

# Tailoring thermal transport in nanomaterials

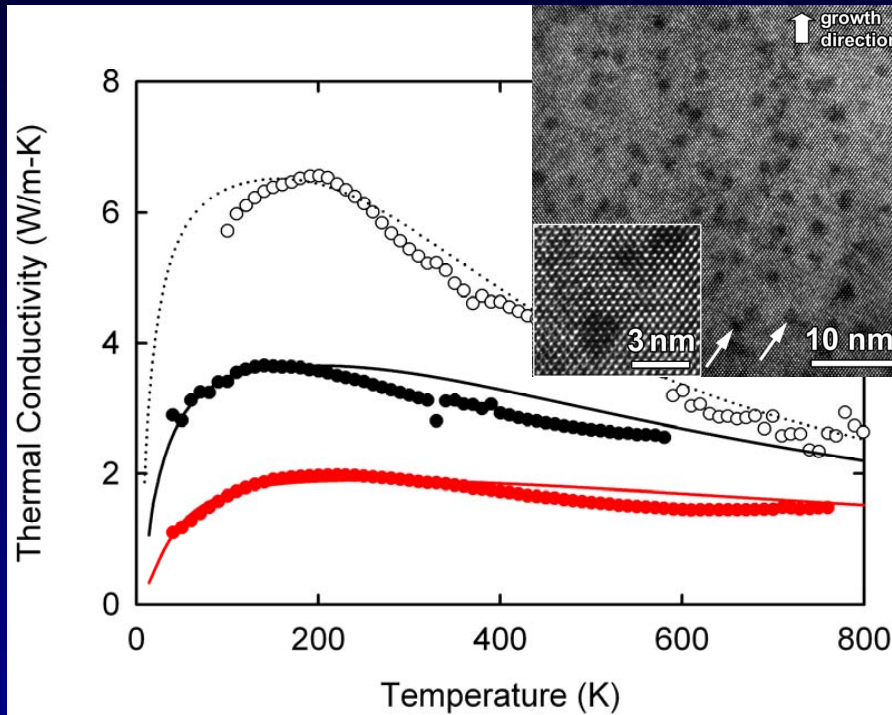
Natalio Mingo

LITEN, CEA Grenoble  
and UC Santa Cruz

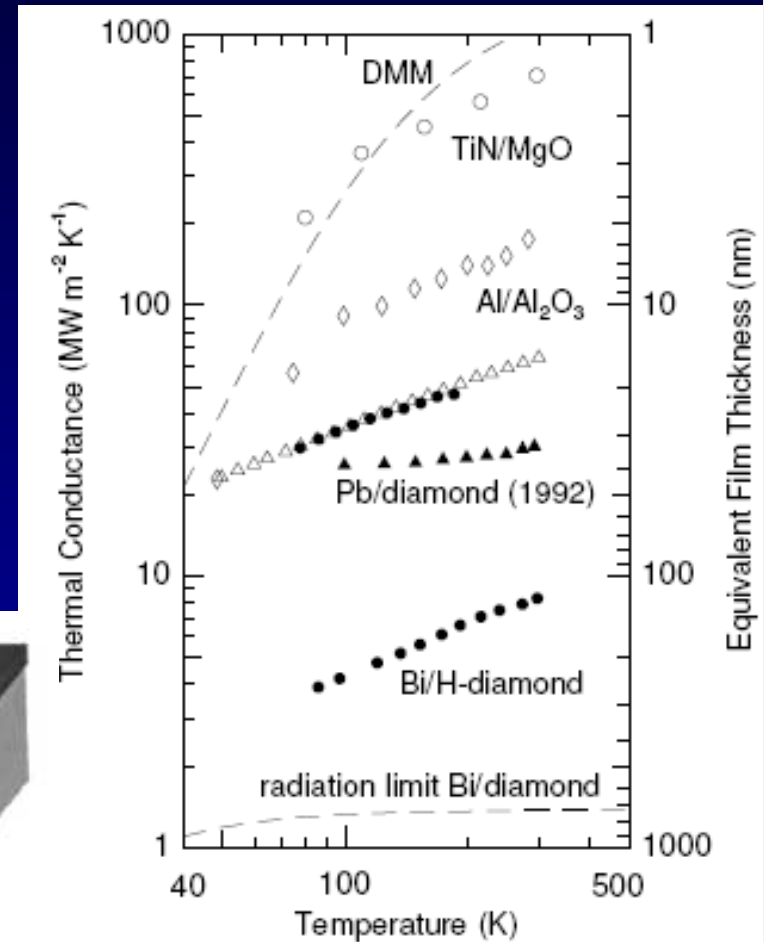


# Nanoscale thermal transport: a recent revolution

3 $\omega$  method

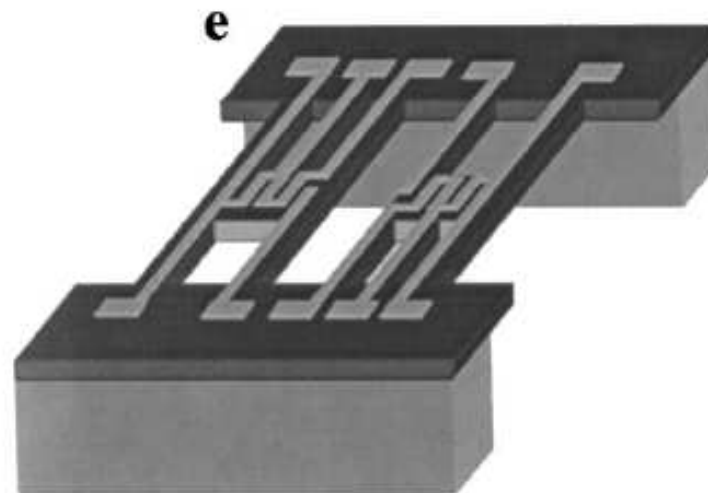


Interface thermal conductance by Time Domain ThermoReflectance



Suspended nano structures

(Shi et al., J. Heat Transfer '03)



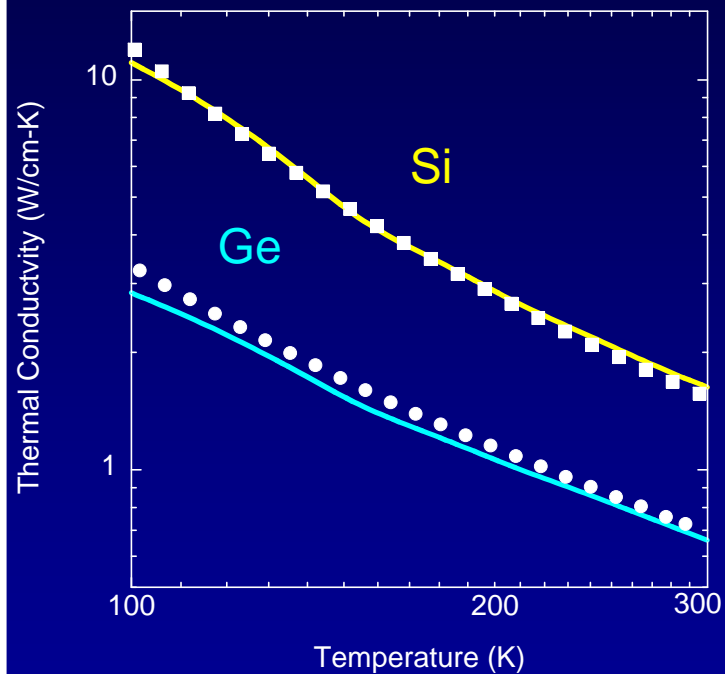
YESS '09

liten

homaterials ».

## Ab-initio Boltzmann Transport Equation

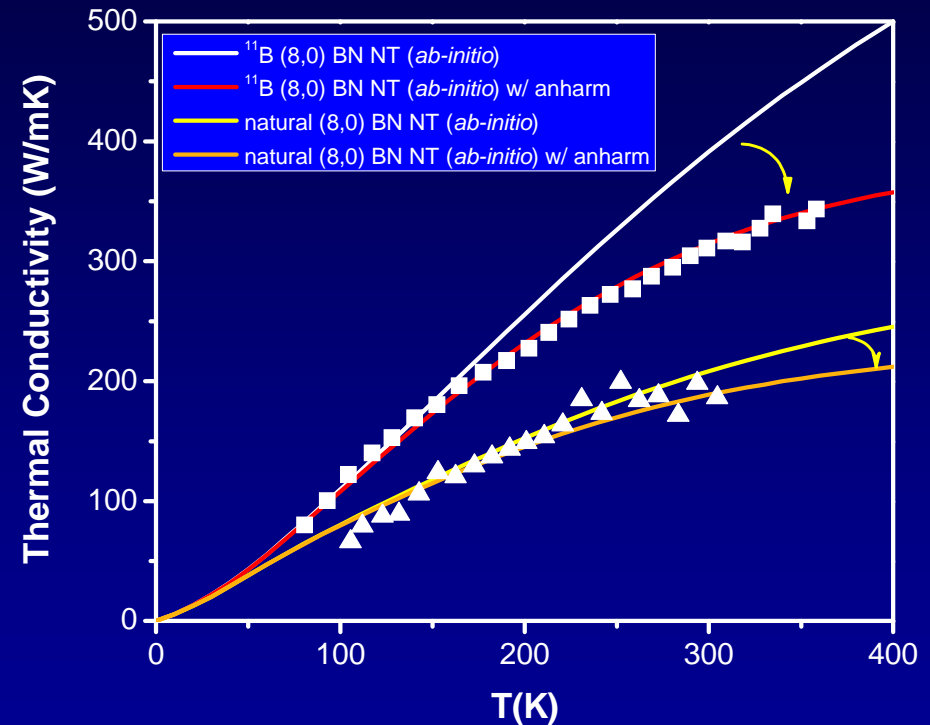
### Thermal conductivity of single crystals



D. A. Broido, M. Malorny, G. Birner, N. Mingo, and D. A. Stewart, *Applied Physics Letters* (2007).

## Ab-initio Green's functions

### Isotope effect in BN nanotubes

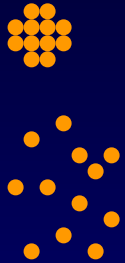


Savic, Stewart and Mingo, *Phys. Rev. Lett.* (2008)

# Sizes

YESS '09. N. Mingo: « Tailoring Thermal Transport in Nanomaterials ».

# How do embedded nanoparticles affect phonon lifetimes?



Low frequency: (Rayleigh scattering)

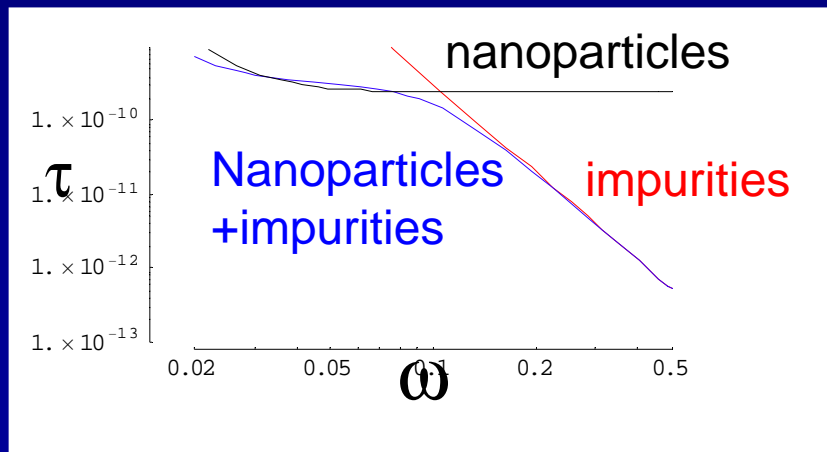
Cluster of N atoms:  $\tau^{-1} \sim N^2$  ← More effective

N independent atoms:  $\tau^{-1} \sim N$

High frequency: (geometric scattering)

Cluster of N atoms:  $\tau^{-1} \sim N^{2/3}$

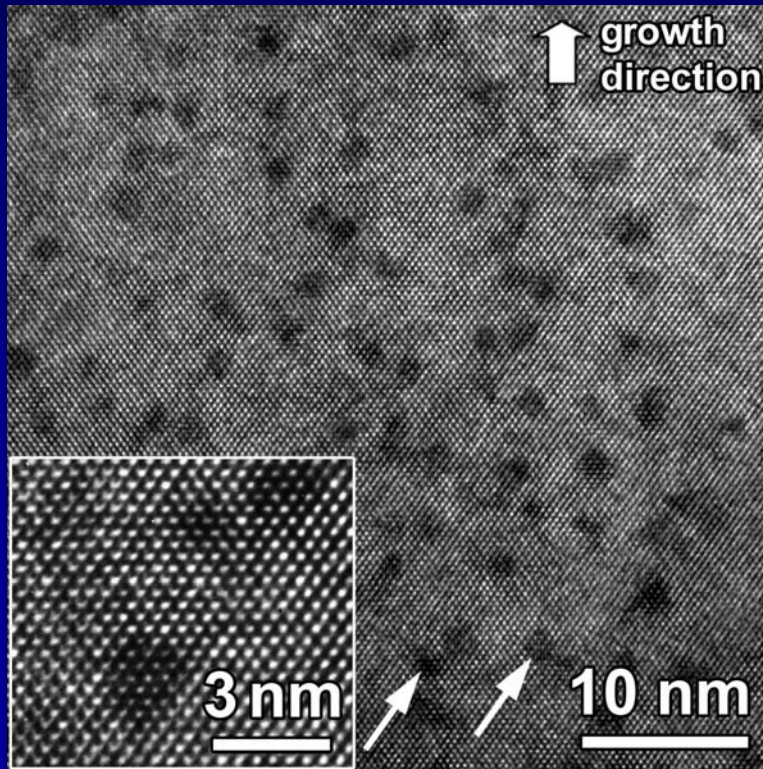
N independent atoms:  $\tau^{-1} \sim N$  ← More effective



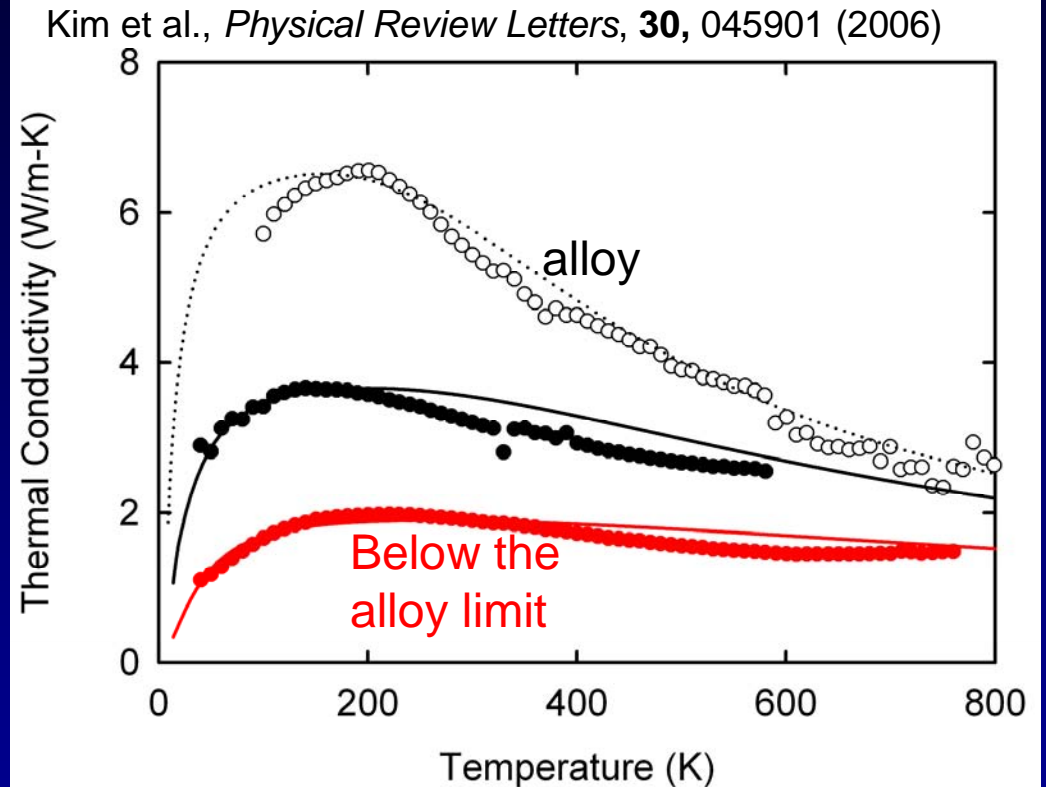
# Tailoring thermal transport by “nanoparticles in alloy”

ErAs (semimetal)  
nanoparticles in InGaAs

Image from D. Klenov  
J.M. Zide, *et. al.* Appl. Phys. Lett. **87**,  
112103 (2005)



Kim et al., *Physical Review Letters*, **30**, 045901 (2006)

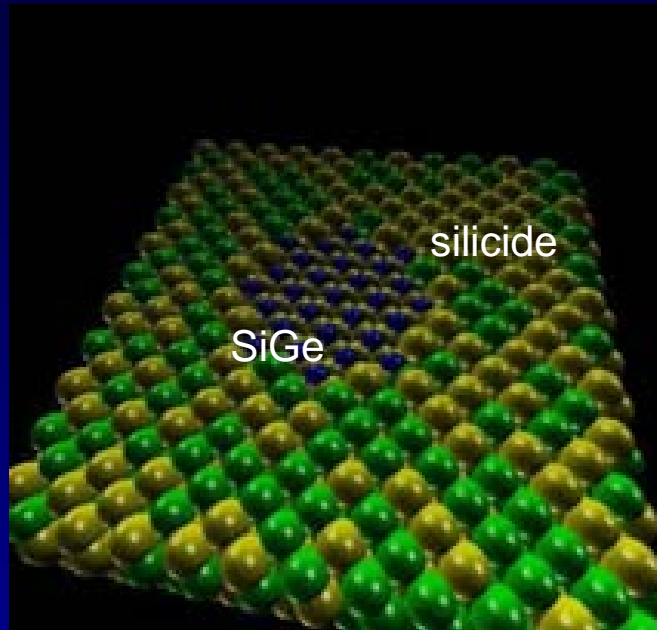


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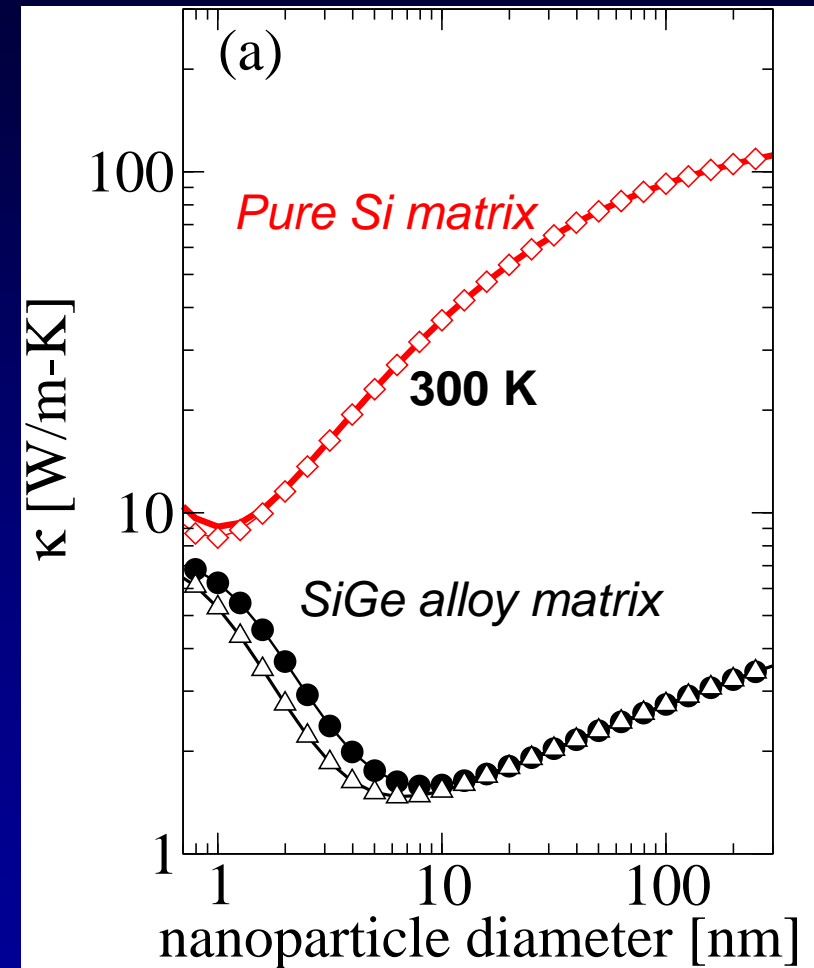
# The interest of an improved SiGe

- SiGe is monolithically integrable into Si technology

Cooling hotspots.



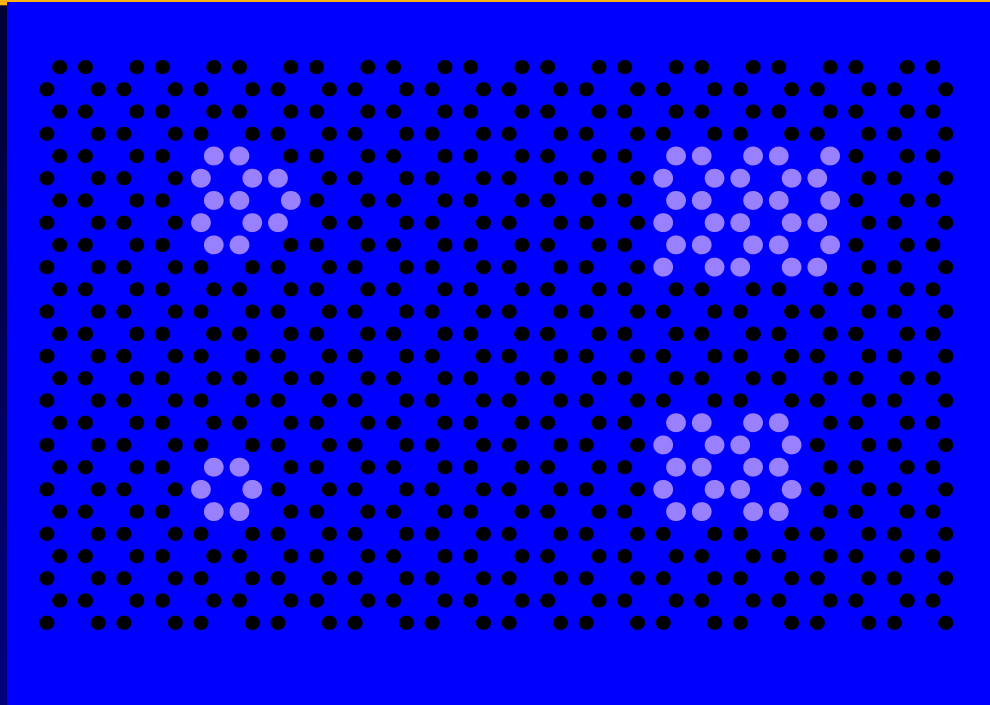
- 10 microns thick,  $50 \times 50 \mu\text{m}^2$  monolithic microrefrigerator with  $ZT \sim 0.5$  can cool a  $1000 \text{ W/cm}^2$  hot spot by  $>15\text{C}$ .



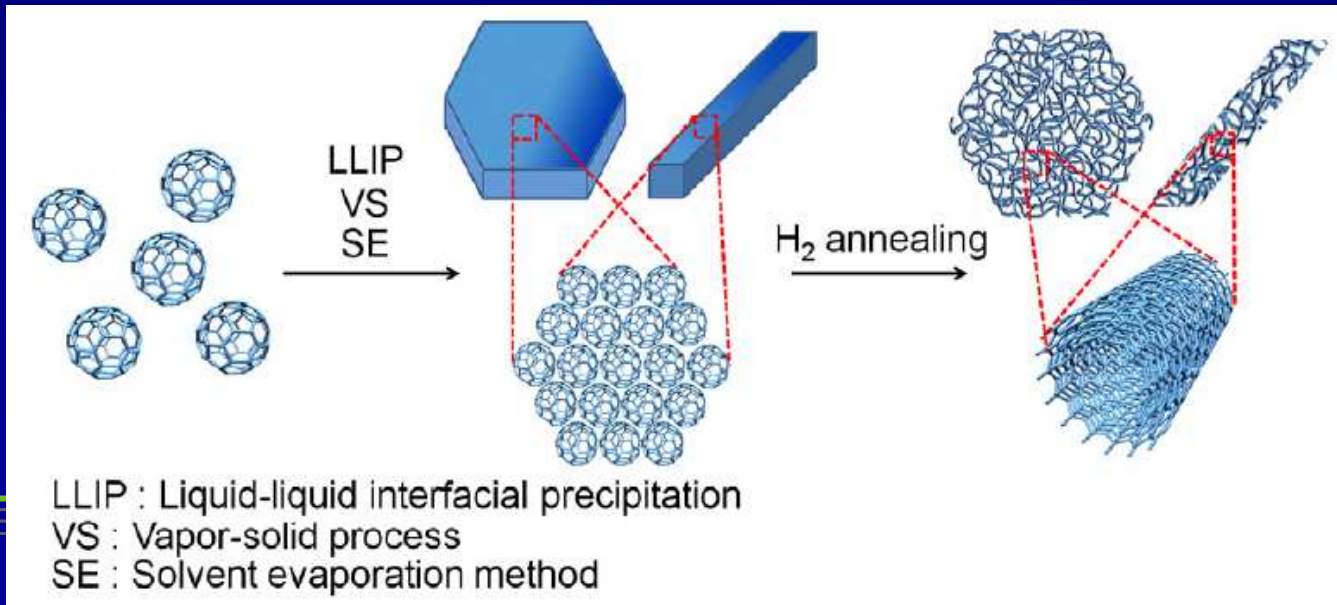
Mingo et al., *Nano Lett.* 9, 711 (2009).

YESS '09. N. Mingo: « Tailoring Thermal Transport in Nanomaterials ».

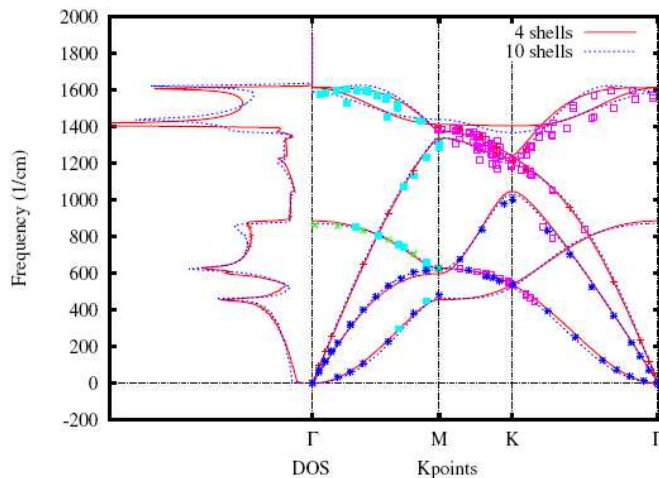
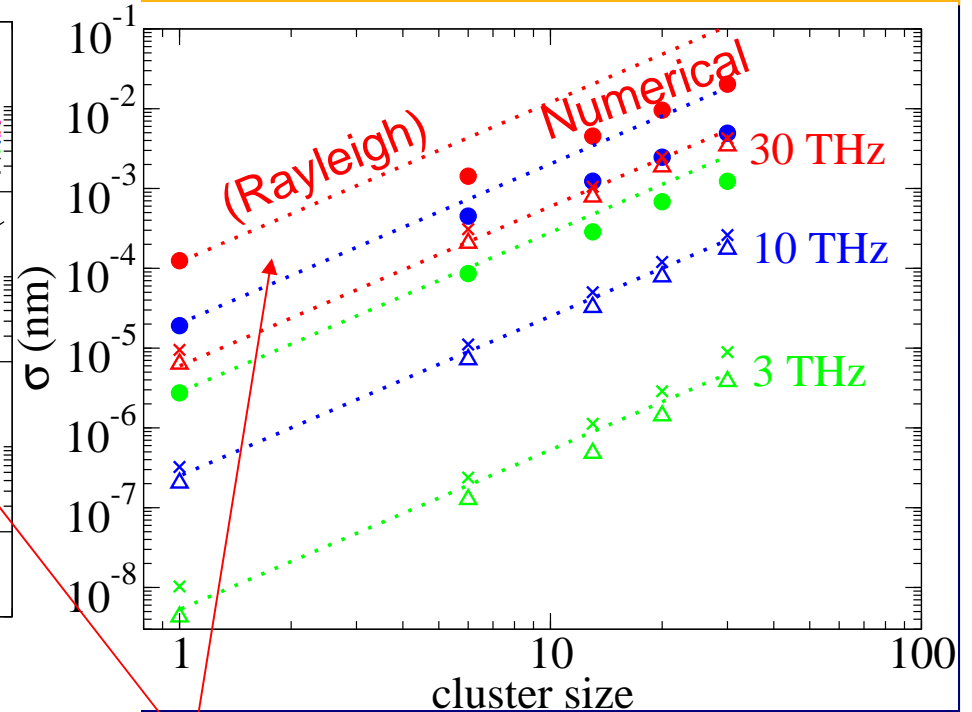
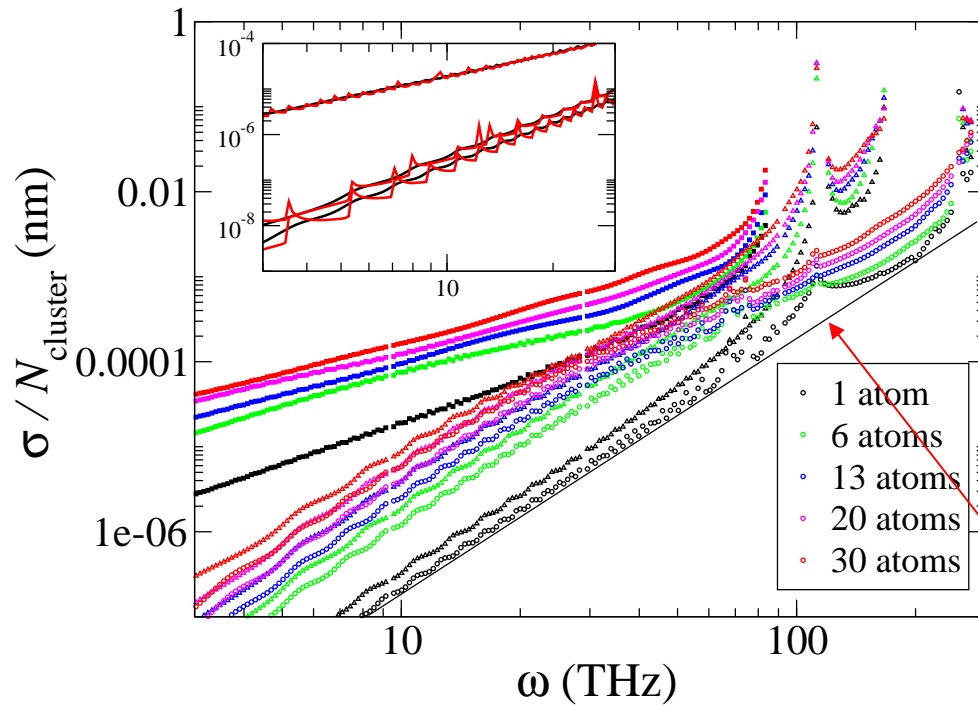
An ideal system:  
 $^{13}\text{C}$  isotopic  
 clusters in  
 graphene



Lim et al.  
 Nanotechnology **20** (2009) 145601

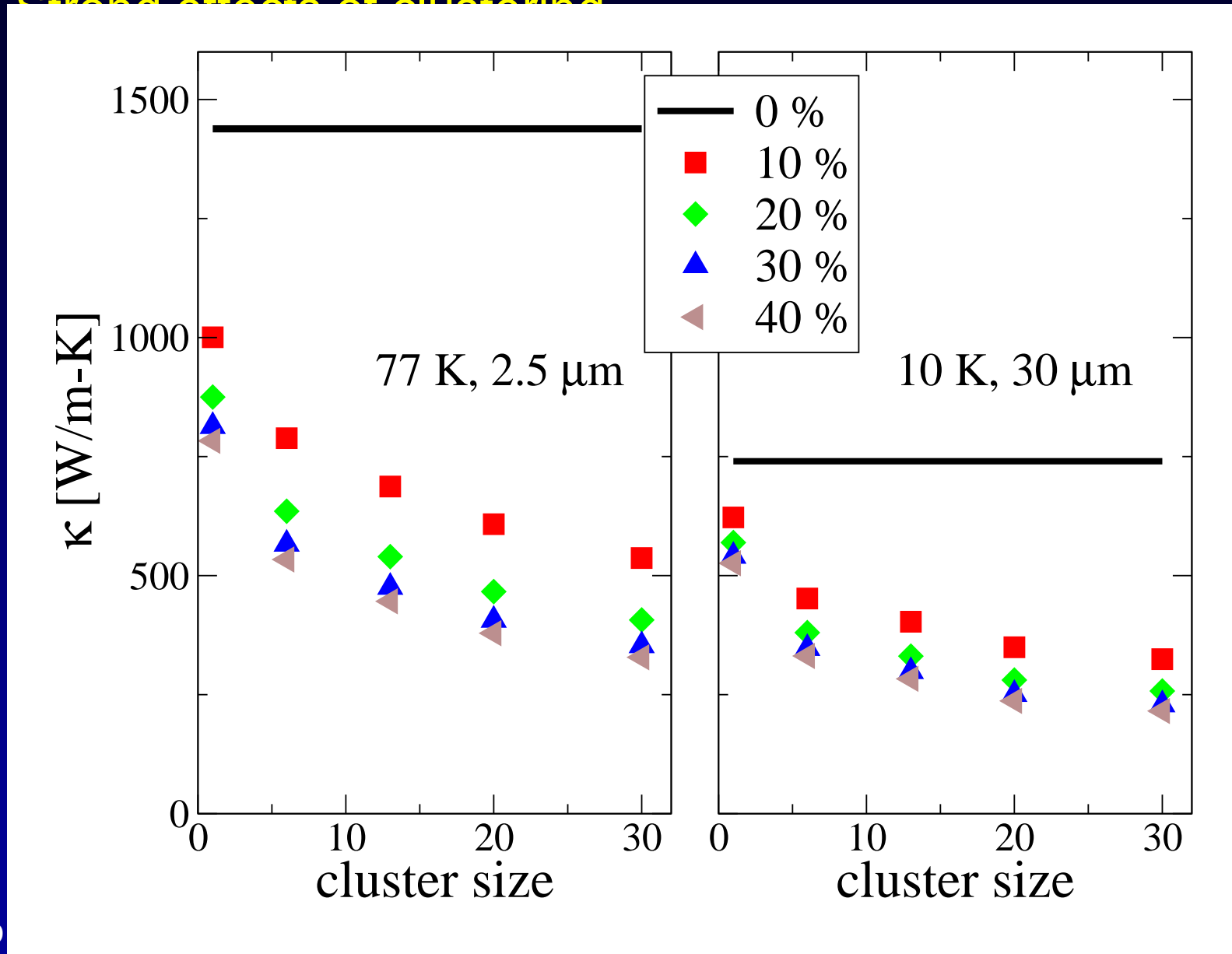


# Computing cross sections « ab-initio »



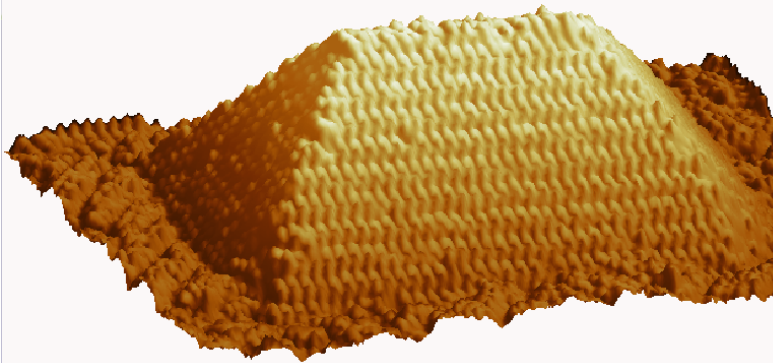
There are important differences between the atomistic calculation and common analytical expressions

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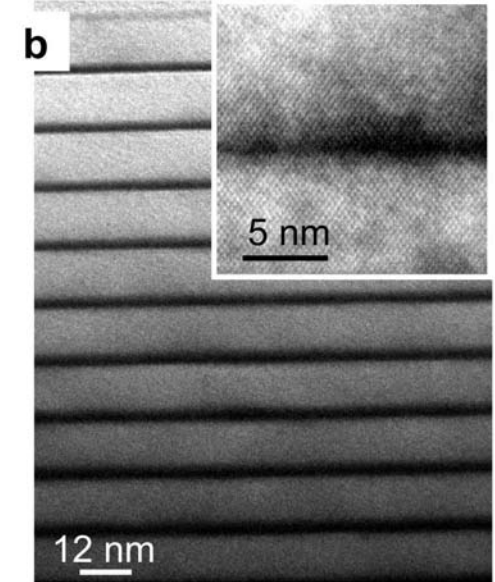
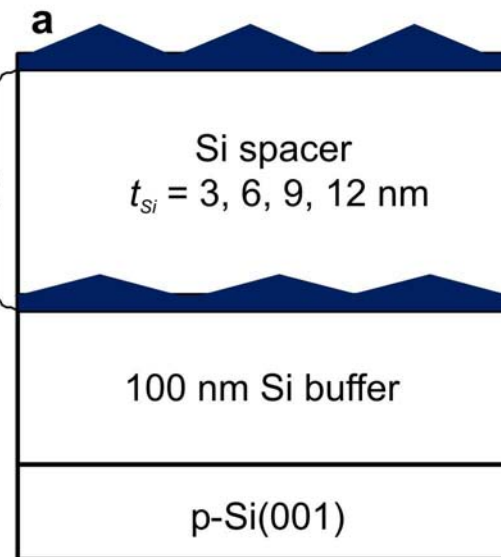


# Textures

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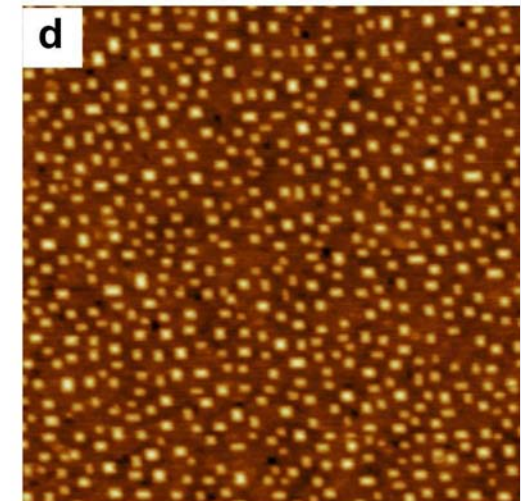
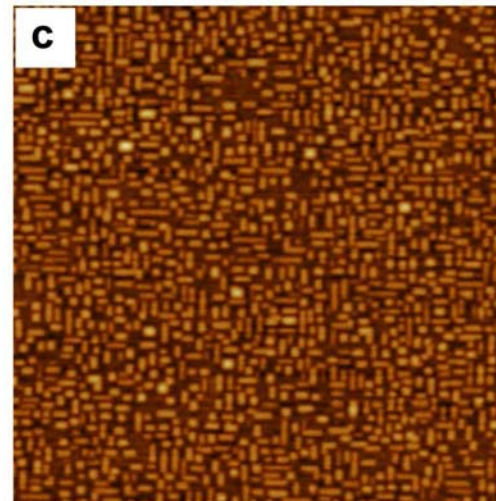
×4  
or  
×10



Growth and  $3\omega$  measurements:  
IFW Dresden (A. Rastelli)

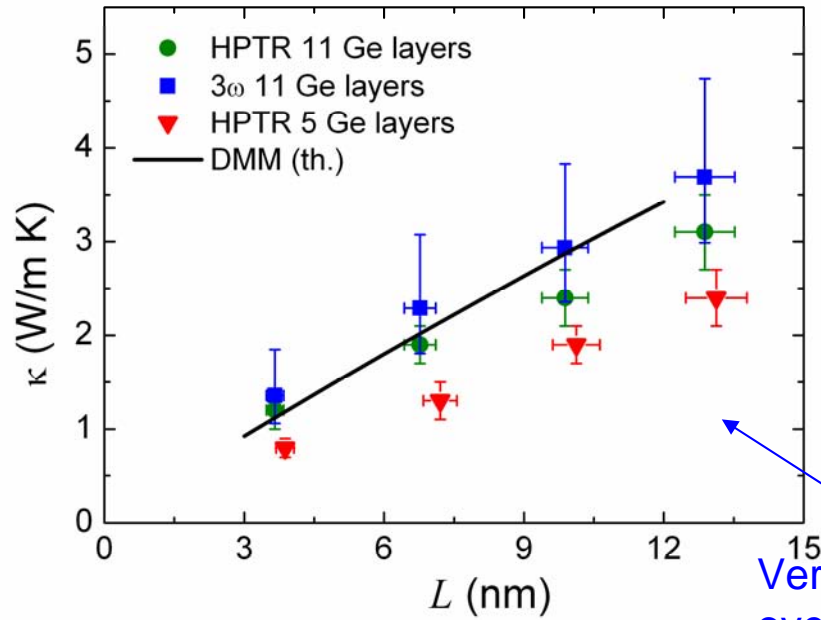
TDTR measurements: U. of  
Bordeaux (S. Dilhaire)

Theory: CEA (Mingo)

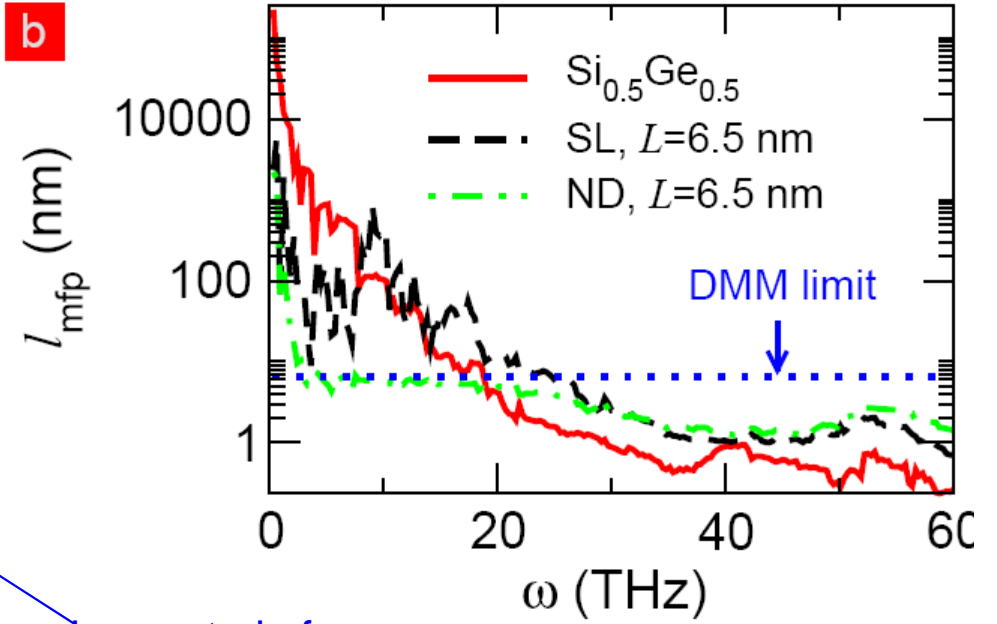


— 100 nm [100] → Height (nm) -1 3 nm

Pernot et al., submitted

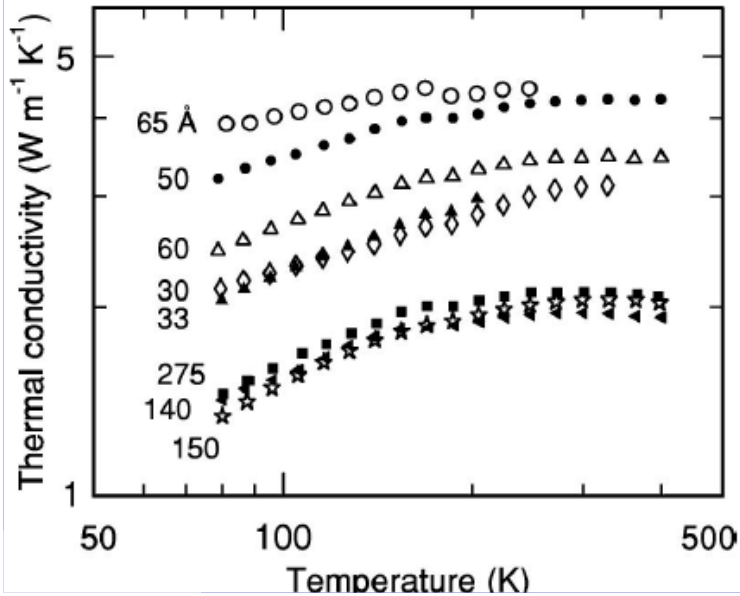


**b**

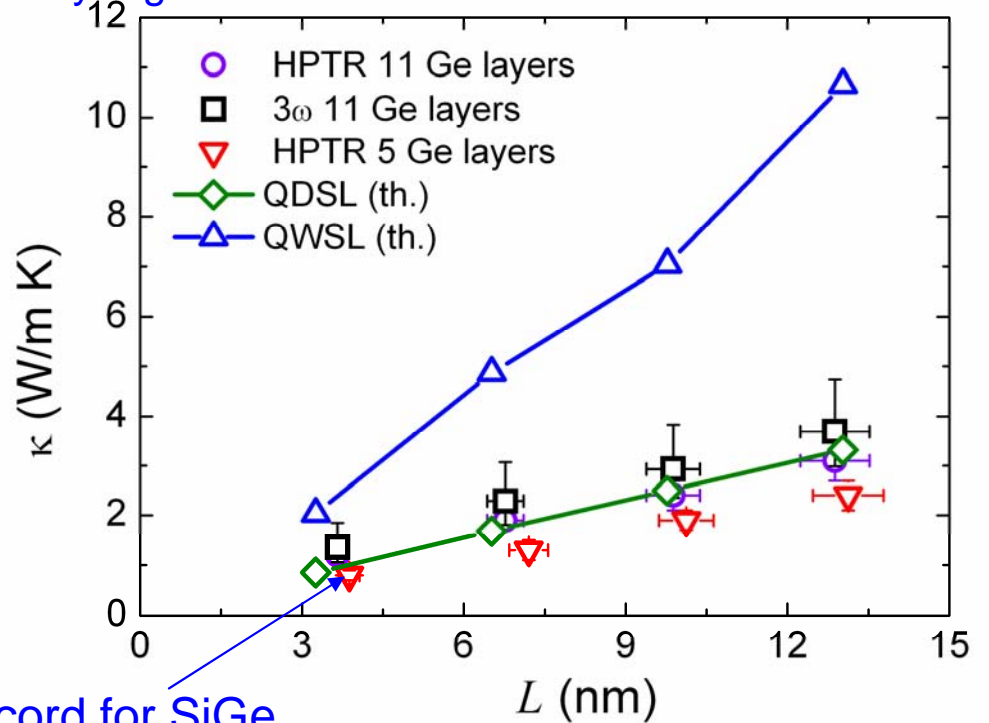


Very precise control of  $\kappa$  over tiny regions

Planar SL (Lee and Cahill APL97)

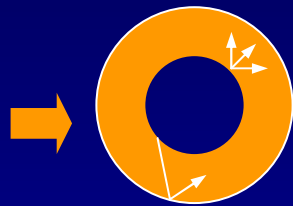
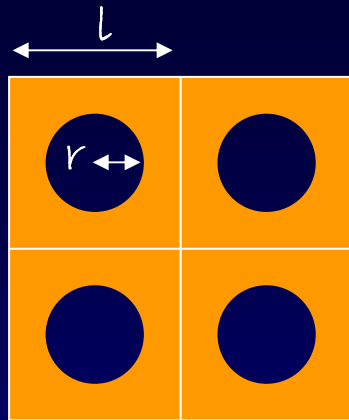


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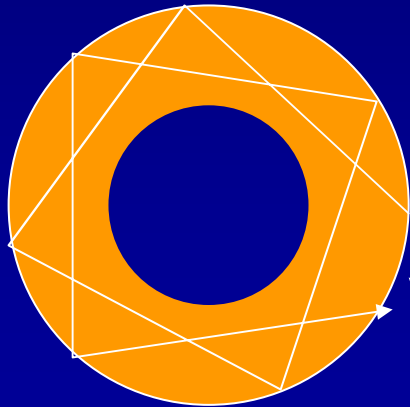
Record for SiGe

# Tailoring phonon transport with nano-pores

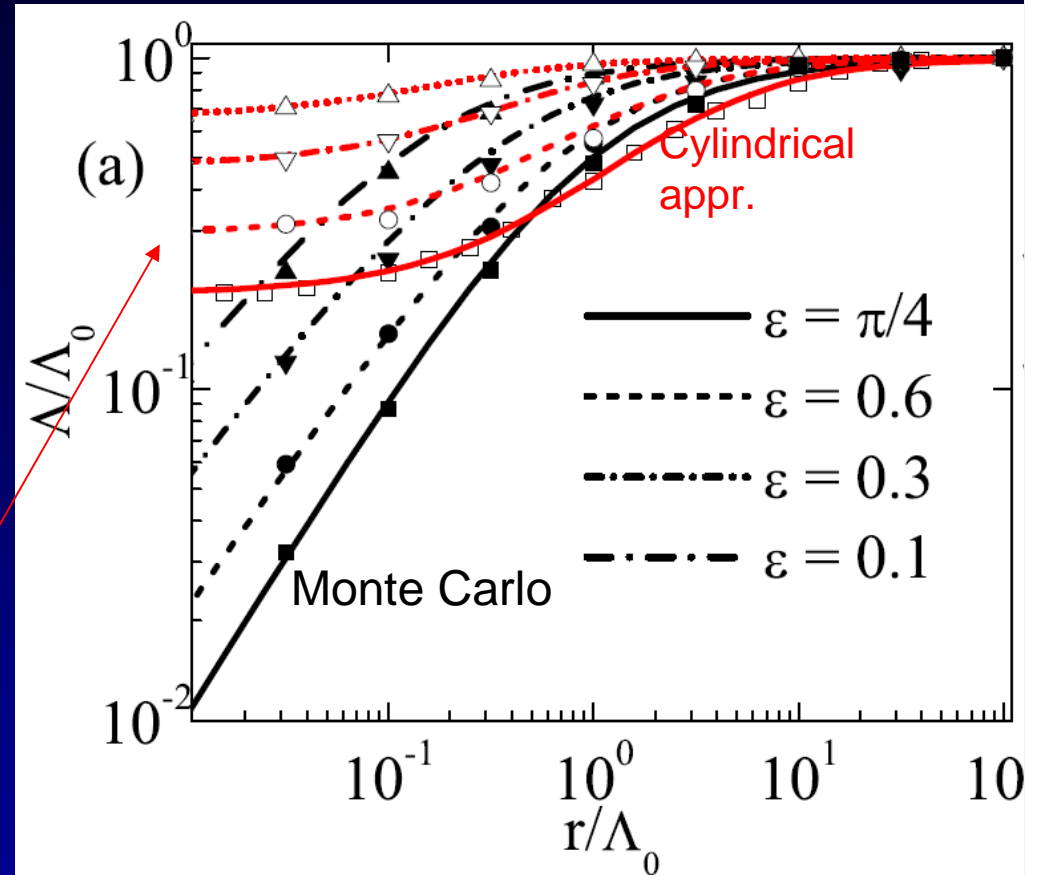


diffusive reflection at inner surface  
 specular reflection at outer surface

R. Prasher (JAP 2005)



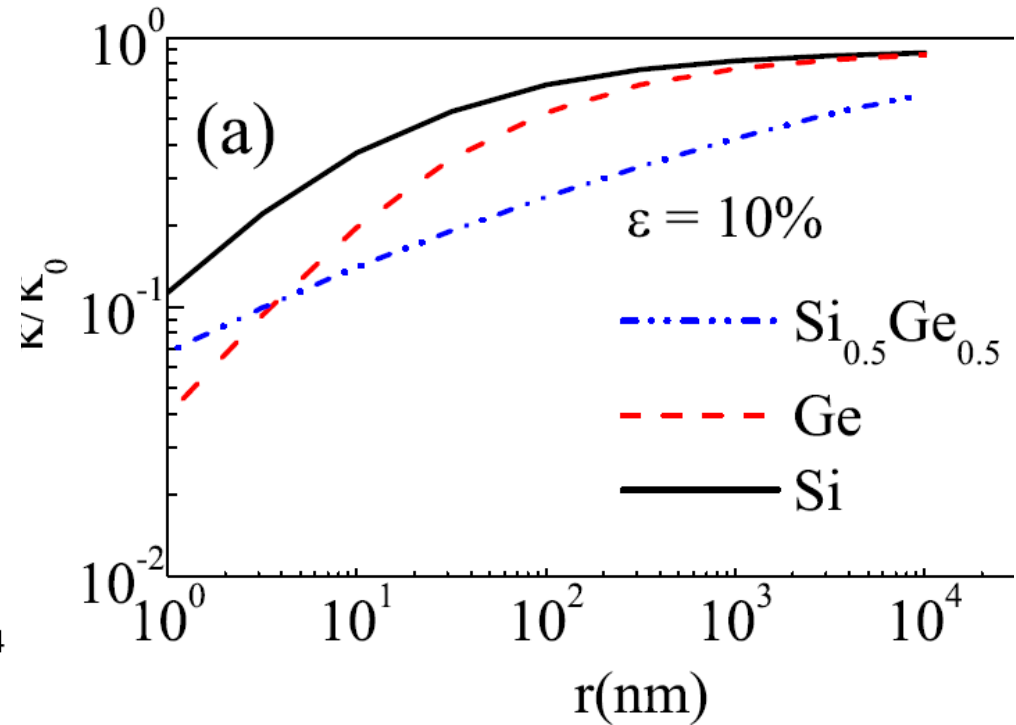
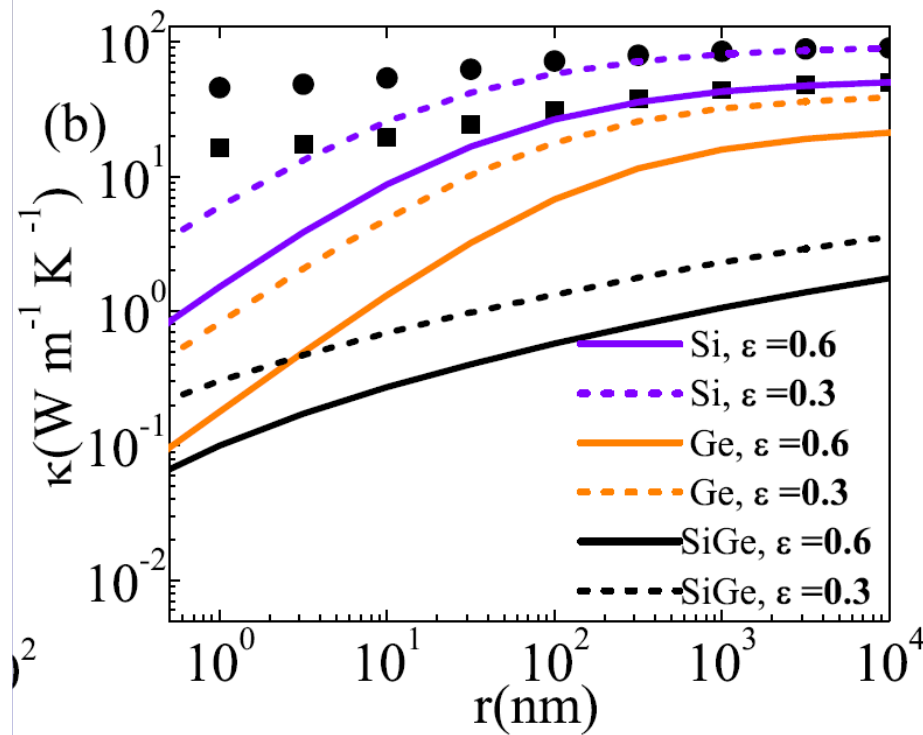
The cylindrical approximation gives spurious results



Bera, Volz, and Mingo, submitted



## Promising nanoporous alloys



Bera, Volz, and Mingo, submitted

# Alloy is better

*Larger pores mean less charge trapping: good for thermoelectrics.*

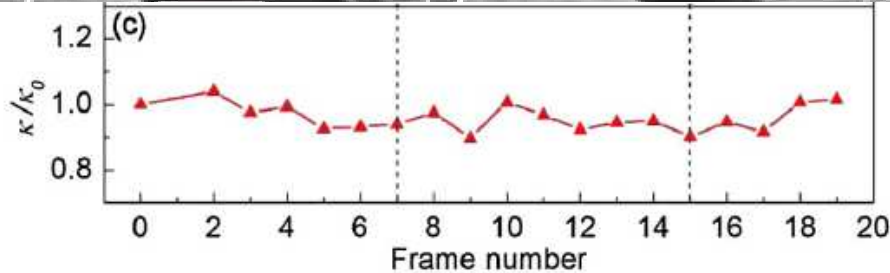
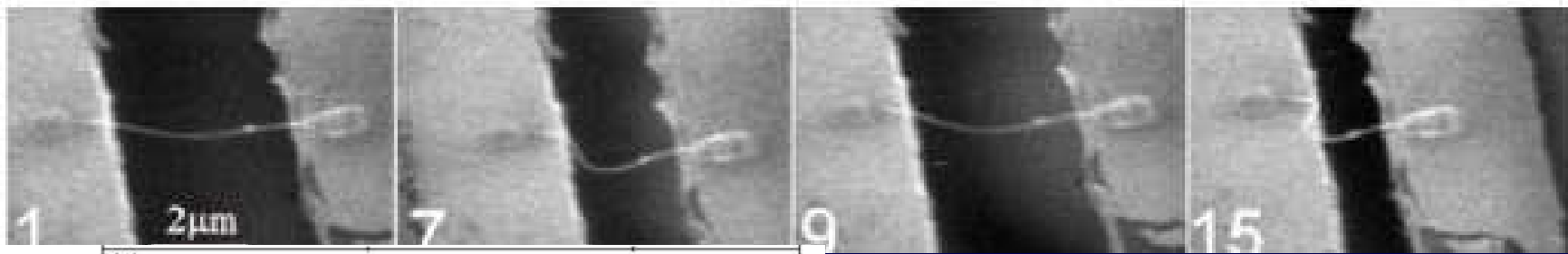
YESS '09. N. Mingo: « Tailoring Thermal Transport in Nanomaterials ».

# Shapes

YESS '09. N. Mingo: « Tailoring Thermal Transport in Nanomaterials ».

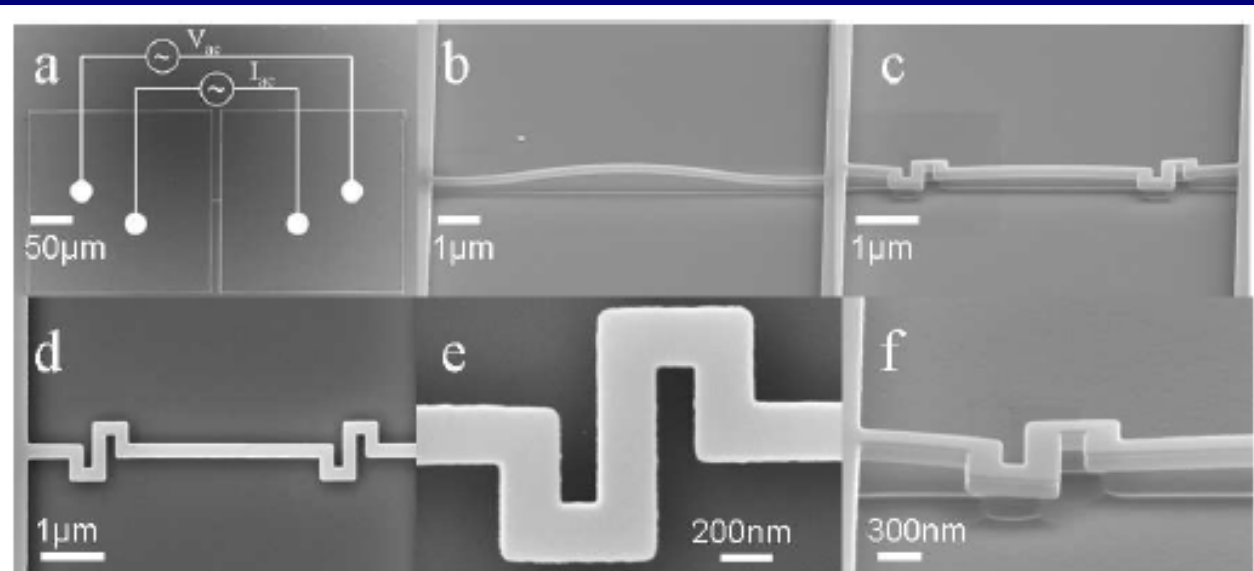


# Tailoring phonon transport via nanoscale geometrical design



Chang et al.: Nanotube phonon waveguide (PRL07)

No effects of bending were observed



Our etched nanowires:

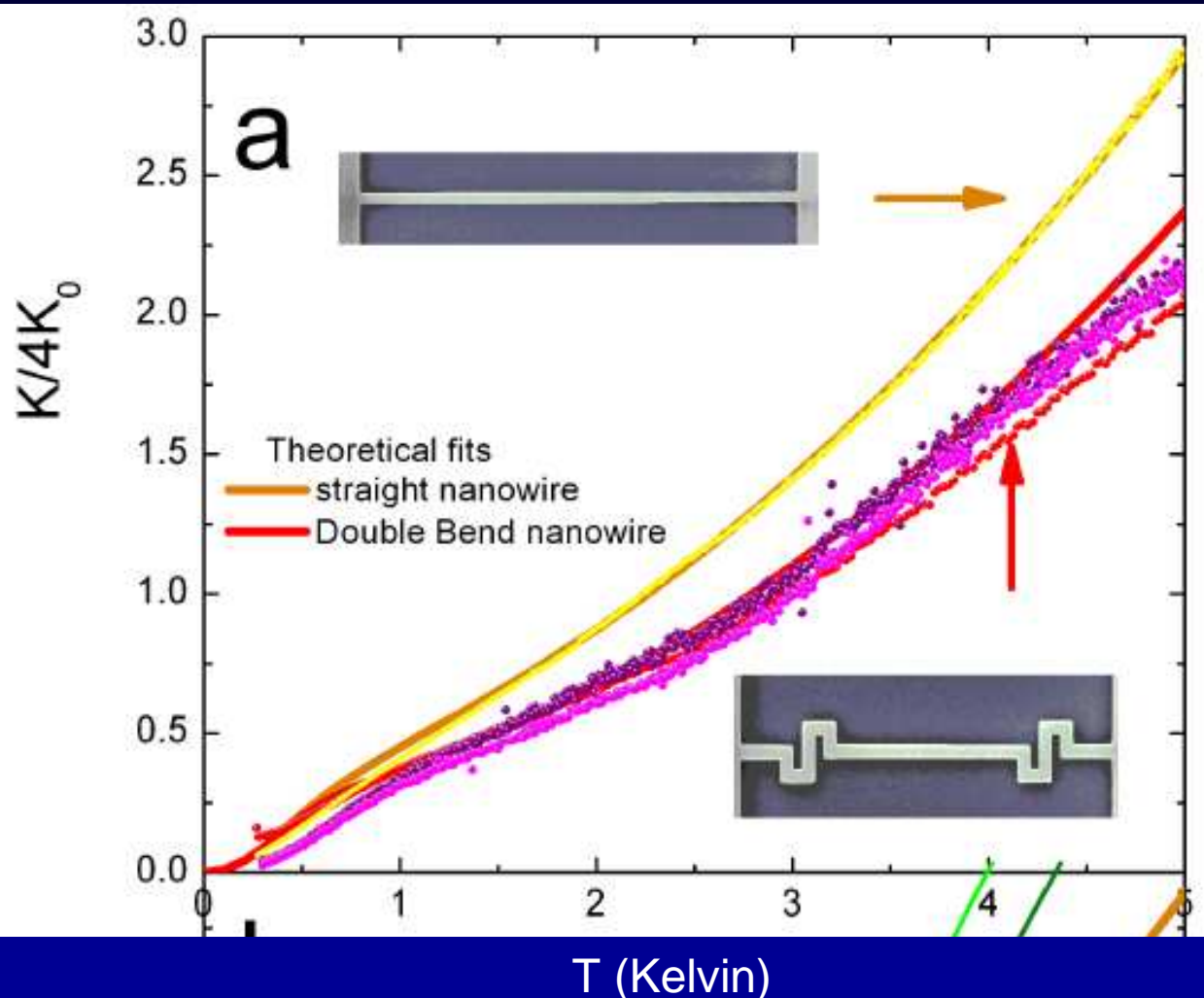
Will they show effects of geometry?

(Experiment by O. Bourgeois, CNRS)

aterials ».



# Tailoring phonon transport via nanoscale geometrical design



The straight nanowire conducts 40 times less than its ballistic limit.

So, how can the serpentine affect so much?

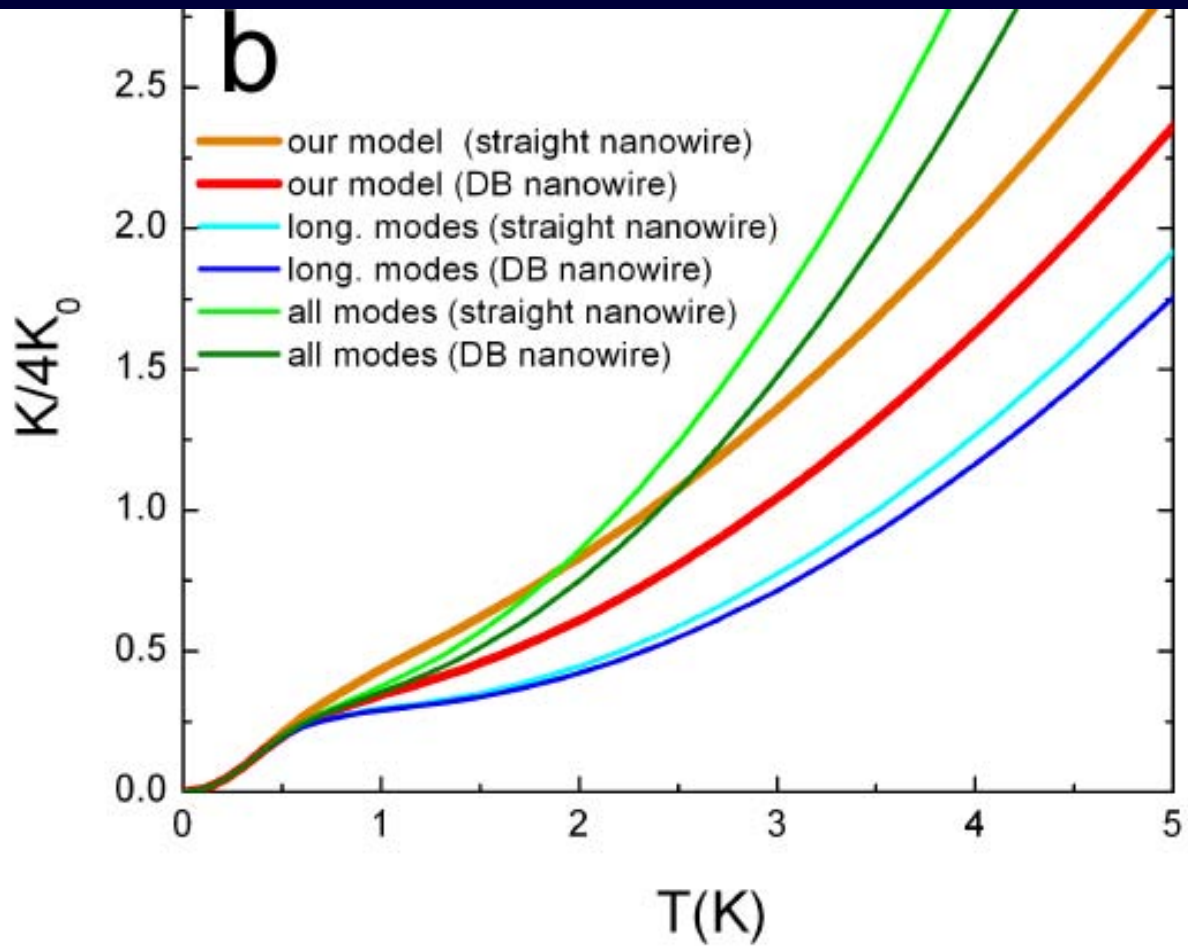
*Because transmission is frequency dependent.*

J.S. Heron, C. Bera, T. Fournier, N. Mingo and O. Bourgeois, manuscript in preparation.

YEISS '09. N. Mingo: « Tailoring Thermal Transport in Nanomaterials ».



## Tailoring phonon transport via nanoscale geometrical design



Theory also tells us that:

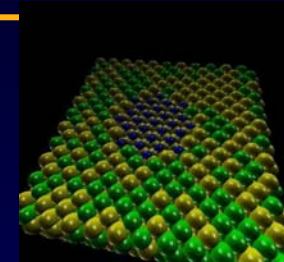
the serpentine's transmission probability is  $\sim 0.2$ .

The T modes are practically absent.

## Conclusions: tailoring phonon transport

- **Sizes**

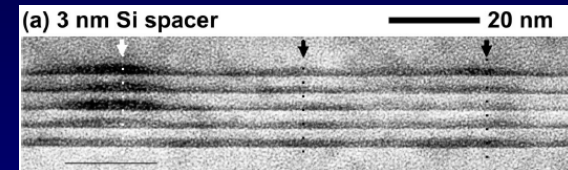
there is always an optimal nanoparticle size that minimizes  $\kappa$ .



- **Textures**

an alloy matrix is much more affected by nanostructuring than a single crystal one. Thus, nanoporous SiGe is a more interesting thermoelectric than nanoporous Si.

Nanodot phonon barriers allow us to precisely control  $\kappa$ .



- **Shapes**

low temperature  $\kappa$  is very sensitive to patterned nanowire shapes.



*There are exciting prospects in the area of nanomaterial thermal conduction. The interplay between theory and experiment will play a major role in this development.*

### Acknowledgements:

D. Broido (Boston College), D. Stewart (Cornell), K. Esfarjani (MIT), S. Volz (EC Paris), C. Bera (CEA), S. Wang (CEA), I. Savic (UCD), A. Rastelli's team (IFW-Dresden), A. Shakouri (UCSC), O. Bourgeois (CNRS), J. S. Heron (CNRS), F. Mauri (Paris VI), N. Vast (E. Polytechnique)

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YESS '09. N. Mingo: « Tailoring Thermal Transport in Nanomaterials ».