Simulating Thermal Transport in Nanostructures from the Ballistic to the Diffusive Regime

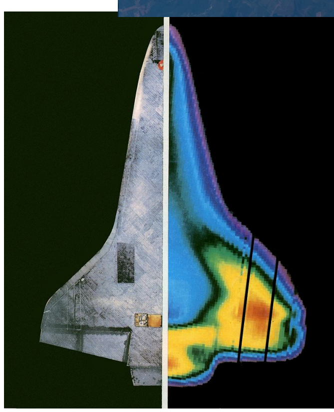
Taishan Zhu, Dinkar Nandwana, Elif Ertekin

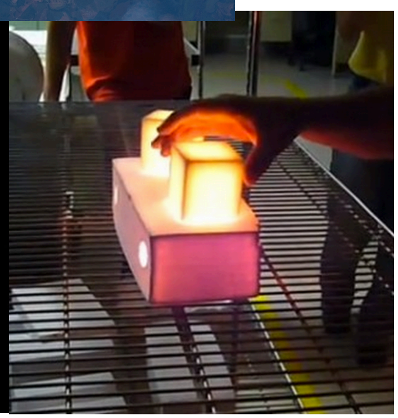
Department of Mechanical Science & Engineering, University of Illinois

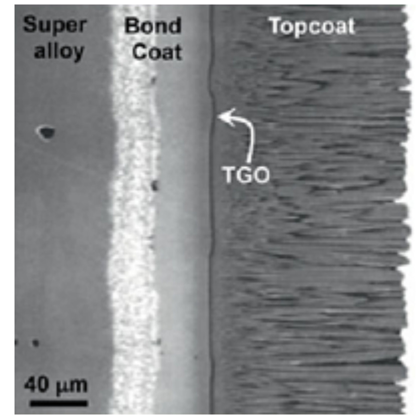
2015 Blue Waters Symposium – Sun River, Oregon– 11-13 May 2015

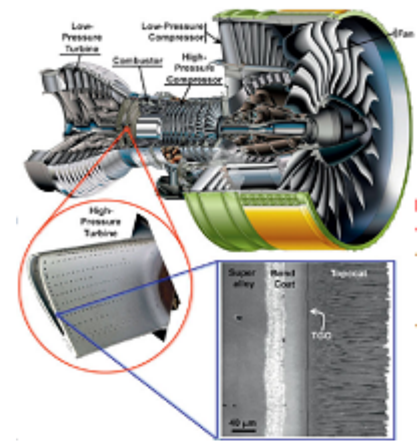
Thermal Transport

Why does it matter?









Heat Transport in Solids

Macroscale

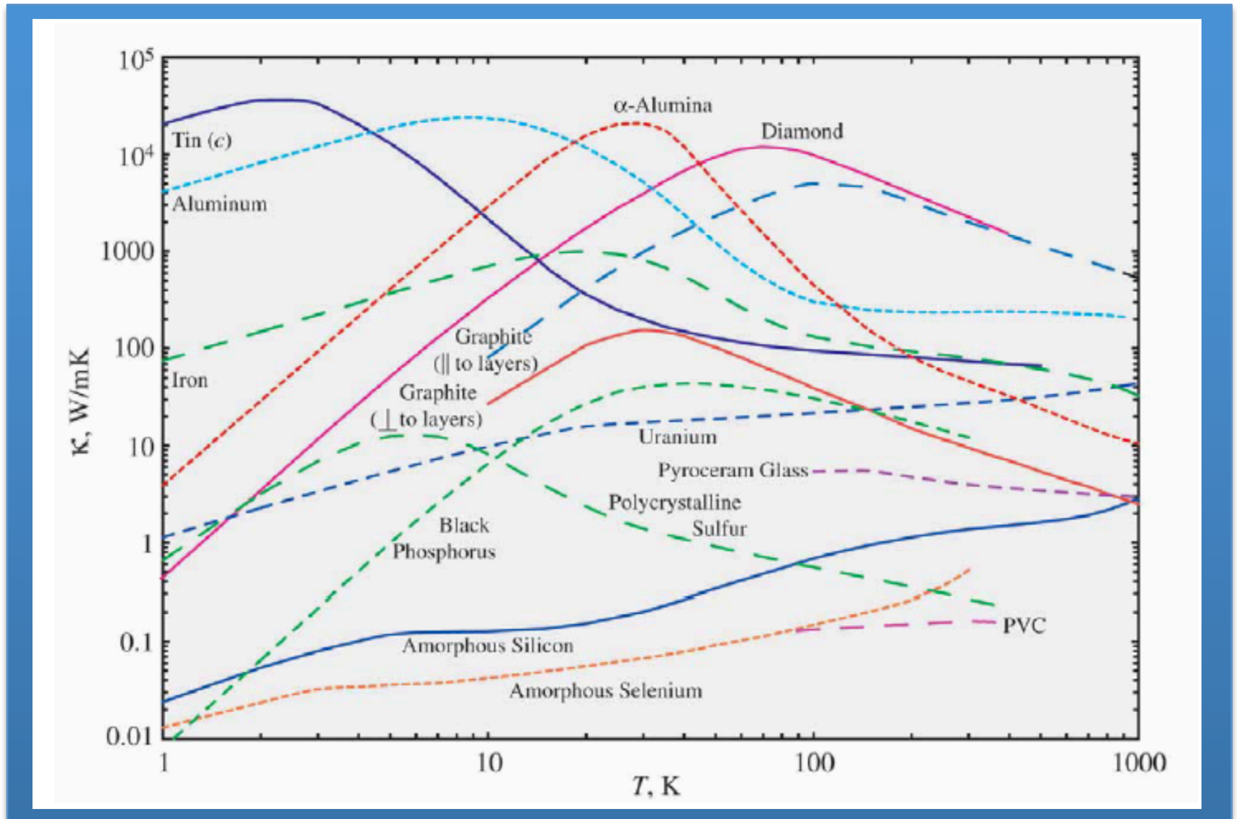
Temperature Gradient

$$Q = -\kappa \nabla T$$

Heat current

Thermal conductivity

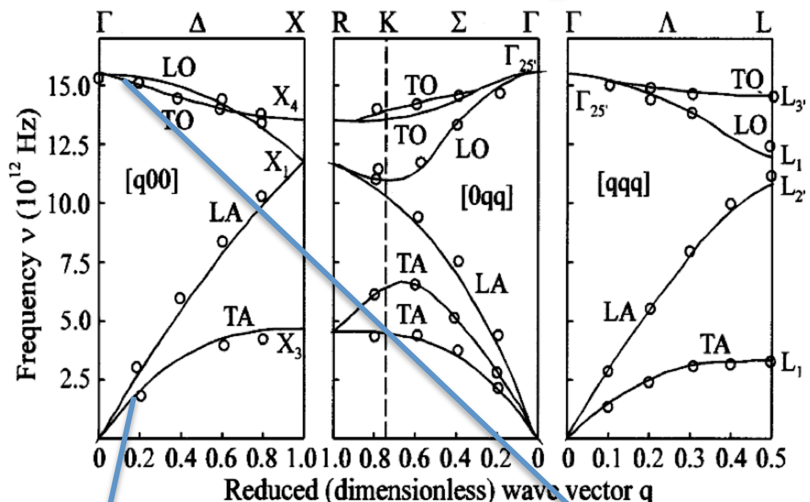
Thermal conductivity of typical solid materials:



Heat Transport in Solids

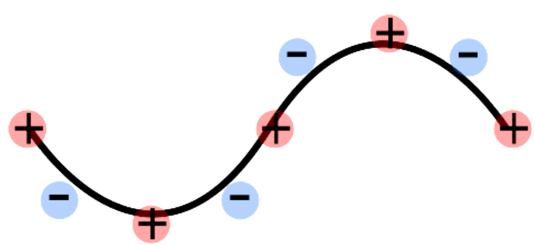
Atomic Scale

Phonons: quantized lattice vibrations

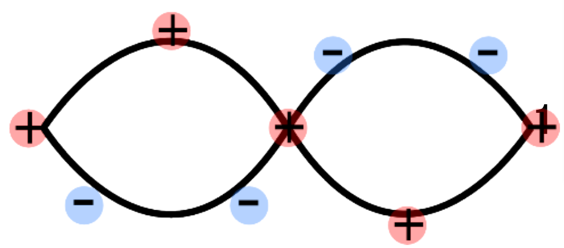


http://www.ioffe.rssi.ru/SVA/NSM/Semicond/SiGe/mechanic.html

Acoustical Mode



Optical Mode



Mechanisms:

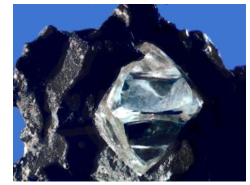
κ (W/mK)

1000

100

10

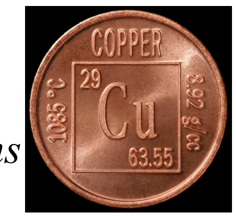
Diamond



phonons

Copper

electrons



Alumina

phonons

phonons

YSZ

polymers

"phonons"

Heat Transport in Nanostructures

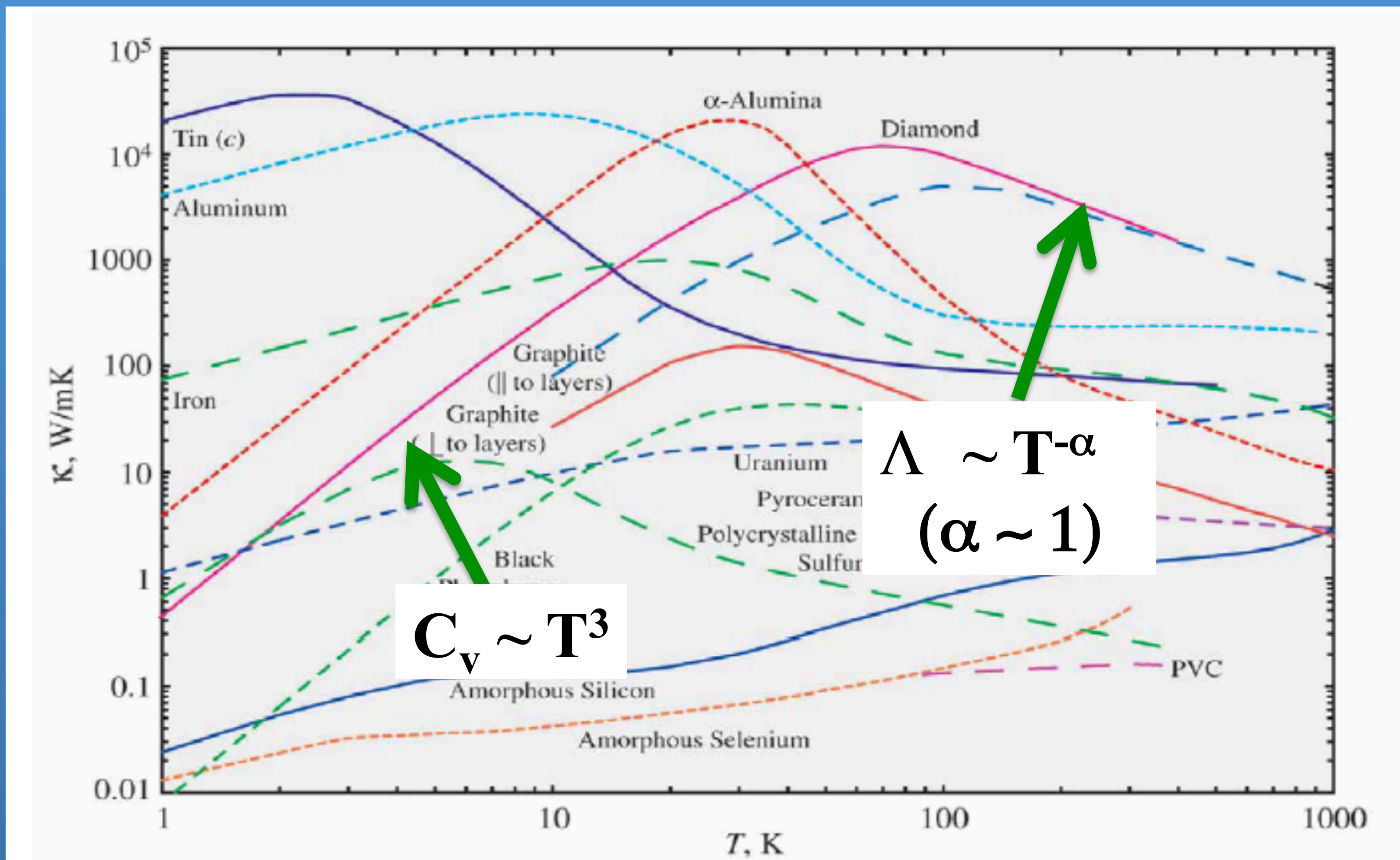
In an infinite solid, scattering of phonons by other phonons, defects, and system boundaries lim

ing

aths

nanoscale.

Thermal conductivity of typical solid materials:

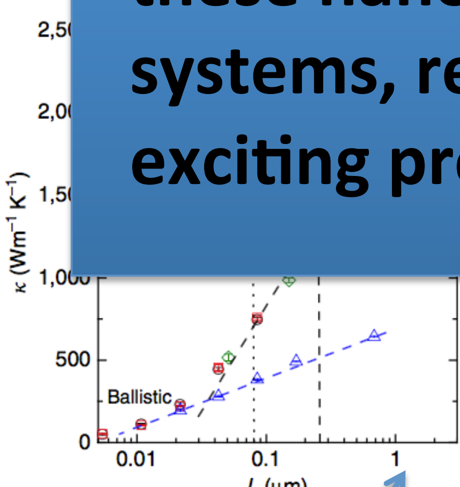


Examples: Transport in Low Dimensions

Diverging thermal conductivity with length (controversial!)

$$\kappa = \int_0^{\omega_{max}} \hbar\omega D(\omega)\frac{\partial f_{BE}}{\partial T} v_g^2 \tau \, d\omega$$

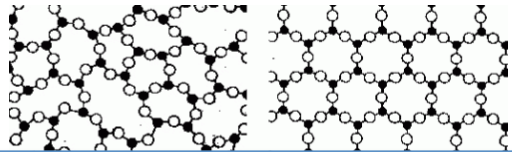
a



Note size of simulated system: 1 μm

X. Xu et al., Nat Comm 5 3689 (2014)

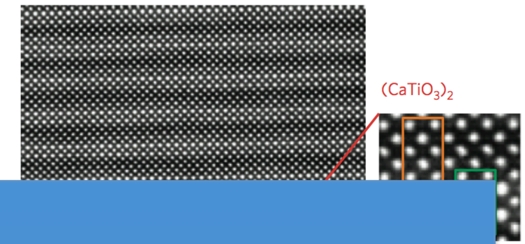
Interactions of Disorder and Low Dimensions

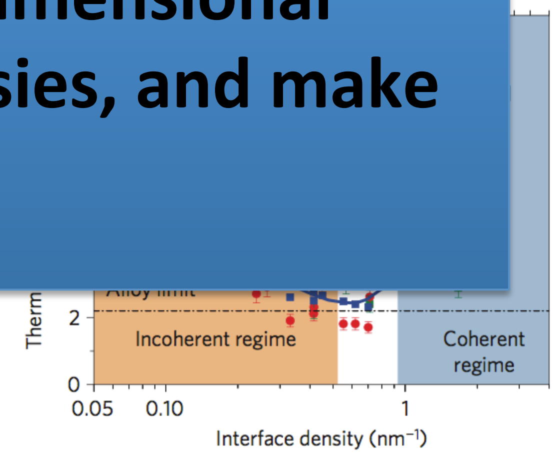


Diamond nanothreads
with ordered
& disordered SW defects

Thomas C. Fitzgibbons, et al, Nat. Mater. 2015

Nanostructured Devices

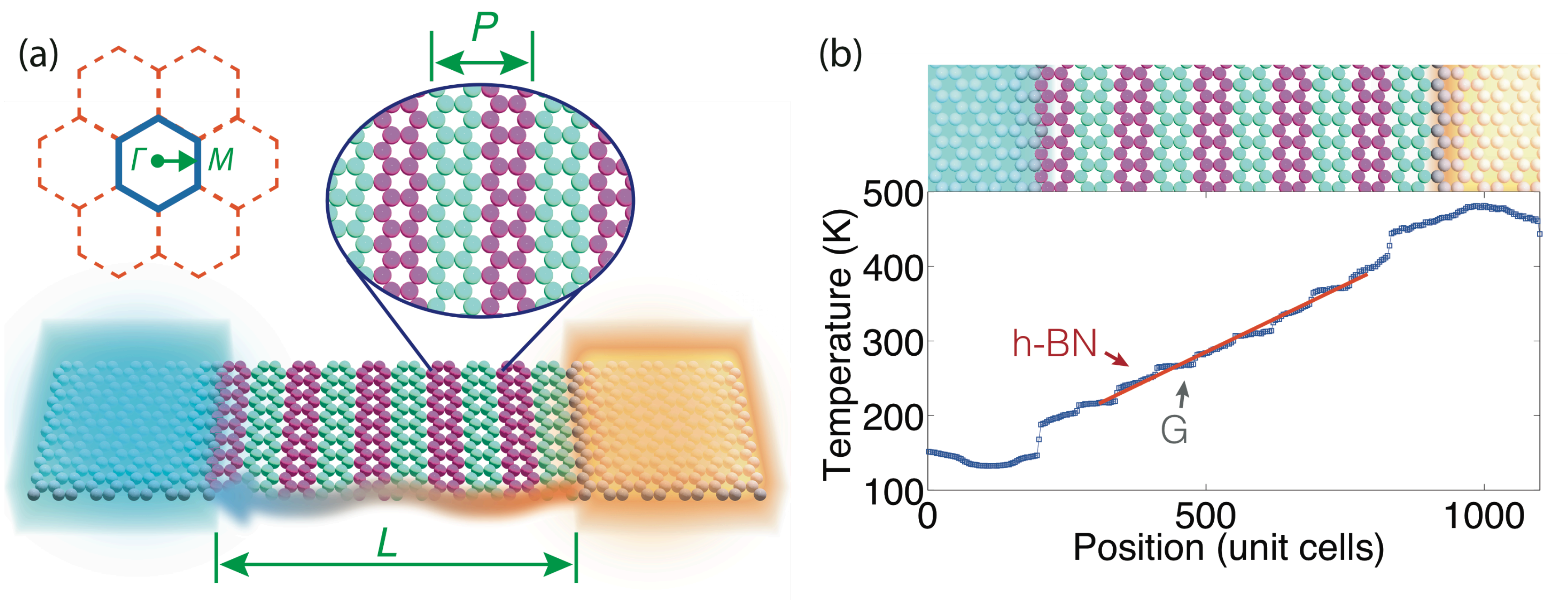




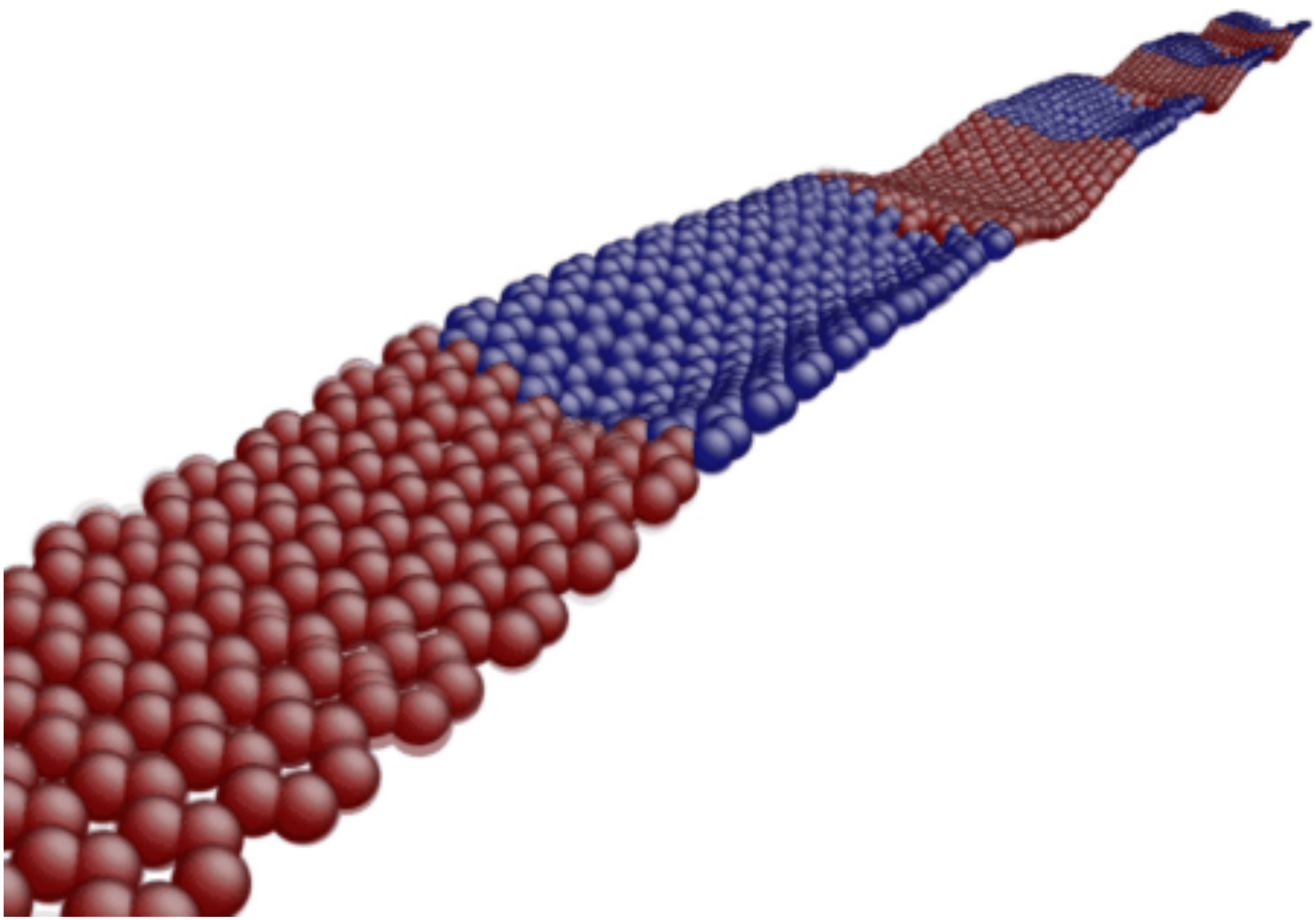
Ravichandaran et al., Nat Materials 13 168 (2013)

In all of these examples, the Blue Waters system has helped us to reveal new underlying physics in these nanostructured and/or low-dimensional systems, resolve existing controversies, and make exciting predictions!

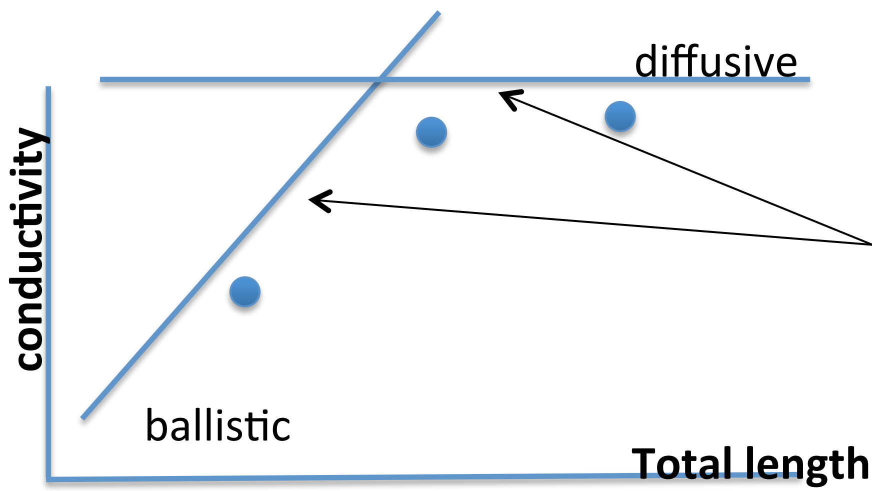
Simulation Methodology



approach: non-equilibrium molecular dynamics … mimic reality!

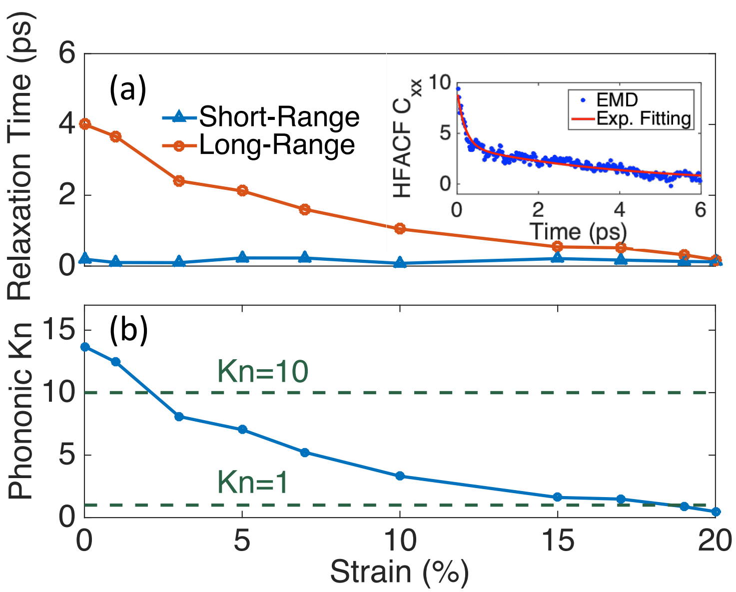


Why Blue Waters? … One example



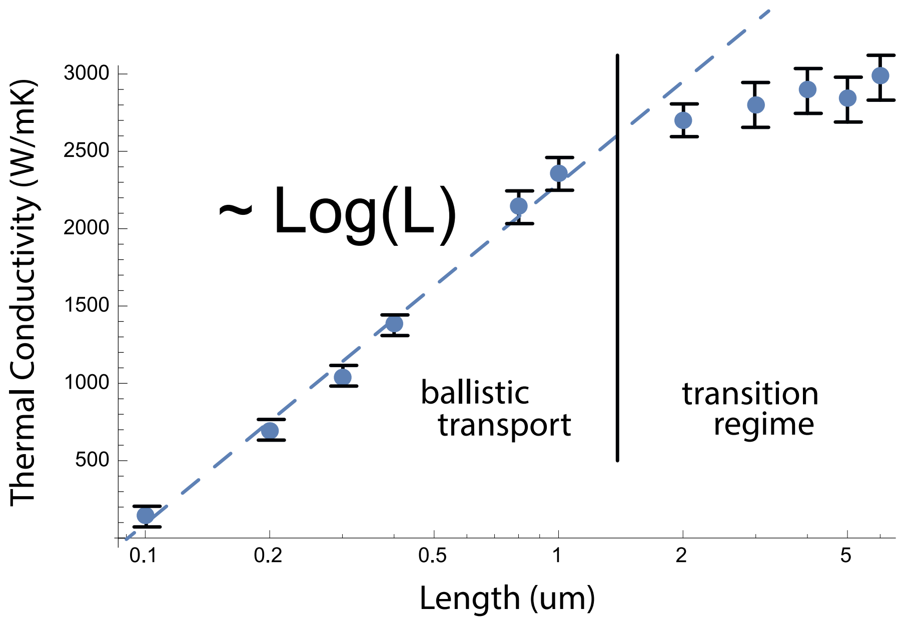
Length < Phonon Mean Free Path

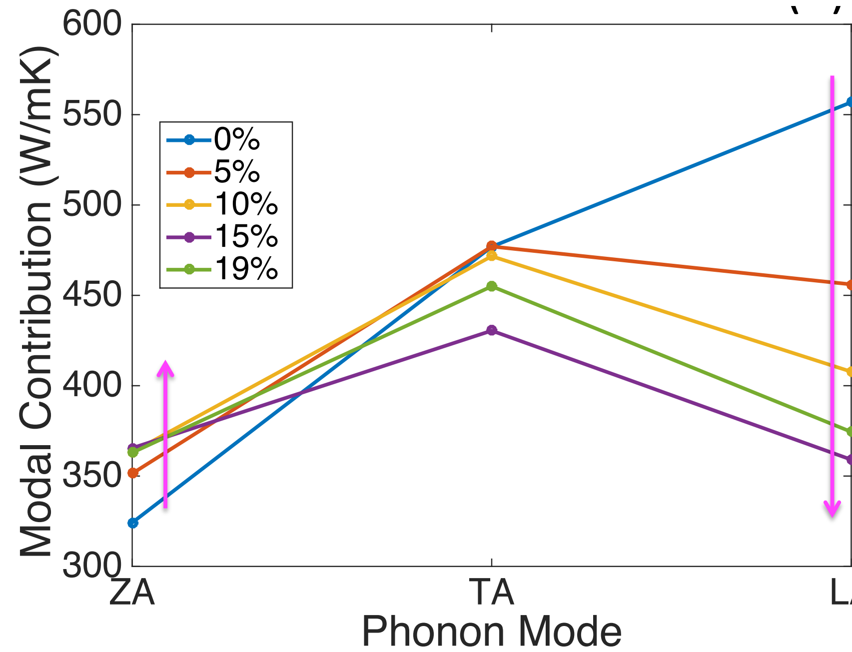
Length > Phonon Mean Free Path



- Extract phonon mean free paths from the heat flux auto correlation function
- For the long ranged phonons, relaxation times around = 4 ps
- Mean free paths are around $\Lambda = v_g\, \tau = 0.10$ μm
- **Purely diffusive transport regime should be visible around Kn = Λ/L = 0.01, L = 10 μm**

Accomplishments - I





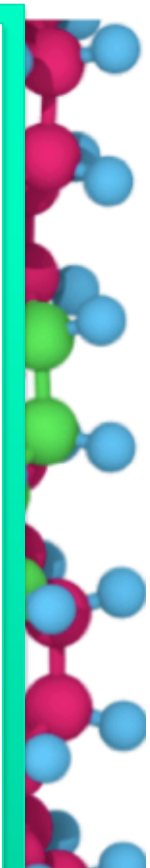
- Demonstration of transition from ballistic to transitional transport regime (required simulations of samples 2 – 6 μm side length! Largest to date.)
- Physical insight … what did we learn? Why is the divergence suppressed?

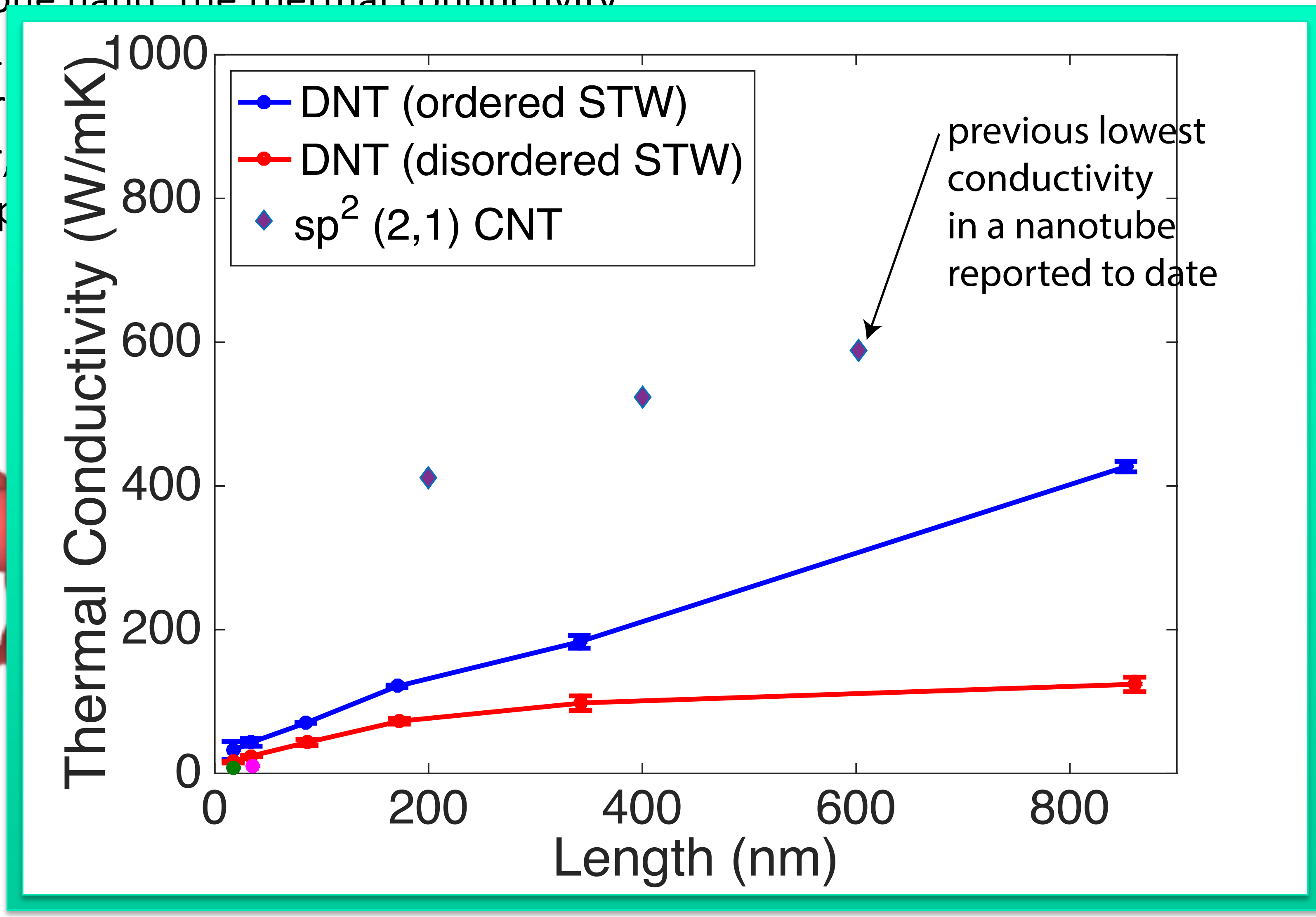
Accomplishments II – Disordered Systems

DNT with ordered
& disordered SWs

sp^3 (3,0) CNT

One one hand, the thermal conductivity
of a 1
linear
other,
transp

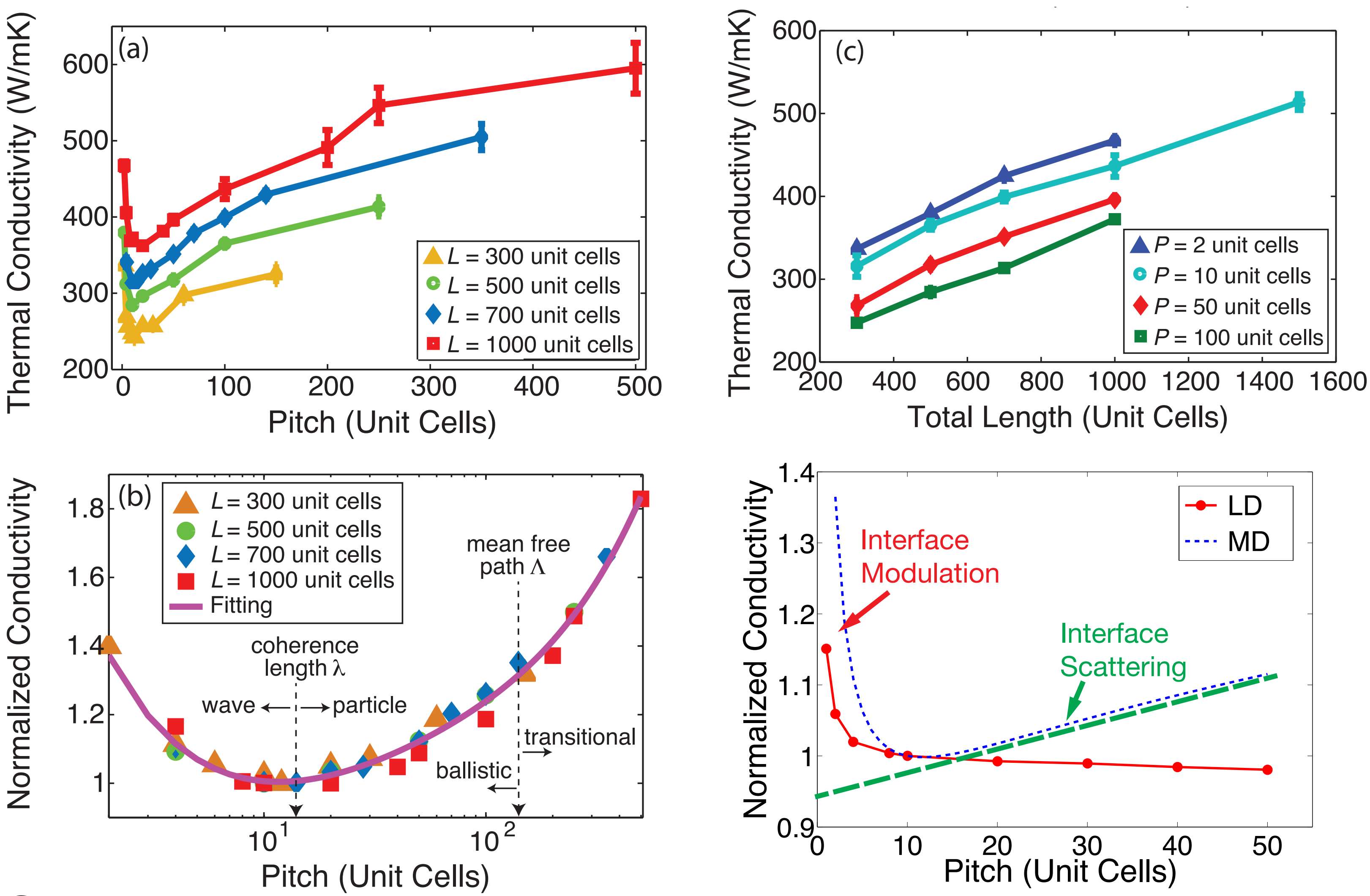




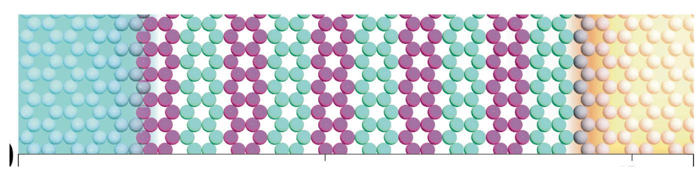
. 2015

, 2015

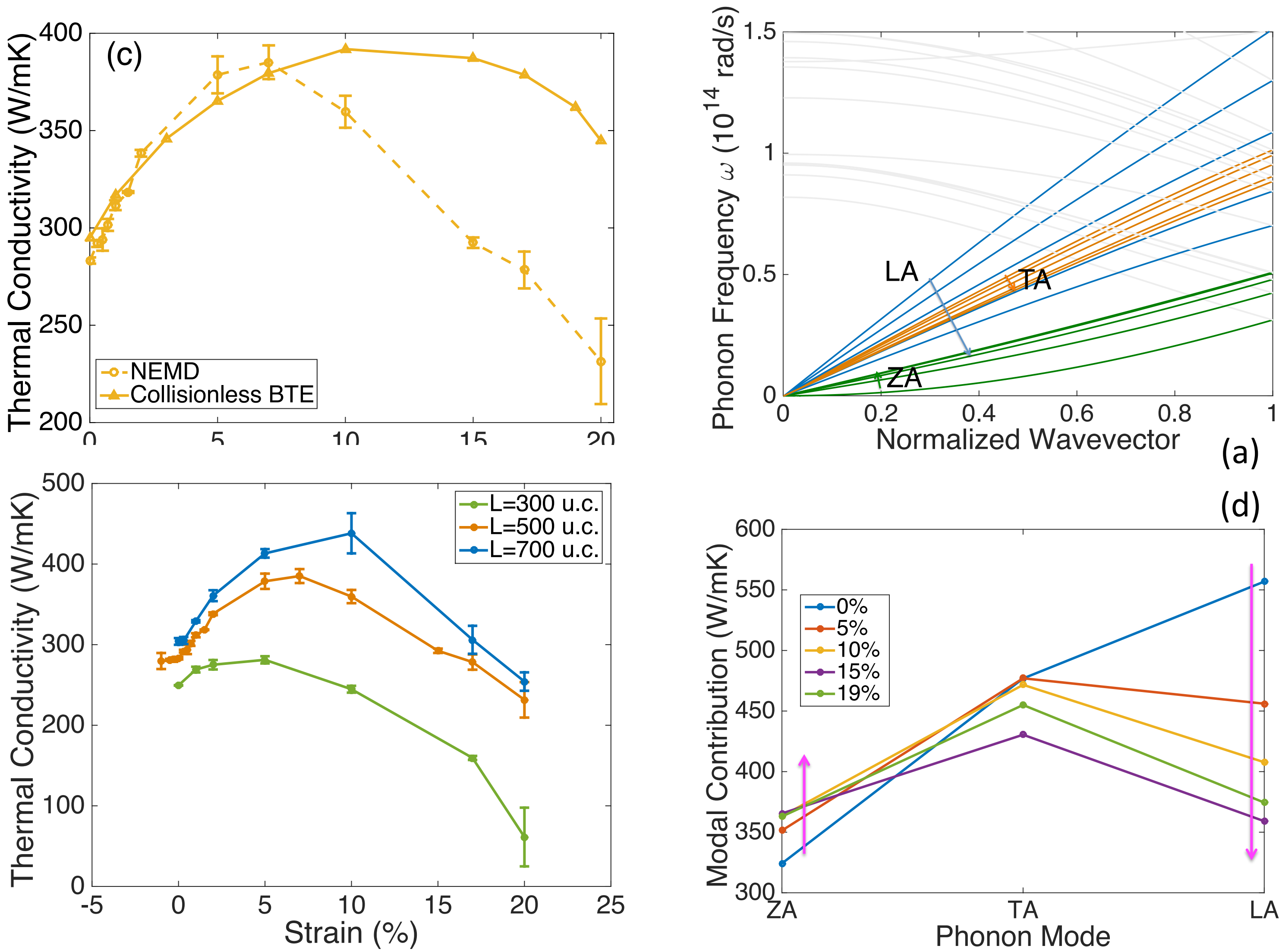
Accomplishments - III



Tuning the thermal conductivity by introducing superlattices into 2D materials



Accomplishments - IV



Conventional wisdom tells us that applying strain (in 3D solids) tends to reduce the thermal conductivity. What about in 2D? Anomalous, non-monotonic trends.

Conclusions/Summary

- The Blue Waters system has enabled us to carry out large scale molecular dynamics simulations to reveal exciting new thermal transport physics in low-dimensional systems
- **Team contributions**: And, thank you to the Blue Waters team for their regular, timely help with out work!

- References:

  - T. Zhu, E. Ertekin. Phys. Rev. B 2014
  - T. Zhu, E. Ertekin. Phys. Rev. B 2015
  - D. Nandwana, E. Ertekin. Nano Lett. 2015
  - T. Zhu, E. Ertekin (submitted for publication)