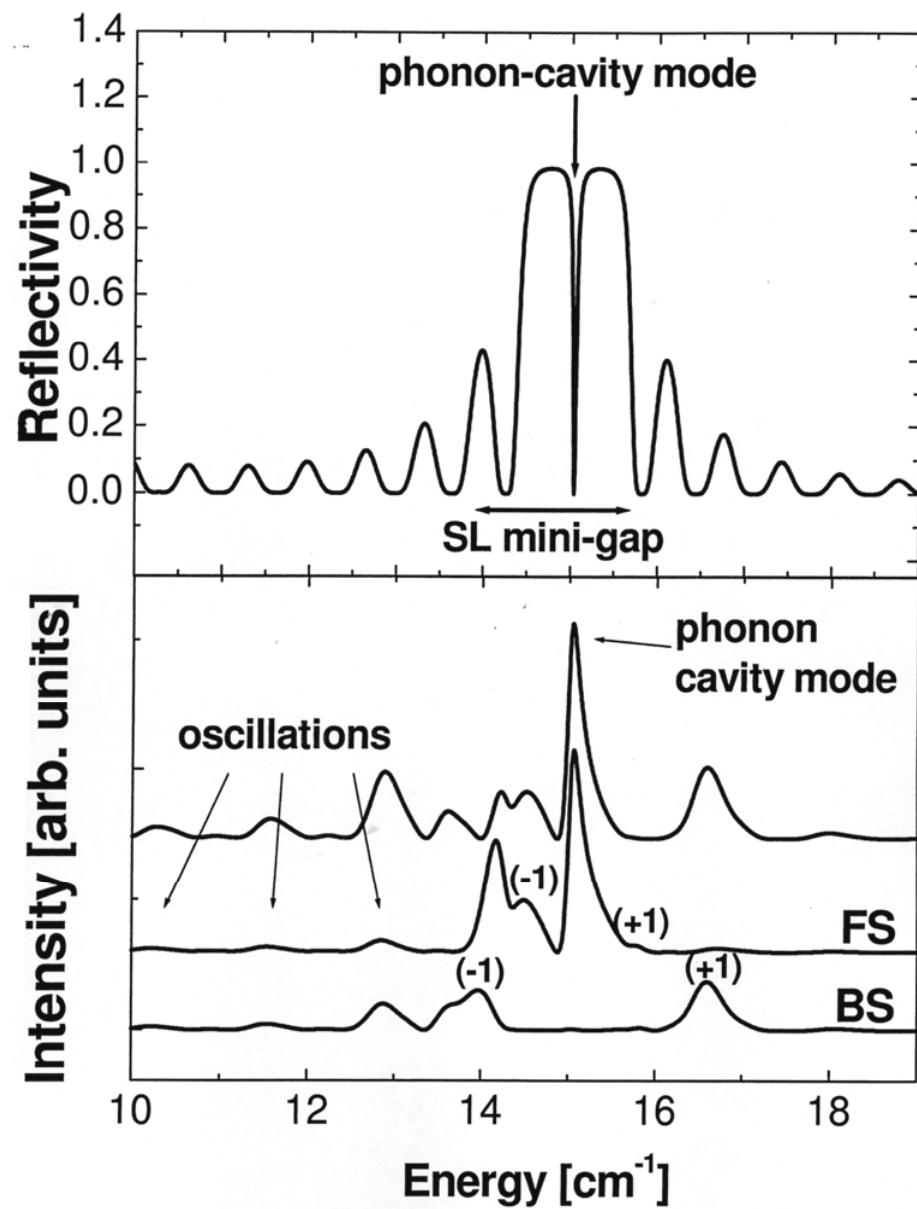
# MOTIVATION



Coupled cavities:  
photon-photon  
cavities.

Trigo et al PRL 2002

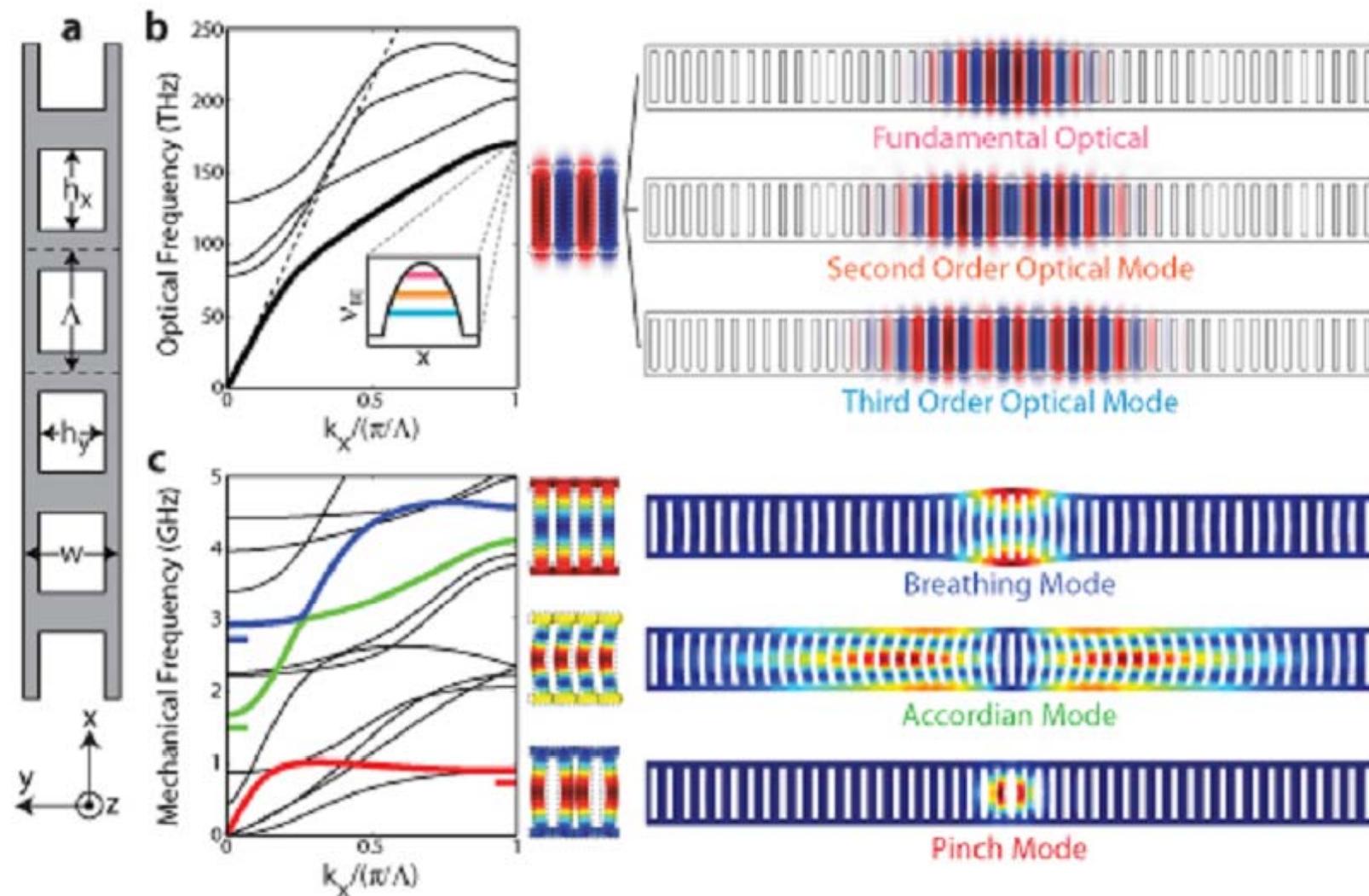
# MOTIVATION



Physics of weak to  
strong coupling  
regimes

Trigo et al PRL 2002

# MOTIVATION



Optical forces control mechanical modes → prospects for cooling, heating, ...

M Eichenfield et al. Optomechanical Crystals, Nature 462, 78-82 (2009)

*Acoustic phonons have also an impact in:*

- Noise and thermal limits in NEMS and nanoelectronics
- Coherence control in quantum information processing
- Phonon engineering: sources, detectors and other components
- Photon-phonon coupling: Phoxonic Crystals and Opto mechanical oscillators
- Energy harvesting and storage
- THz technologies for medical diagnostic and security
- Elastic material parameters down to the nm-scale

# Previous work: 30 nm SOI membrane

phys. stat. sol. (c) 1, No. 11, 2609–2612 (2004) / DOI 10.1002/pssc.200405313

## Observations of confined acoustic phonons in silicon membranes

C. M. Sotomayor Torres<sup>\*1,2</sup>, A. Zwick<sup>2</sup>, F. Poinsotte<sup>2</sup>, J. Groenen<sup>2</sup>, M. Prunilla<sup>3</sup>, J. Ahopelto<sup>3</sup>, A. Mlayah<sup>2</sup>, and V. Paillard<sup>2</sup>

<sup>1</sup> National Microelectronics Research Centre, University College Cork, Lee Maltings, Prospect Row Cork, Ireland

<sup>2</sup> Laboratory of Solid State Physics (LPST), UMR 5477, Paul Sabatier University, 118 route de Narbonne, 31062 Toulouse Cedex 04, France

<sup>3</sup> VTT Centre for Microelectronics, Tietotie 3, 02150 Espoo, Finland

PHYSICAL REVIEW B 77, 045420 (2008)

## Inelastic light scattering by longitudinal acoustic phonons in thin silicon layers: From membranes to silicon-on-insulator structures

J. Groenen,<sup>\*</sup> F. Poinsotte, and A. Zwick

Centre d'Elaboration des Matériaux et d'Etudes Structurales UPR 8011, CNRS-Université Paul Sabatier, 29 Rue Jeanne Marvig, F 31055 Toulouse Cedex 4, France

C. M. Sotomayor Torres

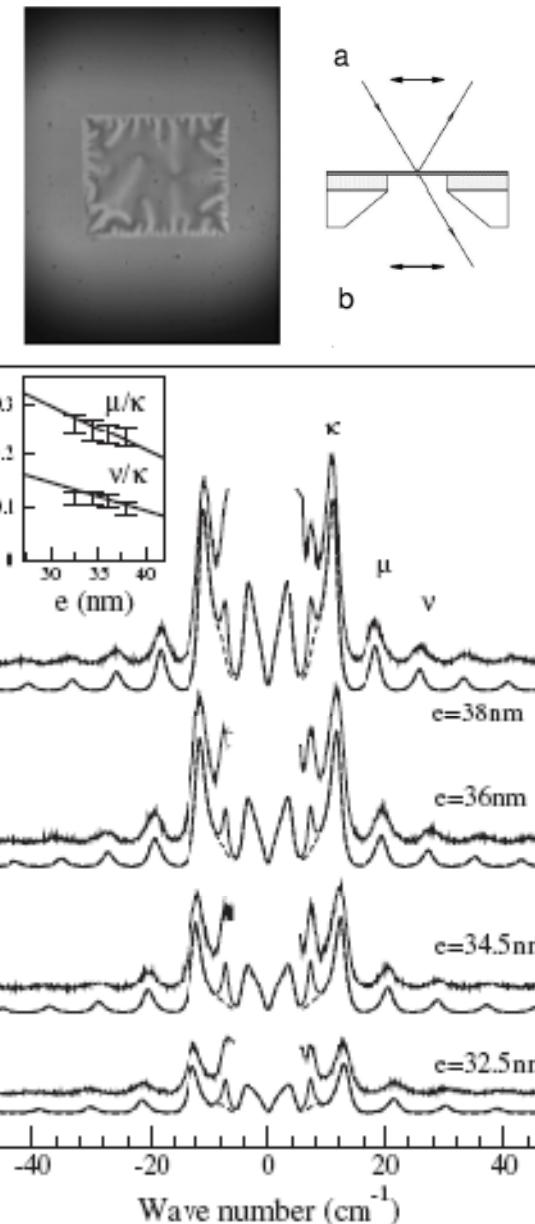
University College Cork, Tyndall National Institute, Lee Maltings, Cork, Ireland;

Catalan Institute of Nanotechnology, Campus de Bellaterra, Edifici CM7, ES 08193 Bellaterra (Barcelona), Spain;  
and ICREA-Catalan Institute for Research and Advanced Studies, 08010 Barcelona, Spain

M. Prunilla and J. Ahopelto

VTT Micro and Nanoelectronics, P.O. Box 1000, FI-02044 VTT, Espoo, Finland

(Received 18 July 2007; published 23 January 2008)



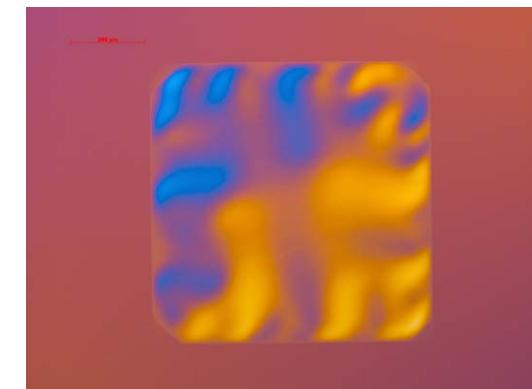
The confinement of phonons modifies their frequencies and density of states affecting group velocities of modes, scattering mechanisms, lifetimes and changes assumptions about boundary conditions and transport properties.

Understanding of acoustic phonons confinement in nanostructures is crucial for phonon engineering and strategies for low power nanoelectronics.

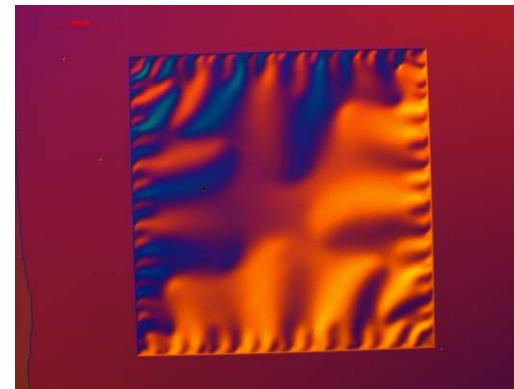
- Motivation
- Methods
  - Membranes
  - Inelastic light scattering
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- Impact on heat transfer
- Perspectives and Conclusions

# MEMBRANES

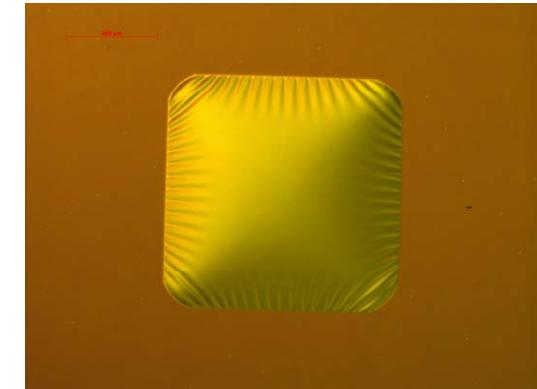
- Free-standing Si membranes
- Corrugation due to residual compressive strain in SOI films
- Methods to avoid corrugation are being developed.



200nm

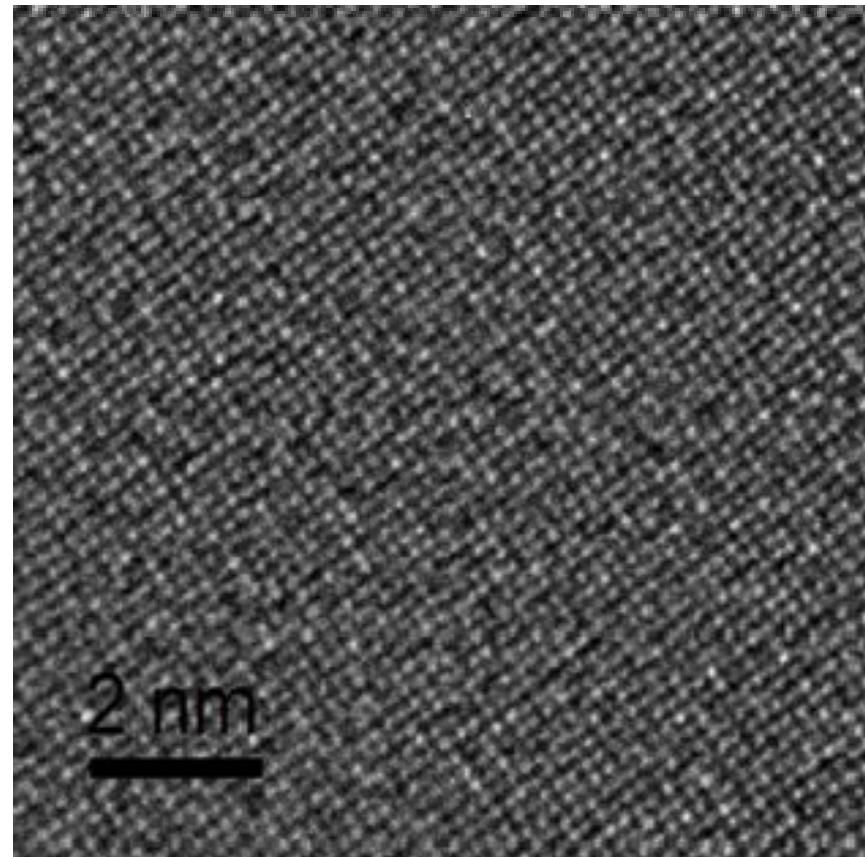


50nm



50nm with weak  
vacuum

HRTEM image of freestanding Si membrane, thickness 6 nm



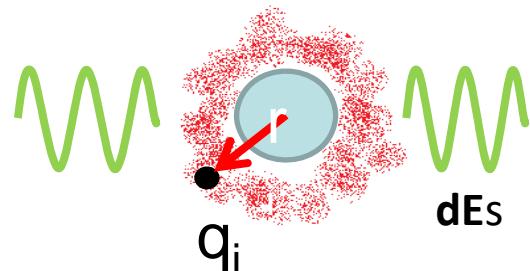
A. Schcepov, M. Prunnila, J. Ahopelto, VTT  
J. Hua, Aalto University

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# Scattering Mechanisms

## Photoelastic Scattering

$$I_s = \alpha \cdot \left| \int_{-\infty}^{+\infty} dz p(z) G(z, z') E(z) \frac{\partial u(z)}{\partial z} \right|^2$$



$$\mathbf{p}(t) = \sum q_i \mathbf{r}_i(t) = \boldsymbol{\alpha} \cdot \mathbf{E}_0 e^{i(\mathbf{k}_i \cdot \mathbf{r} - \omega_0 t)}$$

$$\mathbf{E}_s(\mathbf{R}, t) \sim -\omega^2 \int_V \boldsymbol{\alpha} \cdot \mathbf{E}_0 e^{i(\mathbf{k}_i - \mathbf{k}_s) \cdot \mathbf{r}} d\mathbf{r}$$

$$\boldsymbol{\alpha} = \langle \boldsymbol{\alpha} \rangle + \underline{\delta \alpha(\mathbf{r}, t)}$$

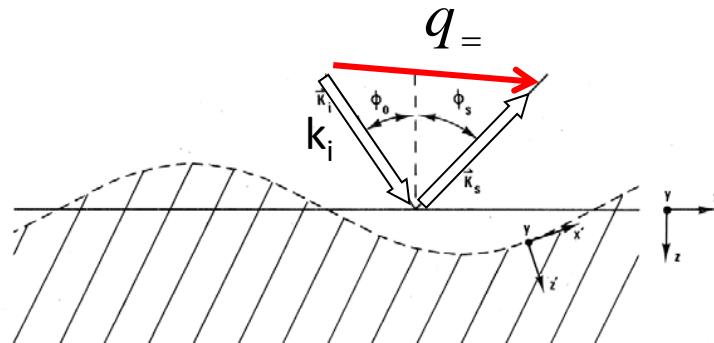
Benedek, G B & Fritsch, K Phys Rev, **149**, 647 (1966)

## Corrugation (Ripple) Scattering

$$I(\omega) = A \frac{T}{\omega} \text{Im}\{G_{33}(k_{||}, x_3 = d, \omega + i0)\}$$

$$LDOS = - \frac{1}{\pi} \text{Im} [G(z, z)]$$

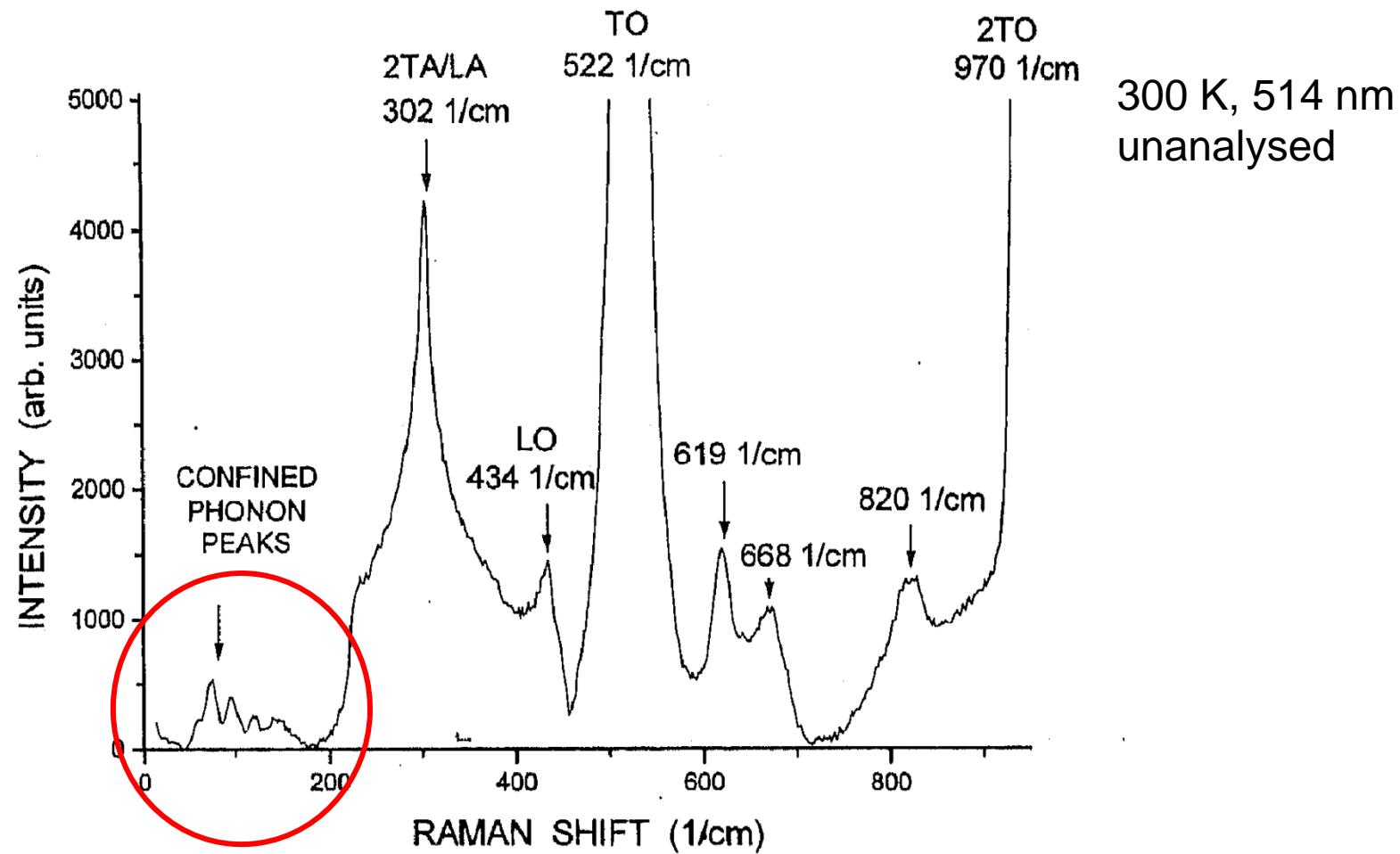
EH El Boudouti et al, Surf Sci Reports **64**, 471 (2009)



Related to power spectrum of normal displacement

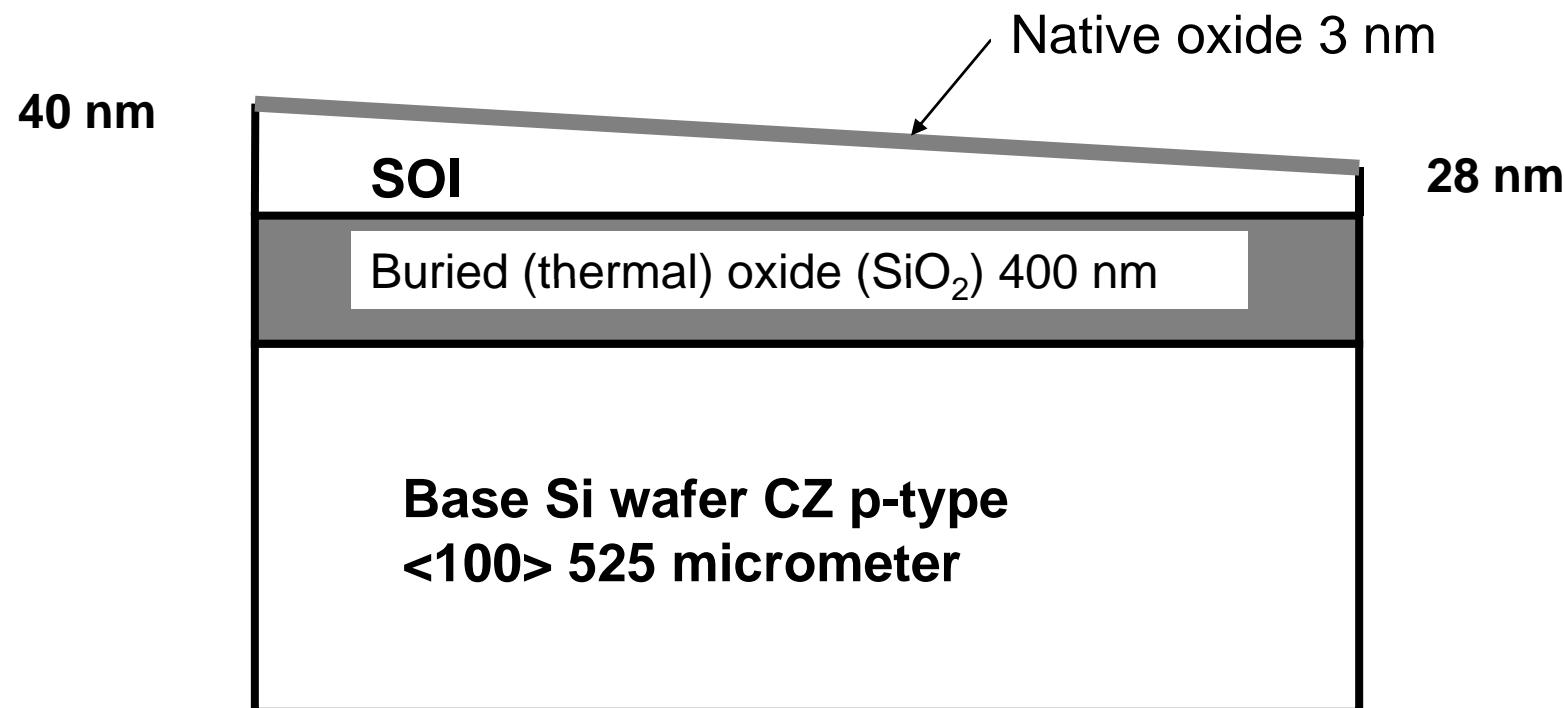
Rowell, N. L. & Stegeman, G. I. PRB **18** 2598 (1978)

# Raman scattering of Silicon



A Balandin 2000

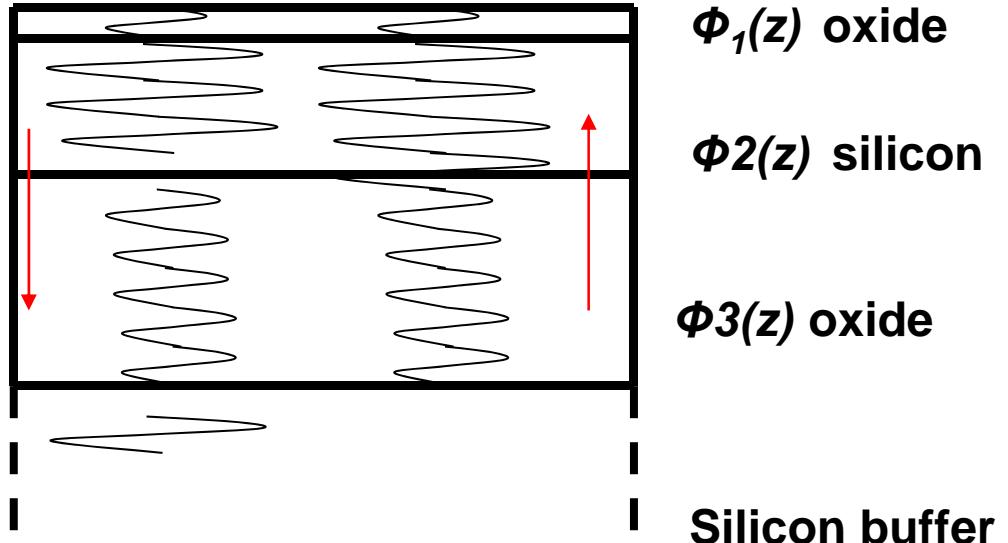
# Thin film SOI sample cross-section



*SOI is a key European technology*

## Photoelastic model for scattering by LA phonos

$$I(\omega_{qz}) \propto \left| \int dz . E_L . E_S^* . p(z) . \frac{\partial \phi(z)}{\partial z} \right|^2$$



$E_L$  ( $E_S$ ) : laser (scattered) field  
 $p(z)$  : photoelastic constant  
 $\phi(z)$  : phonon displacement

# Simulations Raman spectra SOI thin film

- phonons displacement and stress boundary conditions

$$\left\{ \begin{array}{l} \phi_1(z_{Ox/Si}) = \phi_2(z_{Ox/Si}) \\ C_1 \frac{\partial \phi_1}{\partial z}(z_{Ox/Si}) = C_2 \frac{\partial \phi_2}{\partial z}(z_{Ox/Si}) \end{array} \right.$$

## - Assumptions

Phonons stationary waves  $\longrightarrow \phi_1(z) = A_1 e^{iq_1 z} + B_1 e^{-iq_1 z}$

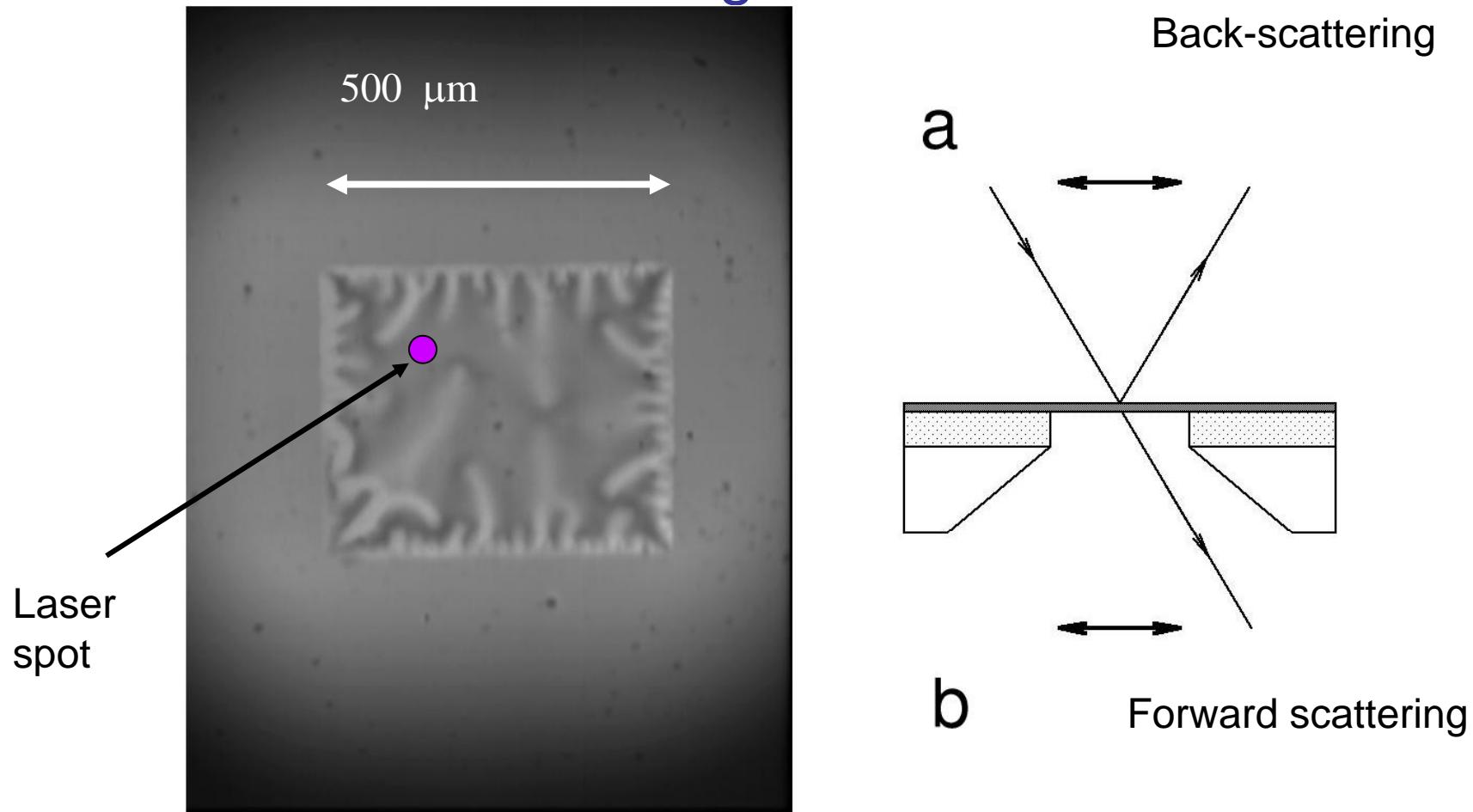
Free surface  $\longrightarrow C_1 \frac{\partial \phi_1}{\partial z}(z_{air/Ox}) = 0$

Dispersion relation  $\omega_{qz} = q_z \cdot v_{ac}$  sound velocity  
Infinite silicon buffer  $Vac(oxide) = 5970 \text{ m.s}^{-1}$   
 $Vac(silicon) = 8433 \text{ m.s}^{-1}$

- Electronic part

$$\left\{ \begin{array}{l} P_{Ox}(z) = 0 \\ P_{Si}(z) = 1 \end{array} \right.$$

## SOI membranes and configuration



Sotomayor Torres et al phys stat sol c 2004

# Simulations of RS spectra of SOI membranes

Treat SOI layer as a cavity for acoustic phonons, ie,  
confined since longitudinal  $v_s$  in Si = 8433 m/s  
(cf. 332 m/s in air at 0 C).

Displacement field of acoustic vibrations in a slab of thickness  $t$  is proportional to:

*n* is the order of the confined frequencies can be derived from LA dispersion branch, considering discrete wave vectors  $q = n \pi/t$

Acoustic vibration  $\rightarrow$  periodic variation of strain  $\rightarrow$  polarisation field in presence of em wave

$$\cos\left(\frac{n \times \pi}{t} z\right)$$

$$P(z,t) = p_s \frac{\partial u_z(z,t)}{\partial z} E_i(z,t)$$

$p_s$  photo-elastic coefficient of slab

$P(z,t)$  OK for anti-Stokes part.  
Obtain Stoke part by changing

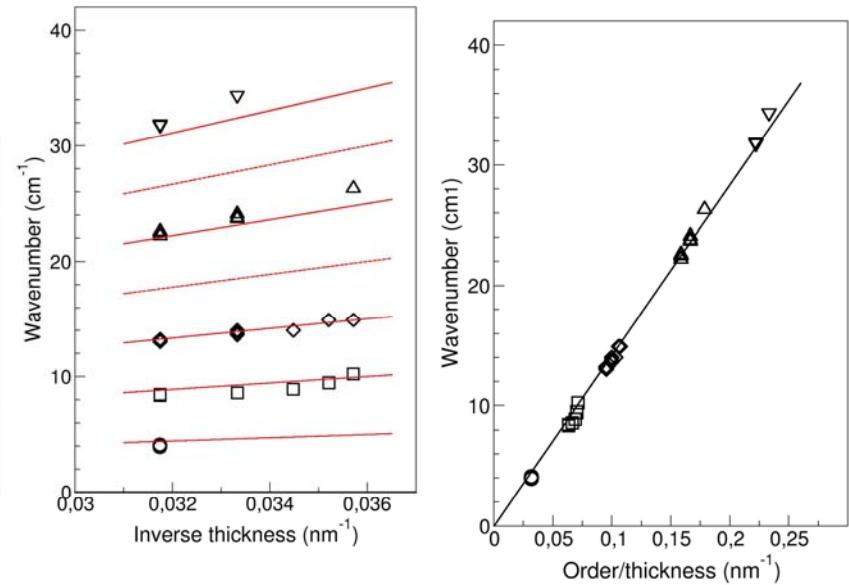
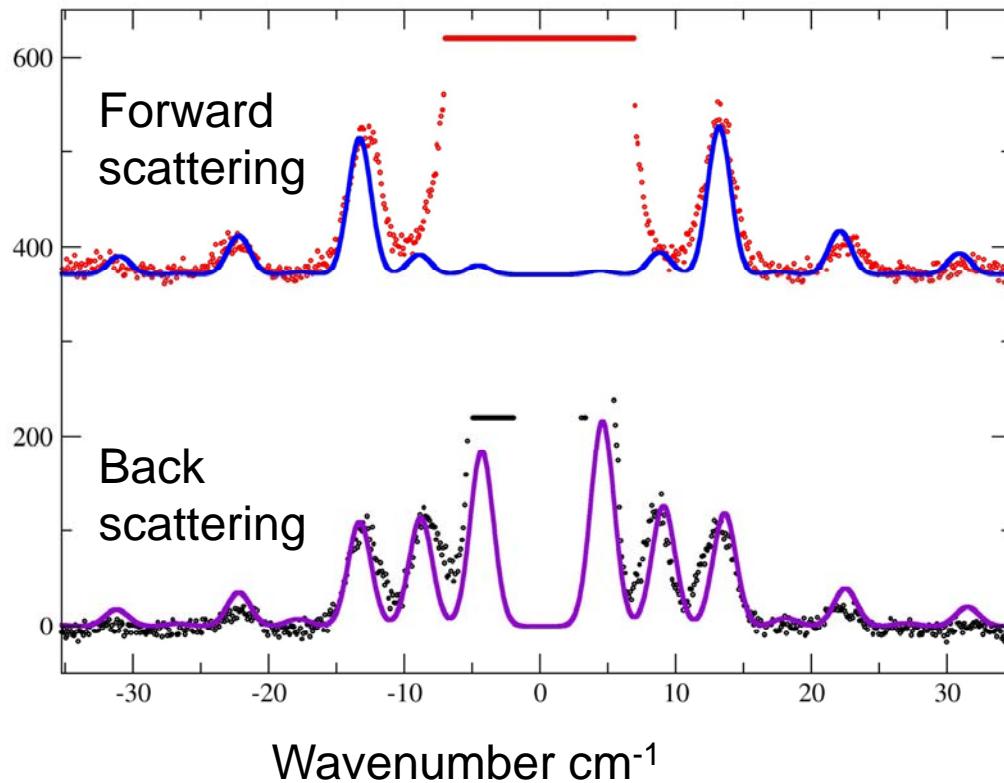
$$\frac{\partial u_z(z,t)}{\partial z} \quad \text{by} \quad \left( \frac{\partial u_z(z,t)}{\partial z} \right)^*$$

# RS spectra of 31.5 nm thick SOI membrane

Thus, scattered field:

$$\frac{\partial^2 Es(z,t)}{\partial z^2} - \frac{n^2}{c^2} \frac{\partial^2 Es(z,t)}{\partial t^2} = \frac{1}{\epsilon_0 c^2} \frac{\partial^2 P(z,t)}{\partial t^2}$$

Where n = slab index of refraction.



J Groenen et al, PRB 2008

- Motivation
- Methods
  - Membranes
  - Inelastic light scattering
- Dispersion relations (mainly by J Cuffe, E Chavez,  
both PhD students at ICN, work unpublished)
- Impact on heat transfer
- Perspectives and Conclusions

# From bulk to membranes

## Elastic continuum approach

### Displacement-Strain Relationship

$$e_{ij} = \frac{1}{2}(\epsilon_{ij} + \epsilon_{ji}) = \frac{1}{2} \left( \frac{\partial R_i}{\partial x_j} + \frac{\partial R_j}{\partial x_i} \right)$$

### Hooke's Law

$$\sigma_{ij} = C_{ijkl} e_{kl}$$

### Newton's Second Law

$$\rho \frac{\partial^2 R_i}{\partial t^2} = \frac{\partial \sigma_{ij}}{\partial x_j}$$

### Membrane (Lamb)

$$z = +a/2 \quad \sigma_{iz} = 0$$



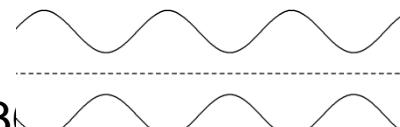
$$\sigma_{iz} = 0$$

$$z = -a/2 \quad \sigma_{iz} = 0$$

### Flexural (Anti-symmetric)

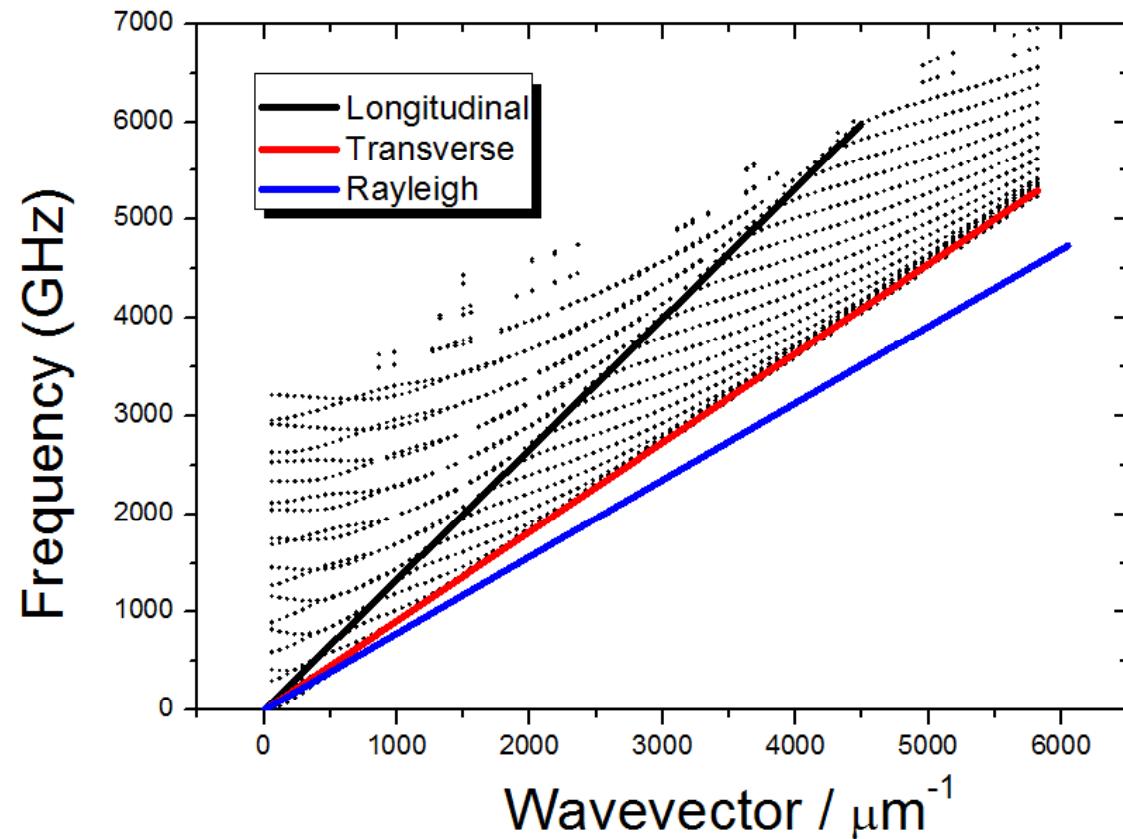


### Dilatational (Symmetric)



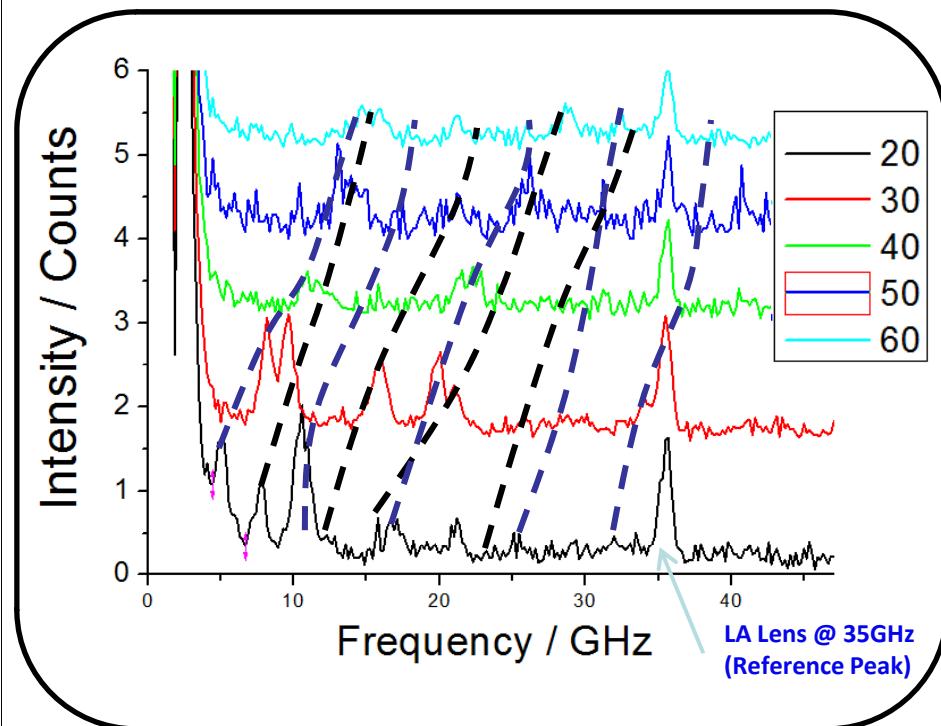
3

### Dispersion Relation

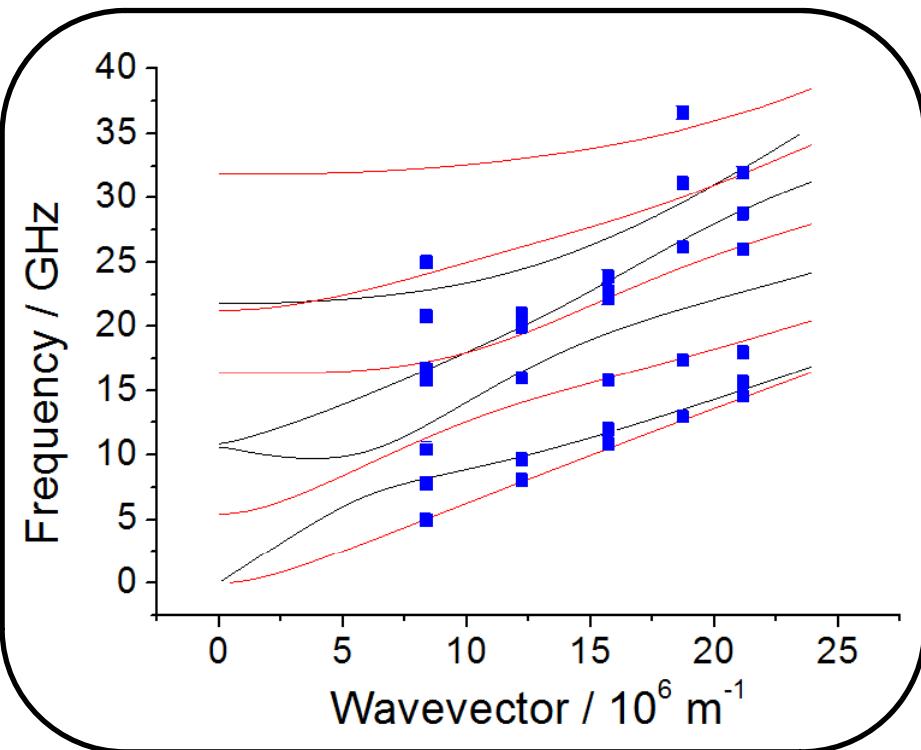


# 430 nm Si Membrane

Spectra at 3mm Mirror Spacing



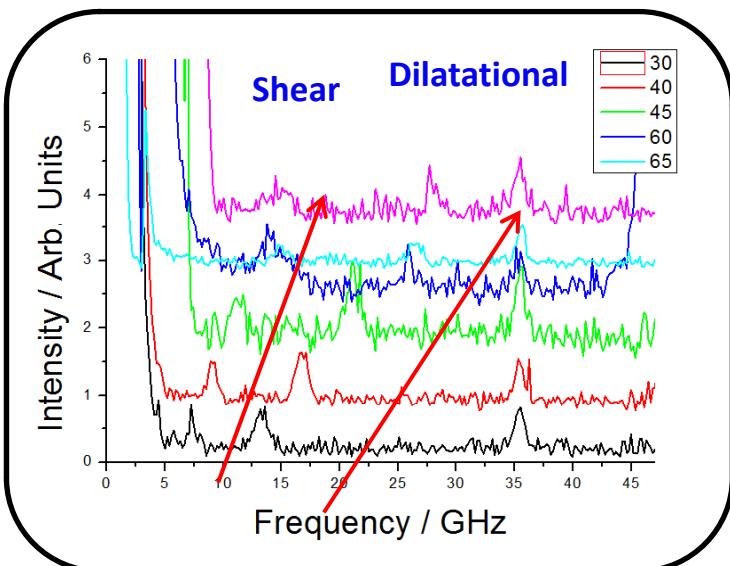
Dispersion Relation



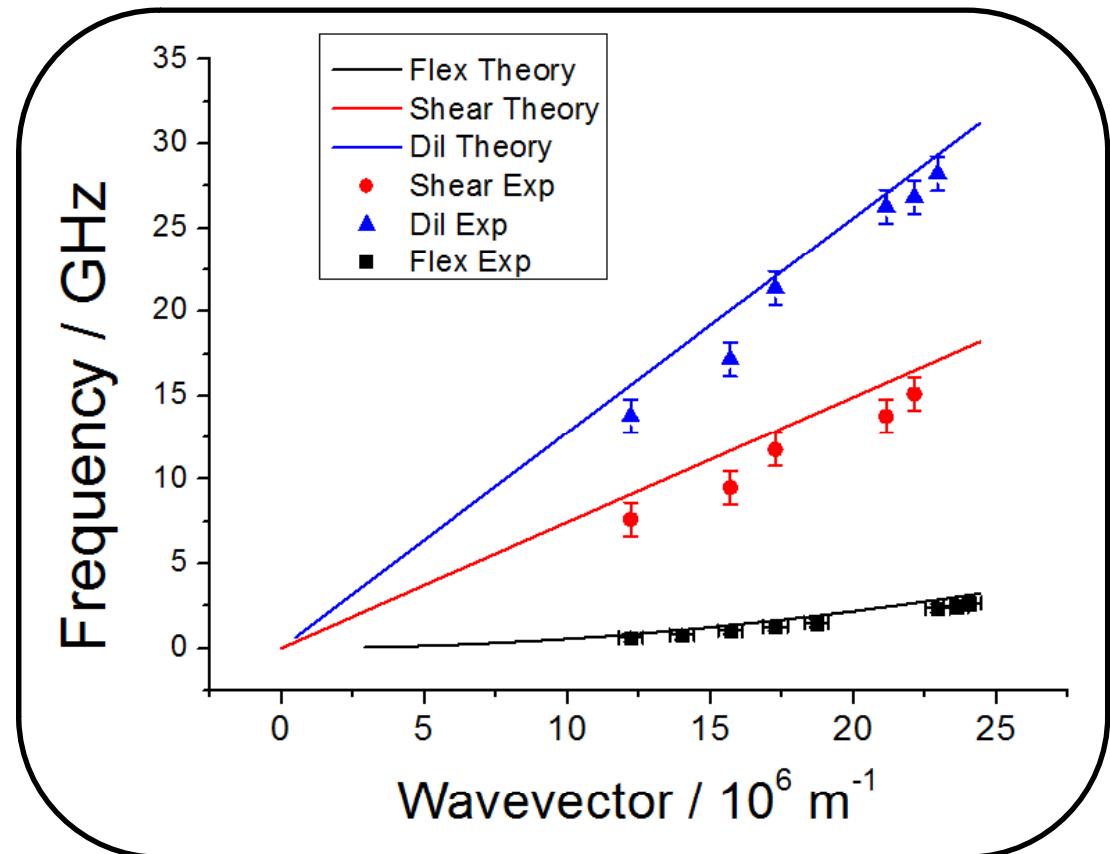
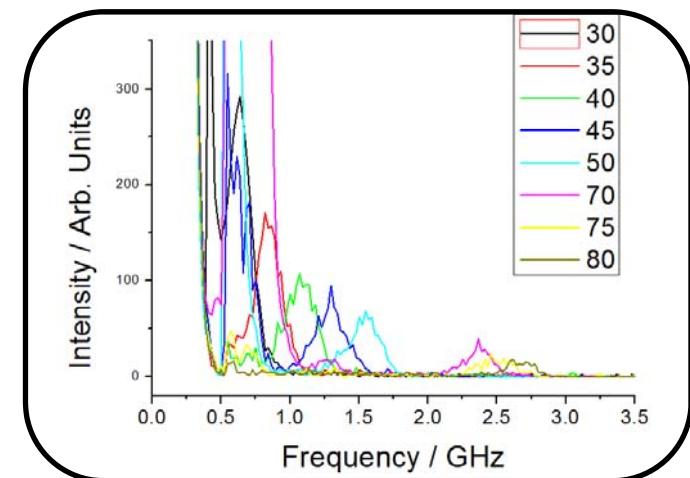
- Spectra observed with Brillouin Light Scattering spectroscopy
- Multiple modes observed (deviation from bulk behaviour)
- Good agreement with theoretical calculations (Lamb waves)

# 10 nm Si Membrane

## Spectra at 3 mm Mirror Spacing



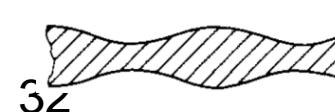
## Spectra at 10 mm Mirror Spacing



Flexural



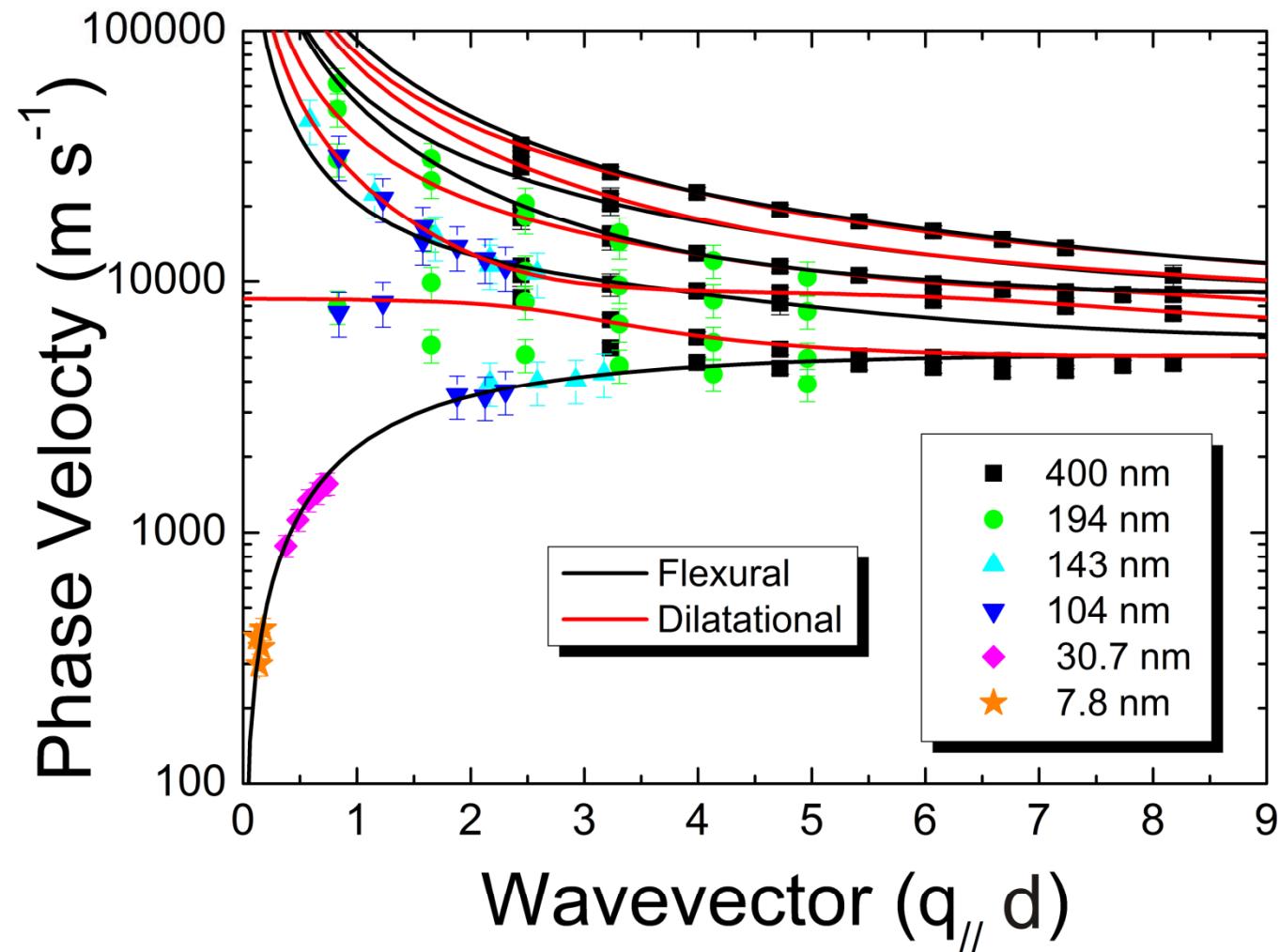
Dilatational



Shear (SH)



# Phase Velocity vs q.a

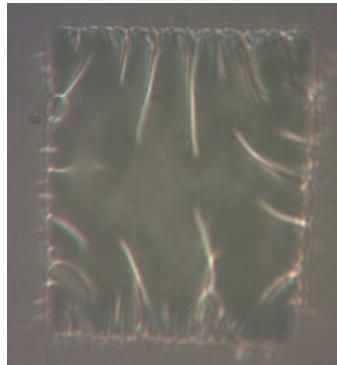


Phase(Group) velocity decreases dramatically for thinner membranes

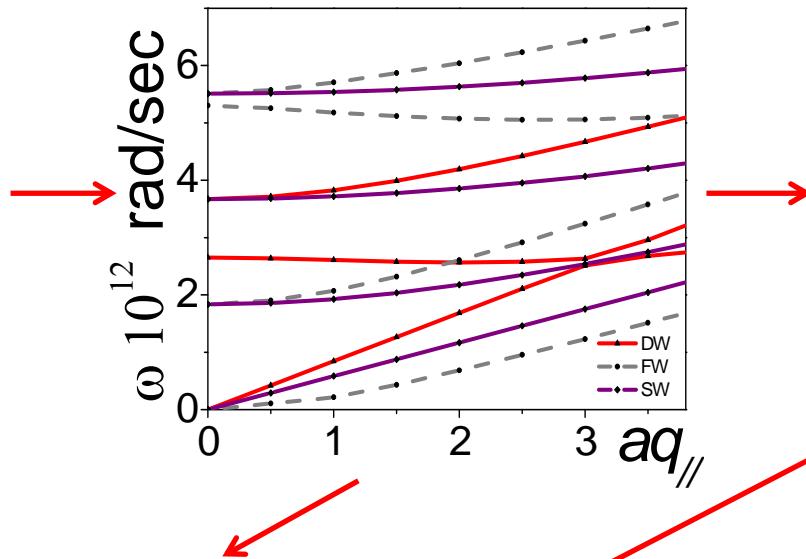
- Motivation
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# Impact on thermal conductivity

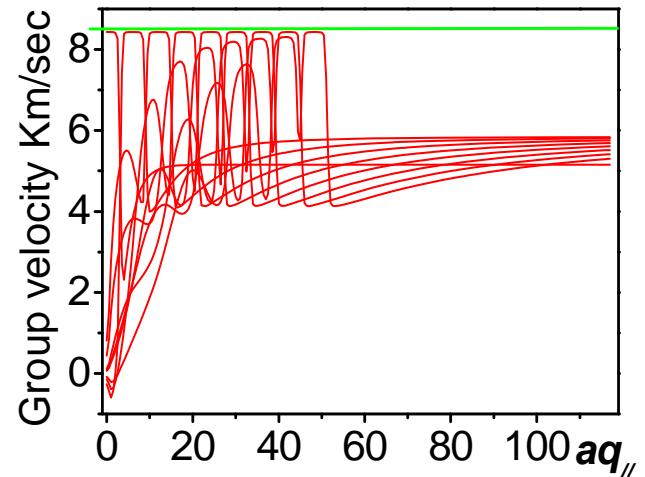
## Spatial confinement



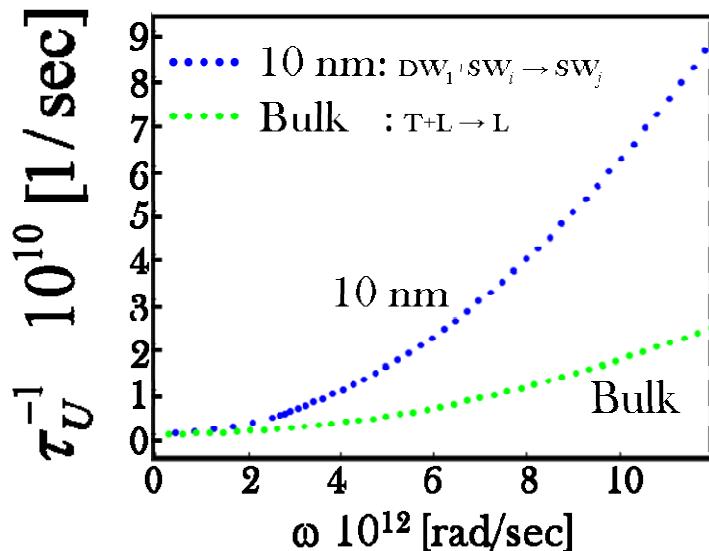
## Modification of dispersion relation



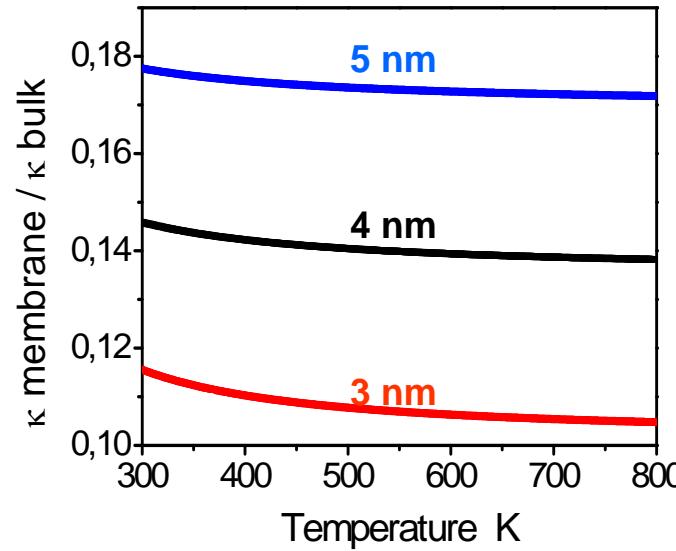
## Modification of group velocity



Increase of relaxation rate



Decrease of thermal conductivity

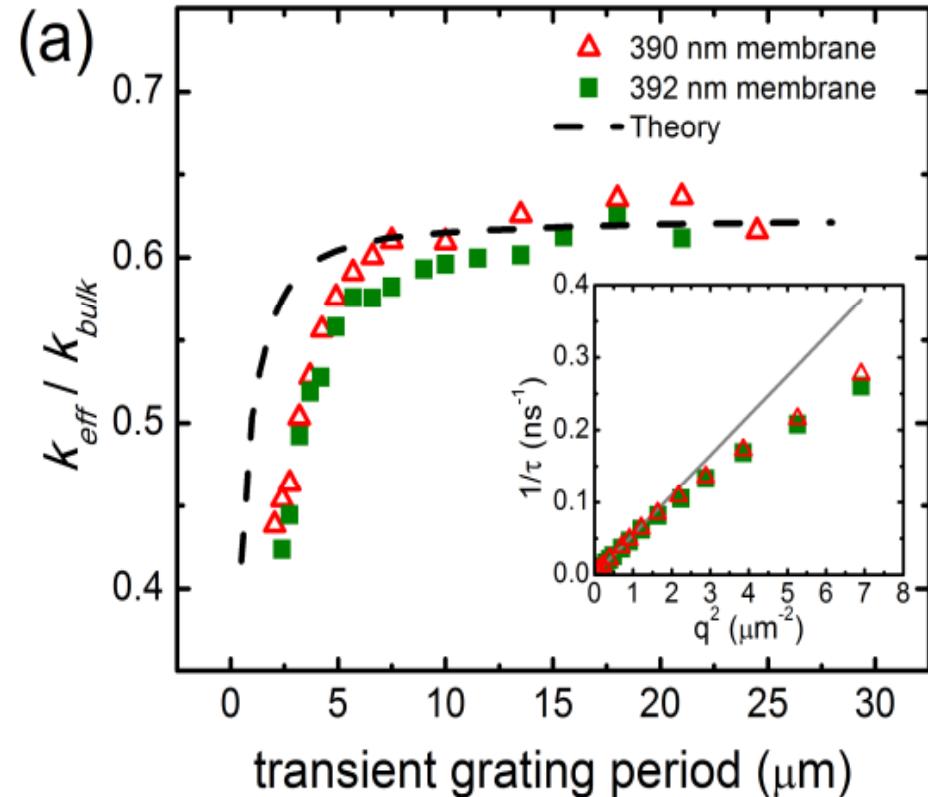


# Impact on thermal conductivity

Change in dispersion relation and the emergence of more branches increases interaction between phonons

→ increase in relaxation rates and a corresponding decrease in the thermal conductivity

→ The thinner the membrane the lower the thermal conductivity  $K$ .

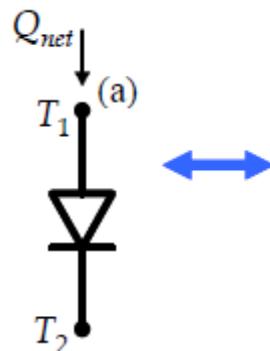


$$K = \frac{\hbar \rho \bar{v}^2}{3\pi \gamma^2 k_B T^2} \sum_{qs} C_{qs}^2 \omega_{qs}^2 n_{qs} (n_{qs} + 1) \left\{ \sum_{q's';q''s''} \omega_{qs} \omega_{q's'} \omega_{q''s''} (n_{q's'} - n_{q''s''}) \delta(\Delta\omega) \right\}^{-1}$$

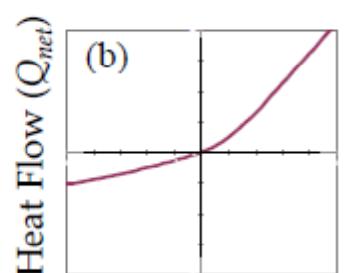
Including all the confined modes and calculating Umklapp processes

# THERMAL RECTIFICATION BY BALLISTIC PHONONS IN ASYMMETRIC NANOSTRUCTURES

John Miller



Wanyoung Jang



Chris Dames

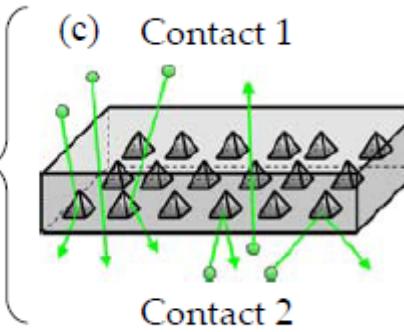
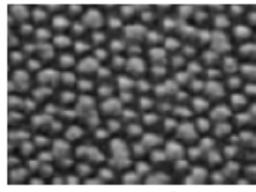


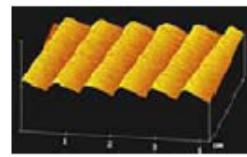
Fig. 1. (a, b) Defining behavior of a thermal rectifier. (c) A thermal rectifier realized through asymmetric scattering of ballistic phonons by pyramidal inclusions.

Quantum dots



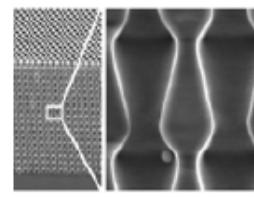
Harman et al., 2000

Blazed Grating



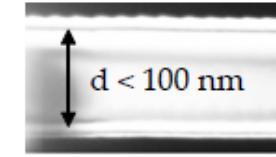
Spectrum Scientific (SSI)

Microporous Si



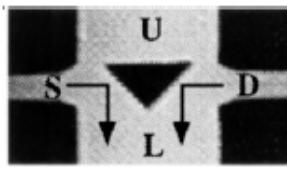
Matthias & Muller, 2003

Sawtooth Nanowire



$d < 100$  nm  
Ross, Terstoff, &  
Reuter, 2005

2D Electron Gas



A. M. Song et al., 1998

Micropatterned membrane

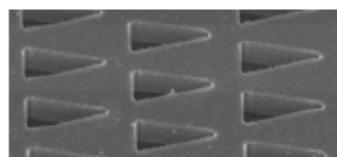
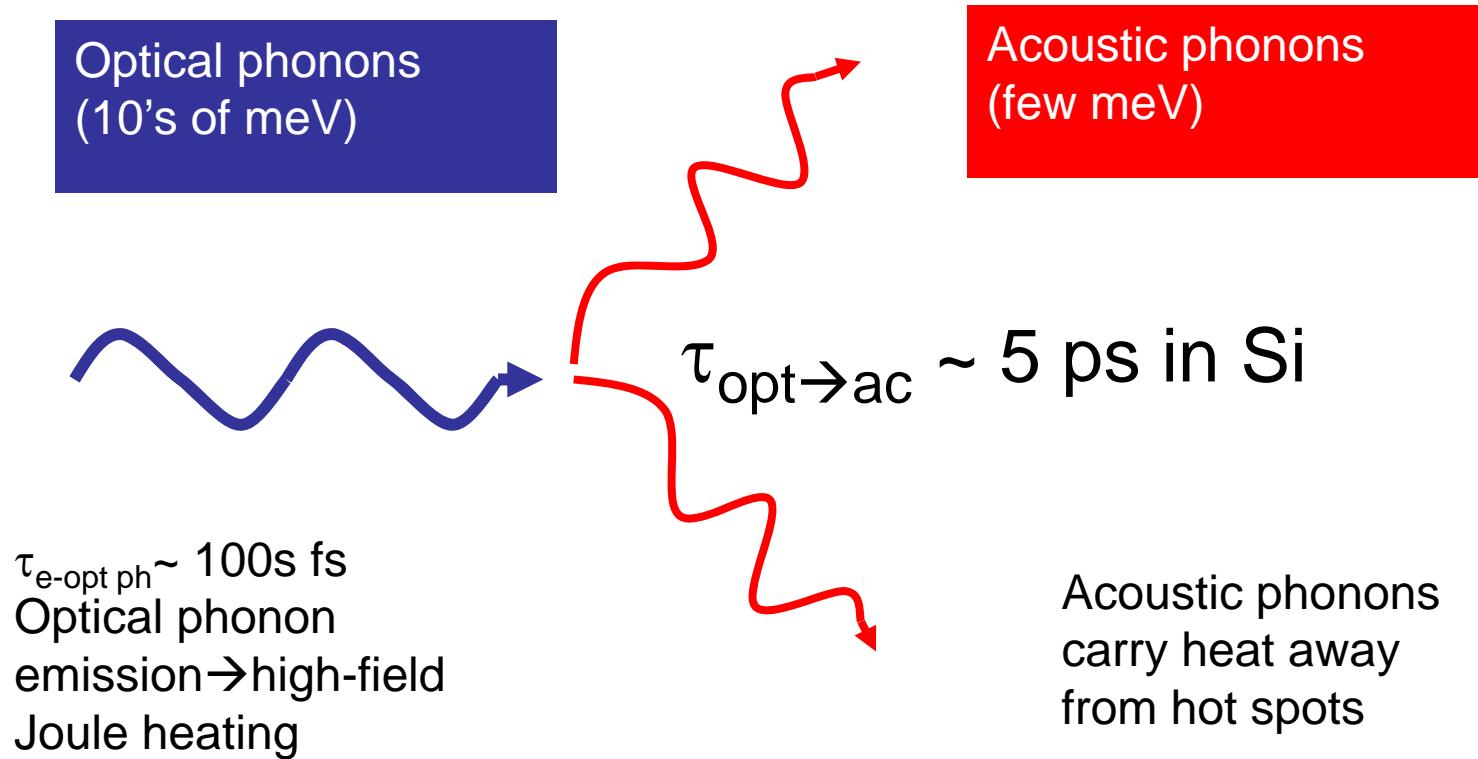


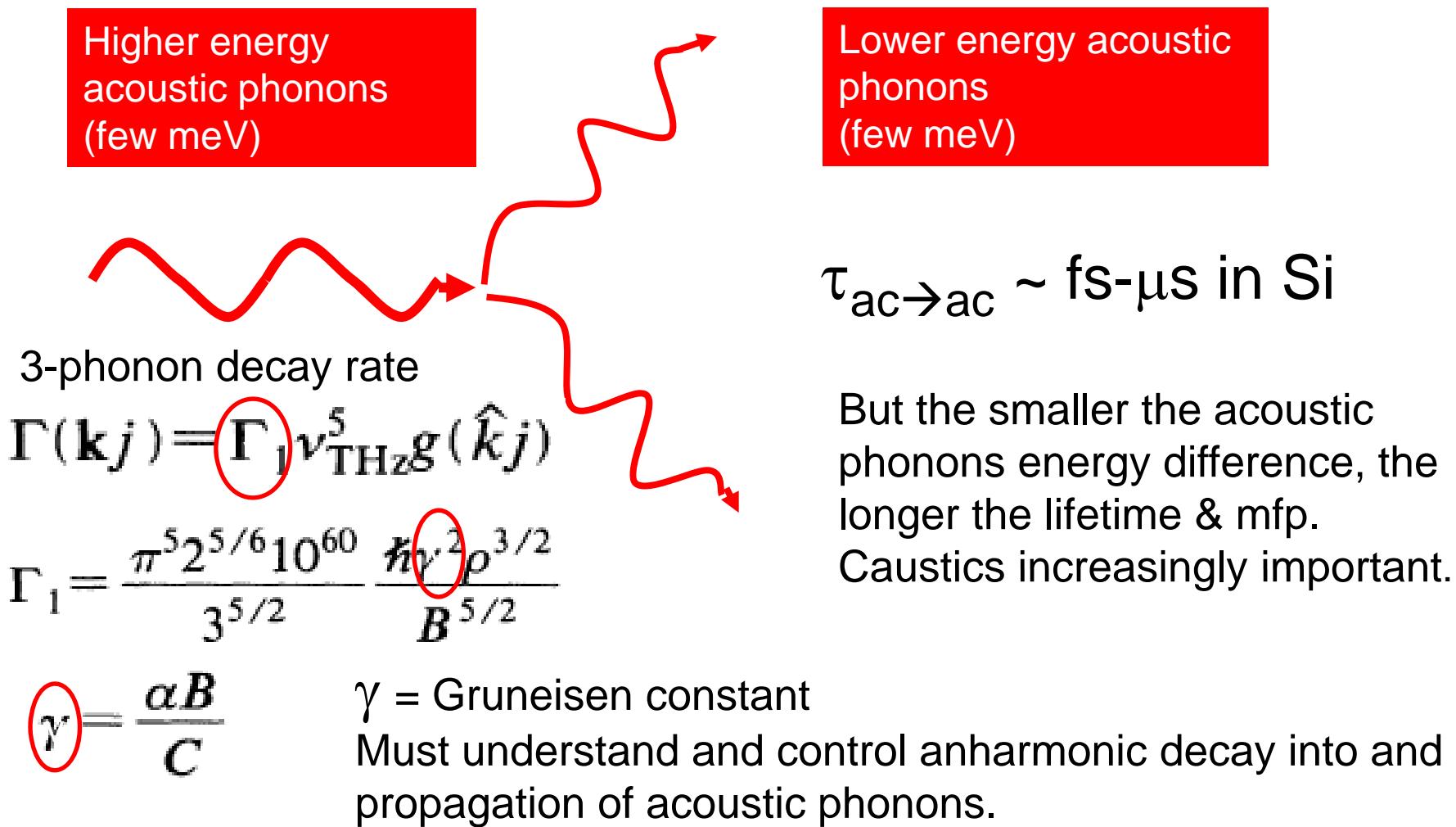
Fig. 3. Various asymmetric nanostructures which could be used for thermal rectification. Refs. [1-7]

# Phonon anharmonic decay



# Phonon anharmonic decay

Decay can involve only acoustic phonons. Cubic case  
 and frequency < Debye frequency



- The Summer School Series Son et Lumiere participating groups
- CA ZEROPOWER partners
- The members of the European CNRS-sponsored Network for Thermal Nanoscience and Nanoengineering
- The Fluctuations and Statistical Physics community
- The Phonons & Fluctuation informal community
- The solid state quantum physics community
- The mechanical engineering heat transfer community
- The multi-scale physics modelling community
- Partners of the EU projects, eg:
  - NANOPOWER –three future scenarios of future heta transport control
  - NANOPACK – thermal management in nanoelectronincs
  - TAILPHOX, MINOS and QNEM – on fluctuations, qbut and phonon engineering
  - CA NANOICT, NoE NANOFUNCTION,

- Motivation
- Methods
  - Membranes
  - Inelastic light scattering
- Dispersion relations
- Impact on heat transfer
- **Perspectives and Conclusions**

# Perspectives & Conclusions

- Dispersion relations of confined acoustic phonons have been measured and simulated in Silicon membranes.
- Phonon engineering is possible with membranes, phononic crystals, cavities and coupled cavities.
- Phonon sources are needed for progress in the field
- Nanofabrication (3D) and nanometrology developments are needed.
- “Heterogeneous” coupled cavities need better description with, e.g., quantum physics and elasticity theory.
- Phonon coherence studies in confined structures unavoidable
- Need contribution from statistical and quantum physics.
- Only then we can seriously address low power electronics.

# Support



Large  
Installation  
IMB-CNM,  
GICSERV  
2010 grant



NANOPOWER

