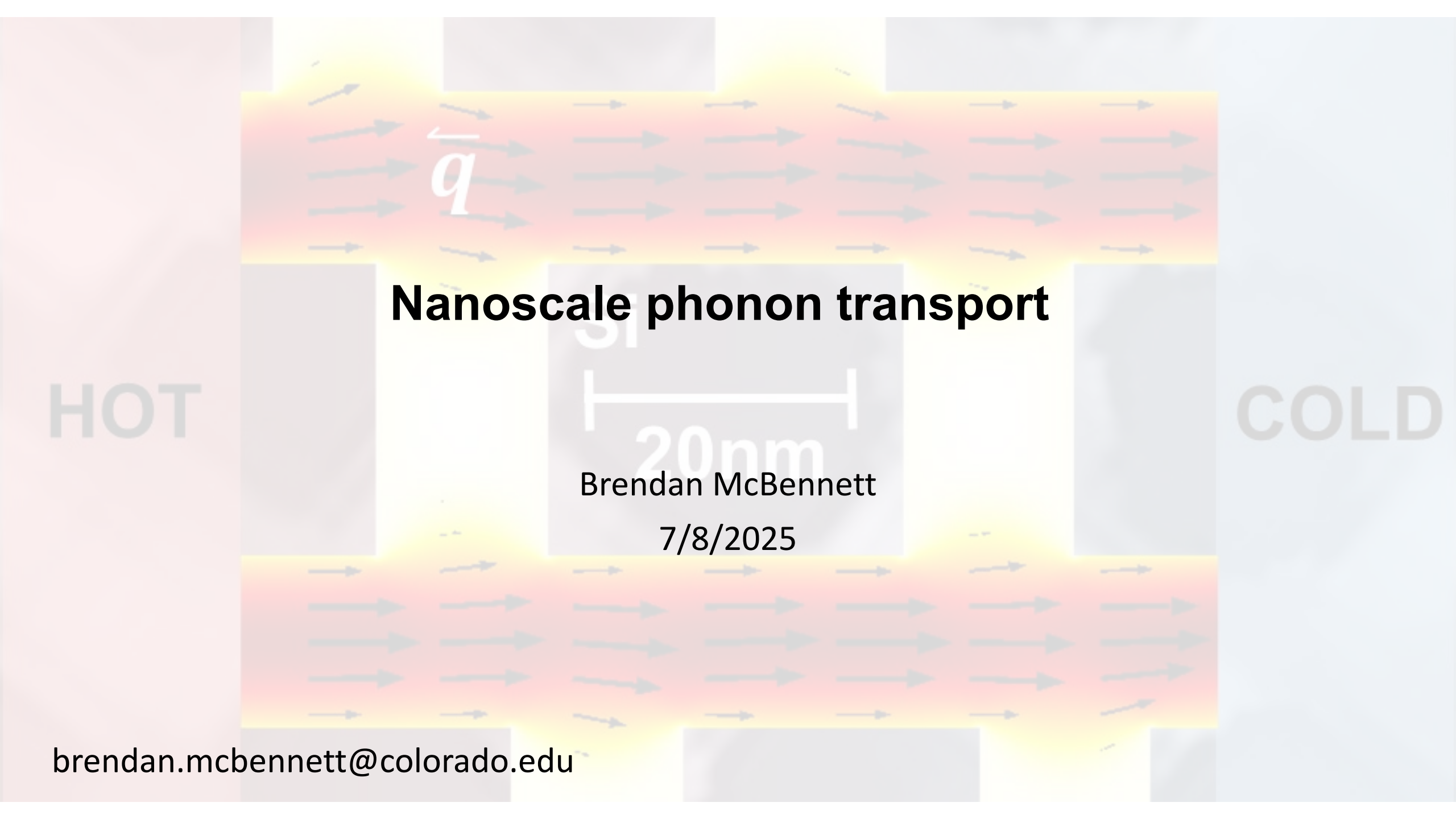




The diagram illustrates phonon transport in a central Silicon (Si) nanowire. The nanowire is shown as a grey rectangular structure with a width of 20 nm, indicated by a scale bar. It is connected to four grey rectangular electrodes at the top, bottom, left, and right. The left side of the device is labeled 'HOT' in large, semi-transparent grey letters, and the right side is labeled 'COLD' in similar letters. A color gradient is applied to the nanowire, transitioning from yellow on the left (hot) to red in the middle to blue on the right (cold). Numerous grey arrows, representing phonons, are shown moving from left to right through the nanowire. A large white arrow labeled with a bold q points to the right, indicating the direction of the phonon current.

Nanoscale phonon transport

Si
20nm
Brendan McBennett

7/8/2025

brendan.mcbennett@colorado.edu

Acknowledgements



JILA

Joshua Knobloch
Albert Beardo
Emma Nelson
Teddy Culman
Travis Frazer
Begoña Abad
J. N. Hernández Charpak
Hossein Honarvar

NIST

Justin Shaw
Michael Tanksalvala
Hans Nembach
Jacob Wisser

Theory

F. Xavier Álvarez
Juan Camacho
Javier Bafaluy
Lluc Sendra
Weinan Chen
Ismaila Dabo
Mahmoud Hussein



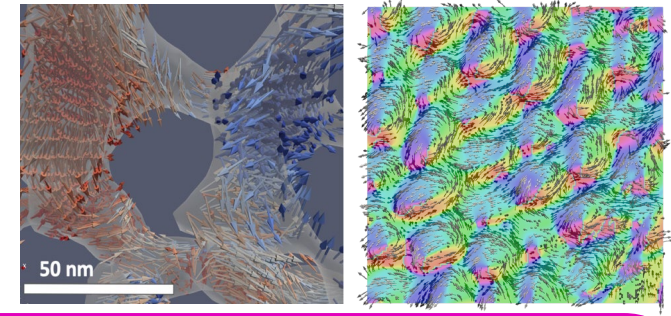
Margaret Murnane



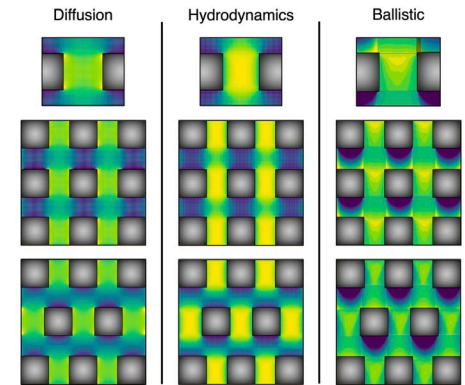
Henry Kapteyn

Outline

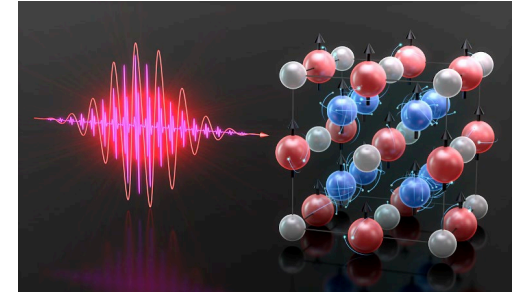
- **Lecture 1 – Brief intro to the physics of High Harmonics (Nobel 2023) and coherent imaging**



- **Lecture 2 – Nanoscale phonon transport** (with Dr. Brendan McBennett, NIST)



- **Lecture 3 – Understanding spin and many-body electron-phonon dynamics** via EUV MOKE and ARPES



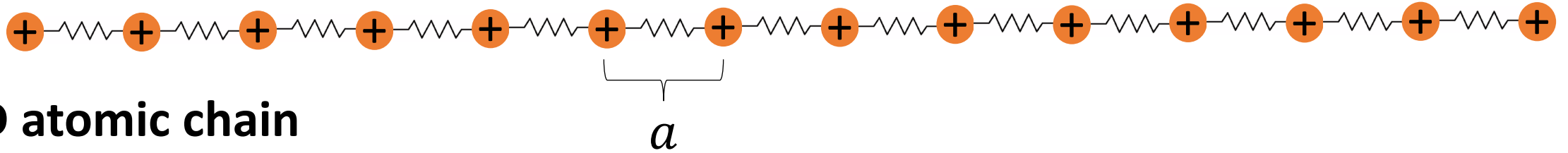
Today's outline

1. Phonons overview

2. Kinetic transport theory

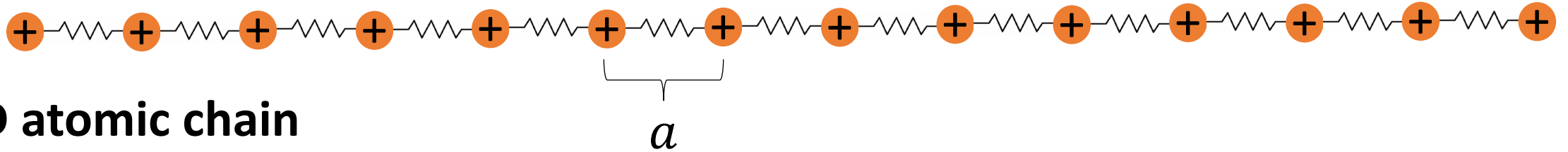
3. Phonon transport at the nanoscale

Phonons



1D atomic chain

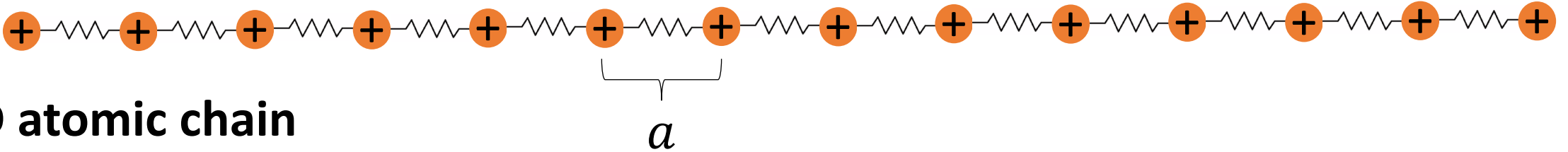
Phonons



1D atomic chain

- N atoms of mass m
- Lattice constant $a = 1$
- u_n is displacement of atom n
- Periodic boundary conditions $u_n = u_{n+N}$

Phonons



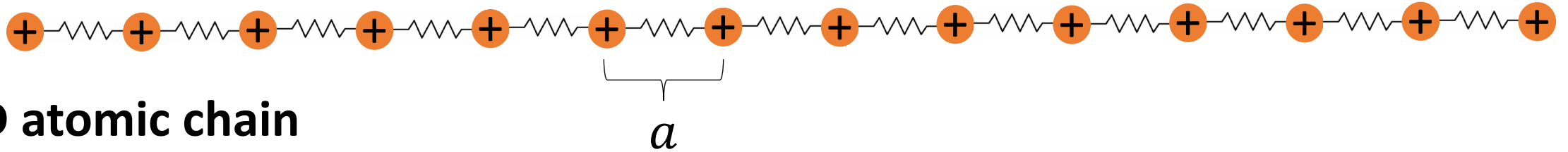
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$$H = \frac{m}{2} \sum_n \dot{u}_n^2 + \omega_0^2 (u_n - u_{n-1})^2$$

$$\ddot{u}_n = \omega_0^2 (u_{n+1} + u_{n-1} - 2u_n)$$

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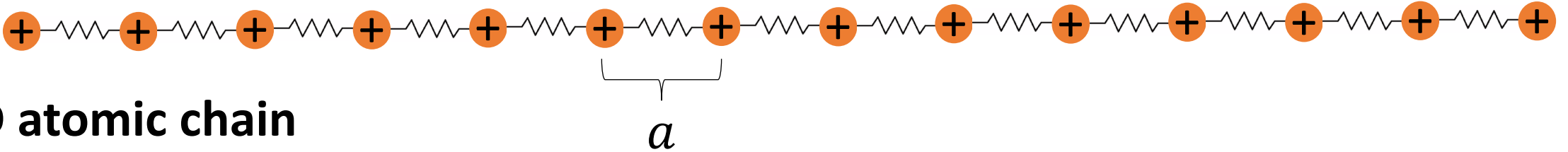
$$u_n \sim e^{ikx - i\omega_k t}$$

$$k = \frac{2\pi}{N} (0, \pm 1, \pm 2 \dots)$$

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$$\omega_k = 2\omega_0 \sin \left| \frac{k}{2} \right|$$

Phonons

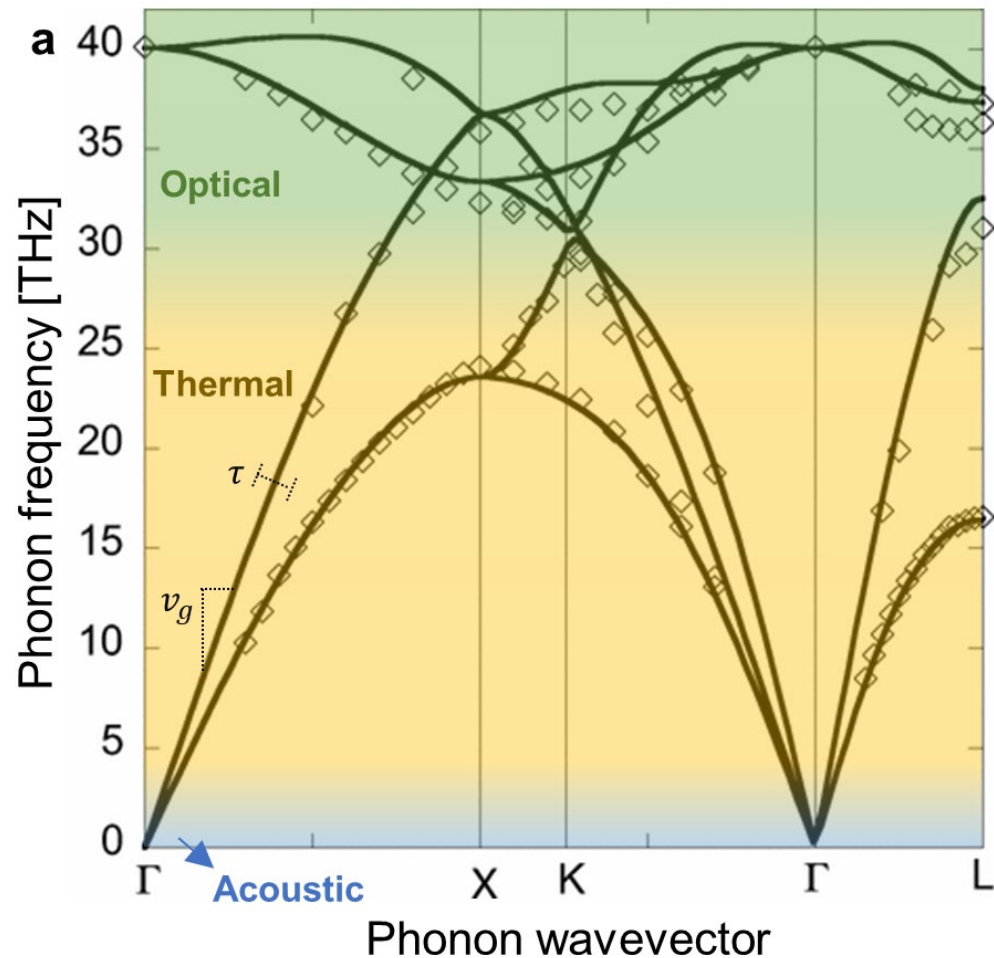
Quantum mechanical approach

$$H = \frac{m}{2} \sum_k \omega_k \left(n_k + \frac{1}{2} \right)$$

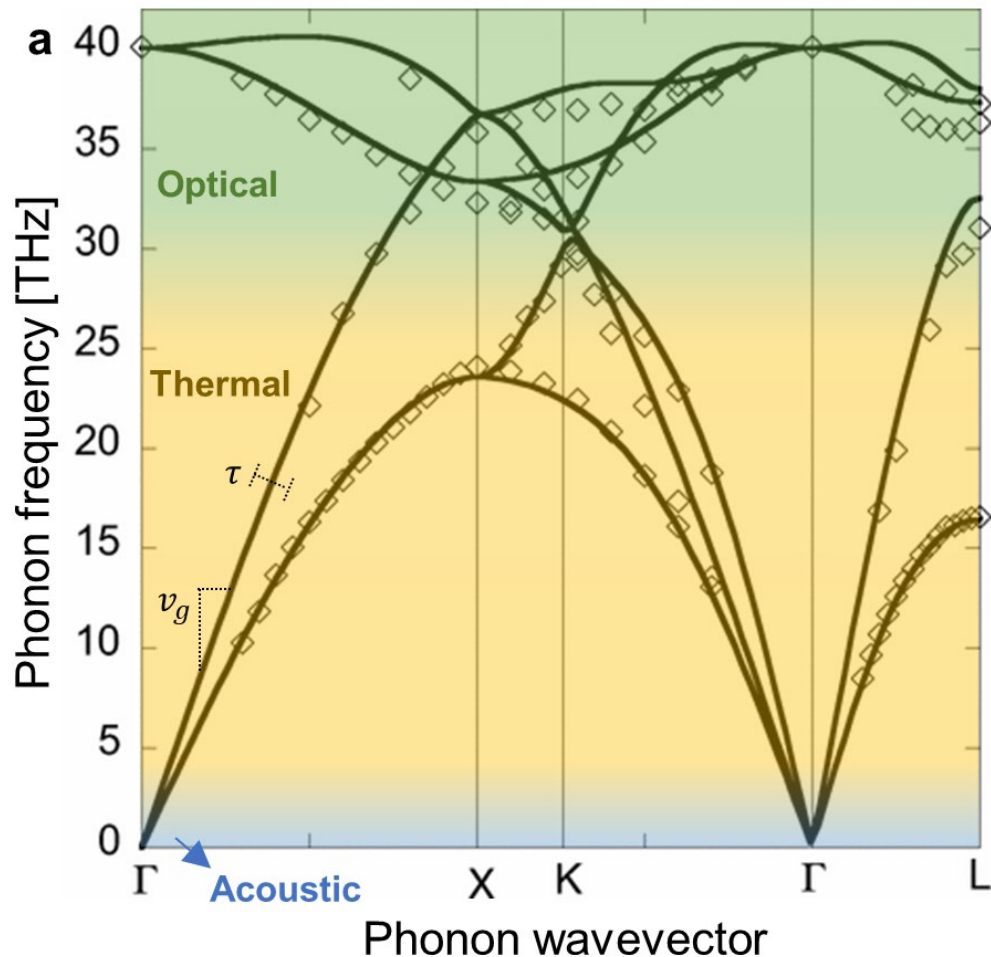
- Superposition of harmonic oscillators
- n_k “phonons” in mode k
- For N atoms in 3D have $3N$ modes

Phonons correspond to eigenstates of the **harmonic** Hamiltonian. Real crystals are not harmonic and so phonons will have finite lifetimes

Phonons in real crystals



Phonons in real crystals



Acoustic phonons (sound) – long wavelength, linear dispersion (kHz-GHz)

Optical phonons – very high frequency, low group velocity

Thermal phonons – heat carriers (THz)

Mean free path: $\Lambda = v\tau$

Macroscopic thermal transport

$$\vec{q} = -\kappa \nabla T$$

Fourier's law

$$\frac{\partial T}{\partial t} = \alpha \nabla^2 T$$

Heat equation

$\vec{q}$

Heat flux

∇T

Temperature gradient

κ, α

Thermal conductivity, diffusivity

Macroscopic thermal transport

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Fourier's law

$$\frac{\partial T}{\partial t} = \alpha \nabla^2 T$$

Heat equation

$$\vec{q}$$

Heat flux

$$\nabla T$$

Temperature gradient

$$\kappa, \alpha$$

Thermal conductivity, diffusivity

How to relate macroscopic variables to microscopic quantities like $v_k, \tau_k, \omega_k, \Lambda_k$?

Today's outline

1. Phonons overview
- 2. Kinetic transport theory**
3. Phonon transport at the nanoscale

Distribution functions

- Treat phonons as particles ($\sim 1\text{nm}$ wavelengths at RT)
- Energy is conserved, but not much else
- $n_k(\mathbf{x}, t)$: number of phonons in mode k at location $\mathbf{x}$ at time t
- In equilibrium, $n_k^0 = [e^{\hbar\omega_k/k_B T} - 1]^{-1}$ (phonons are bosons)

Momentum conservation

- Phonons have zero average “real” momentum (the atoms in a crystal experience no net displacement as a phonon propagates)
- Instead they have crystal momentum $\hbar \vec{k}$

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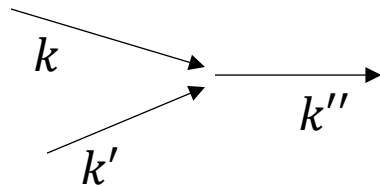


Boltzmann transport equation

$$\frac{\partial n_k(\mathbf{x}, t)}{\partial t} + \underbrace{\vec{v}_k \cdot \nabla n_k(\mathbf{x}, t)}_{\text{Drift}} = \underbrace{C[n_k(\mathbf{x}, t)]}_{\text{Collisions}}$$

C is the collision operator representing all the possible scattering events which can alter the distribution function. In general it is very difficult to calculate

$$C[n_k(\mathbf{x}, t)] \sim \int dk' dk'' |M(k, k', k'')|^2 \omega \omega' \omega'' \delta(\omega + \omega' - \omega'') (n + 1)(n' + 1)n''$$



Energy and heat flux

$$u(\mathbf{x}, t) = V^{-1} \sum_k \hbar \omega_k n_k(\mathbf{x}, t)$$

Energy density

$$\vec{q}(\mathbf{x}, t) = V^{-1} \sum_k \hbar \omega_k \vec{v}_k n_k(\mathbf{x}, t)$$

Heat flux density

These are very fundamental expressions – no assumptions yet

Boltzmann to Fourier

$$\frac{\partial n_k(\mathbf{x}, t)}{\partial t} + \vec{v}_k \cdot \nabla n_k(\mathbf{x}, t) = C[n_k(\mathbf{x}, t)]$$



- Relaxation time approximation
- Local equilibrium approximation
- Steady state

$$\vec{q} = - \underbrace{\left(\sum_k v_k \Lambda_k c_k \right)}_{\text{thermal conductivity}} \nabla T$$

thermal conductivity

Can calculate v_k, Λ_k, c_k from first principles

Bulk thermal conductivity calculations

Intrinsic lattice thermal conductivity of semiconductors from first principles

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(Received 30 October 2007; accepted 19 November 2007; published online 7 December 2007)

We present an *ab initio* theoretical approach to accurately describe phonon thermal transport in semiconductors and insulators free of adjustable parameters. This technique combines a Boltzmann formalism with density functional calculations of harmonic and anharmonic interatomic force constants. Without any fitting parameters, we obtain excellent agreement (<5% difference at room temperature) between the calculated and measured intrinsic lattice thermal conductivities of silicon and germanium. As such, this method may provide predictive theoretical guidance to experimental thermal transport studies of bulk and nanomaterials as well as facilitating the design of new materials. © 2007 American Institute of Physics. [DOI: [10.1063/1.2822891](https://doi.org/10.1063/1.2822891)]

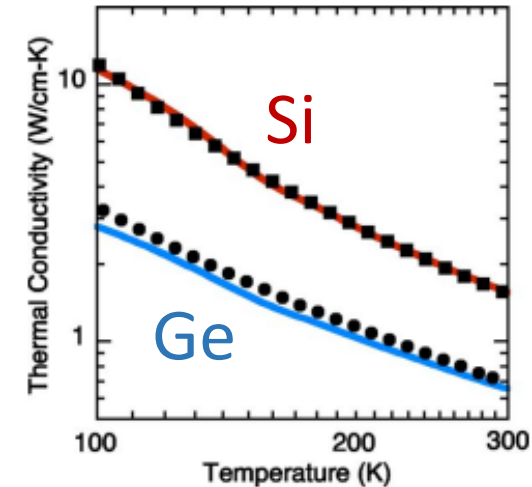


FIG. 1. (Color online) Lattice thermal conductivity $\kappa^{(l)}$ as a function of temperature. The red line and solid squares are the calculated and measured thermal conductivities of silicon, respectively, while the blue line and the solid circles are the corresponding quantities for germanium.

This works for bulk materials with dimensions $\gg$ mean free paths (100s of nm at room temperature). What about at the nanoscale?

Today's outline

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Length scales on the order of phonon mean free paths, time scales on the order of phonon lifetimes

Example: second sound

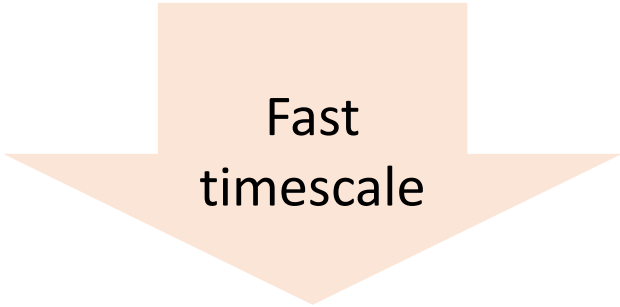
$$n_k = f(\omega_k, T)$$

Arbitrary initial distribution function (ex. from ultrafast laser excitation)

Example: second sound

$$n_k = f(\omega_k, T)$$

Arbitrary initial distribution function (ex. from ultrafast laser excitation)



Fast
timescale

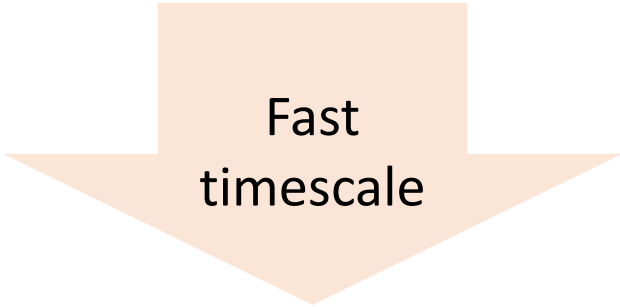
$$n_k = \left[e^{(\hbar\omega_k - \hbar\vec{k} \cdot \vec{u}) / k_B T} - 1 \right]^{-1}$$

Suitable intermediate distribution function

Example: second sound

$$n_k = f(\omega_k, T)$$

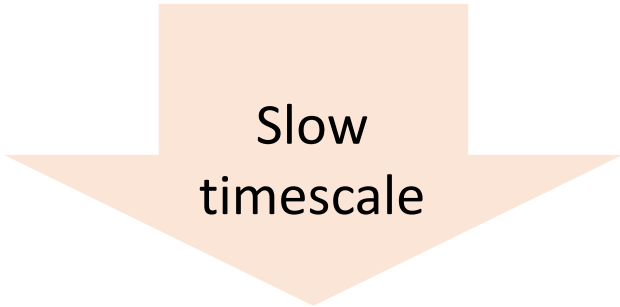
Arbitrary initial distribution function (ex. from ultrafast laser excitation)



Fast
timescale

$$n_k = \left[e^{(\hbar\omega_k - \hbar\vec{k}\cdot\vec{u})/k_B T} - 1 \right]^{-1}$$

Suitable intermediate distribution function



Slow
timescale

$$n_k^0 = \left[e^{\hbar\omega_k/k_B T} - 1 \right]^{-1}$$

Equilibrium distribution function

Example: second sound

$$n_k = f(\omega_k, T)$$

Fast
timescale

$$n_k = \left[e^{(\hbar\omega_k - \hbar\vec{k}\cdot\vec{u})/k_B T} - 1 \right]^{-1}$$

Slow
timescale

$$n_k^0 = \left[e^{\hbar\omega_k/k_B T} - 1 \right]^{-1}$$



$$\tau_{ss} \frac{\partial T}{\partial t} + \frac{\partial T}{\partial t} = \alpha \nabla^2 T$$

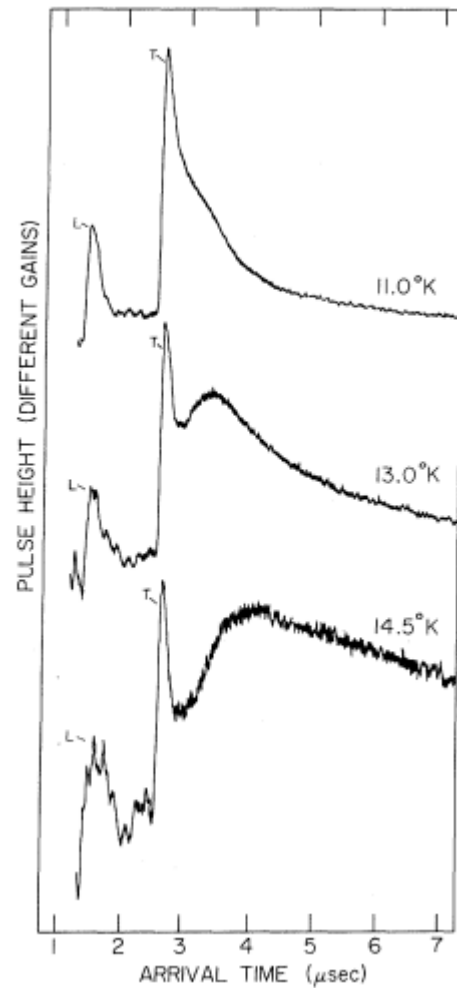
Damped wave equation for temperature!



$$\frac{\partial T}{\partial t} = \alpha \nabla^2 T \quad \text{Heat equation}$$

Example: second sound

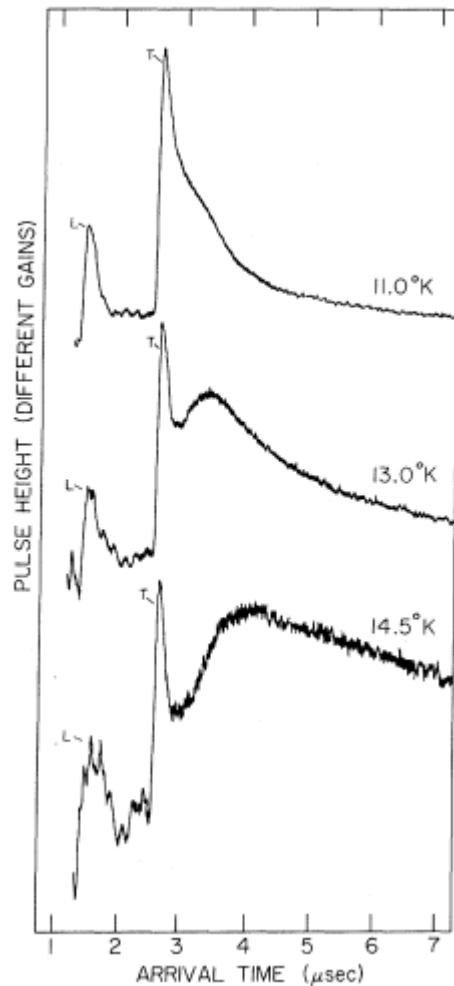
NaF, 13K (1971)



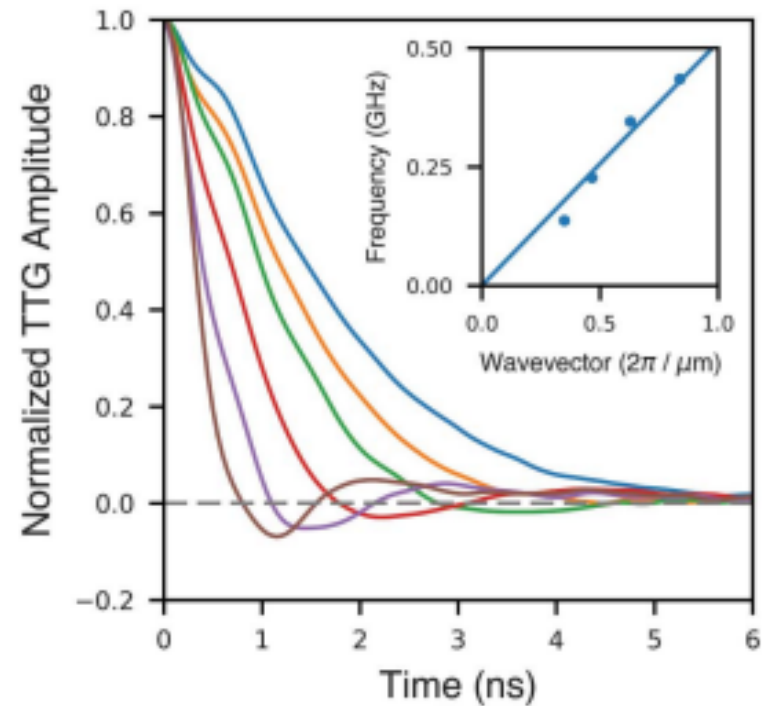
Phys. Rev. B 3 1428 (1971)

Example: second sound

NaF, 13K (1971)

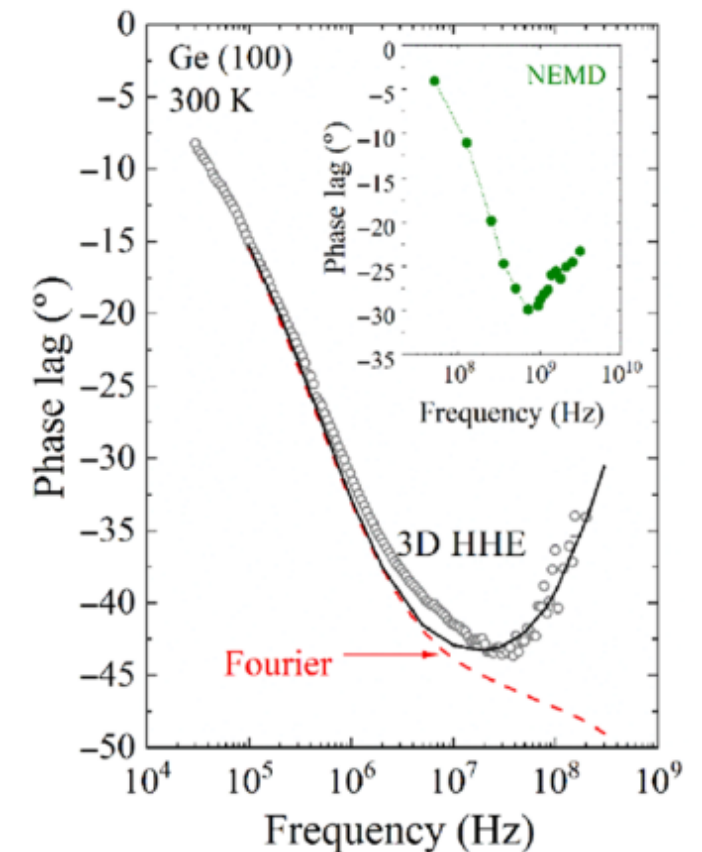


Graphite, 100K (2019)



1970s: exotic
2010s: 2D materials,
higher temperatures

Ge, 300K (2021)



Phys. Rev. B **3** 1428 (1971)
Science **364**, 375–379 (2019)
Sci. Adv **7** eabg4677 (2021)

Example: confinement

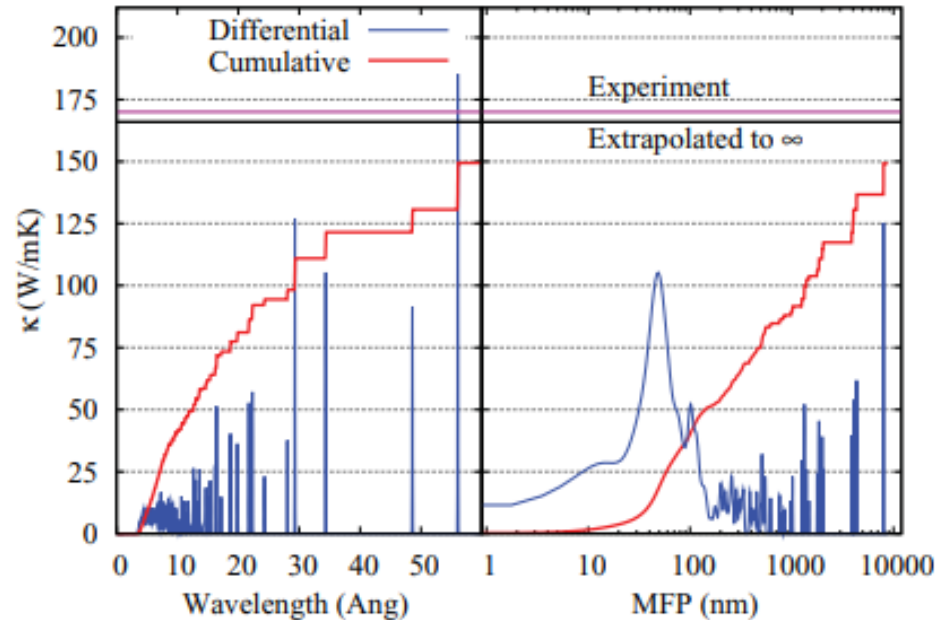


FIG. 6. (Color online) Cumulative contributions of phonons to the thermal conductivity at 277 K from the $18 \times 18 \times 18$ k -point mesh data. Left plot is according to the wavelengths, and right plot is according to the MFPs. Both differential and cumulative thermal conductivities are shown in blue and red, respectively. For comparison, the extrapolated (to infinite k -point mesh) and experimental κ are also shown with horizontal lines at 166 and 174 W/mK, respectively.

- Phonon mean free paths in bulk silicon are 10s of nm to microns

Example: confinement

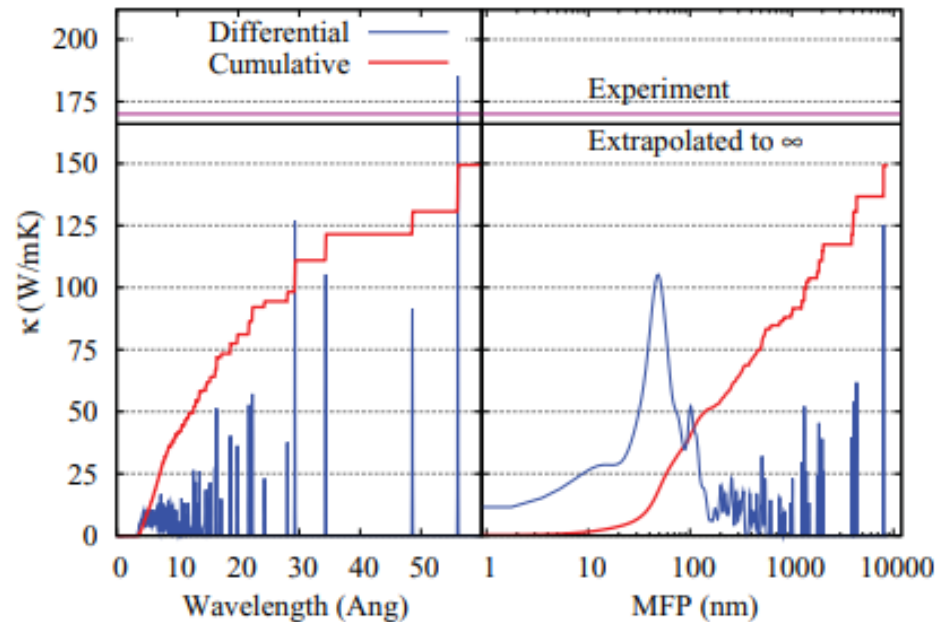
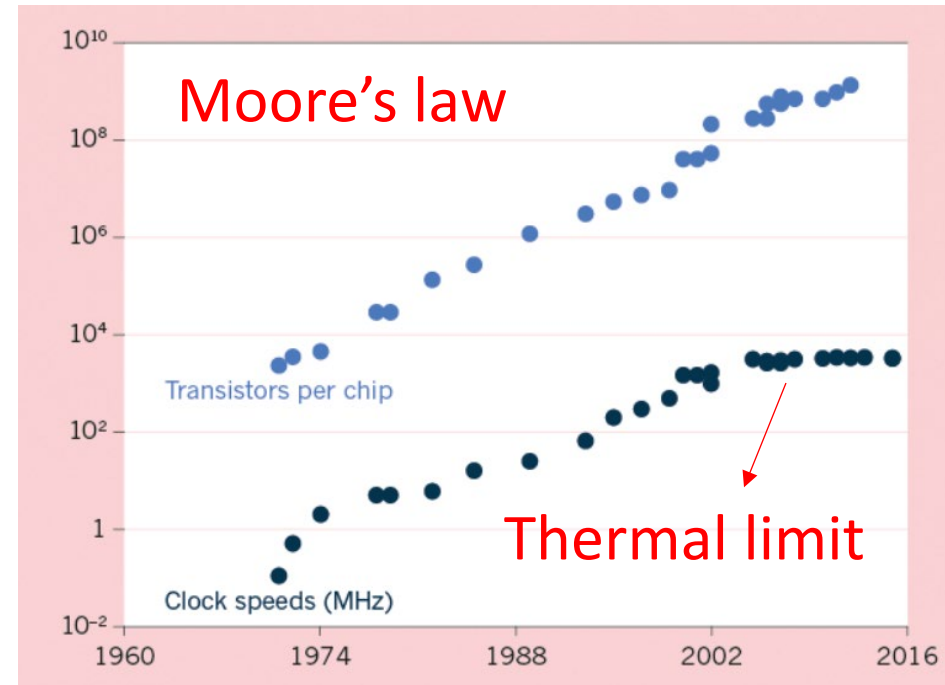
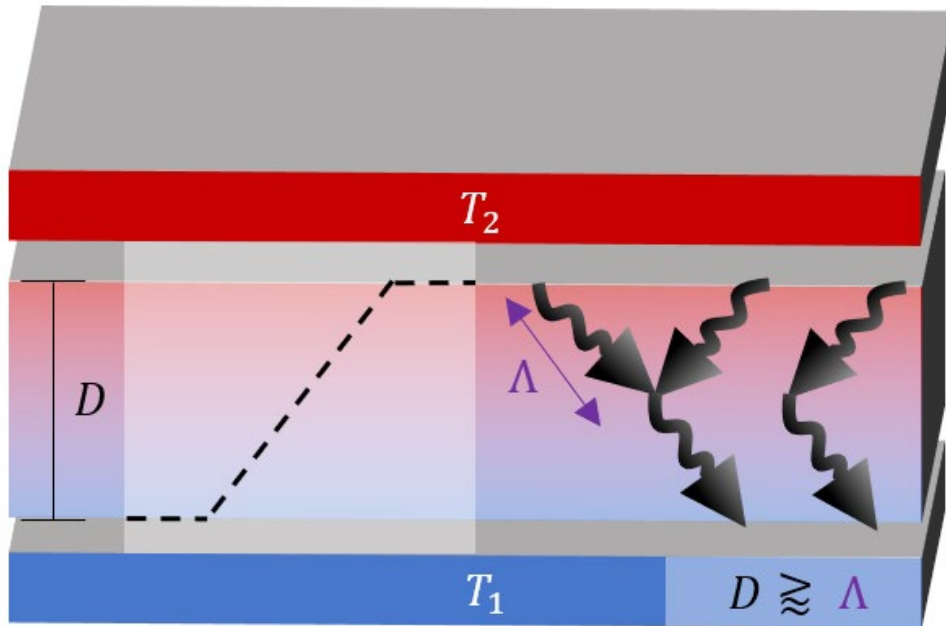


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- Phonon mean free paths in bulk silicon are 10s of nm to microns
- Dimensions in nanoelectronics are much smaller



Example: confinement

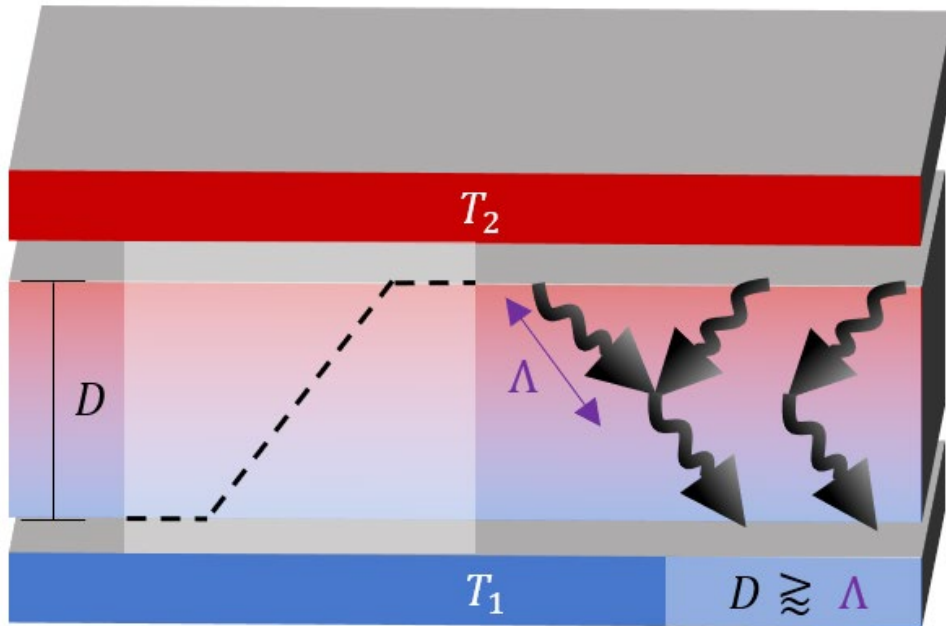


Naïve approach
“ballistic” model

Heat flow across a film of similar thickness to the phonon mean free path

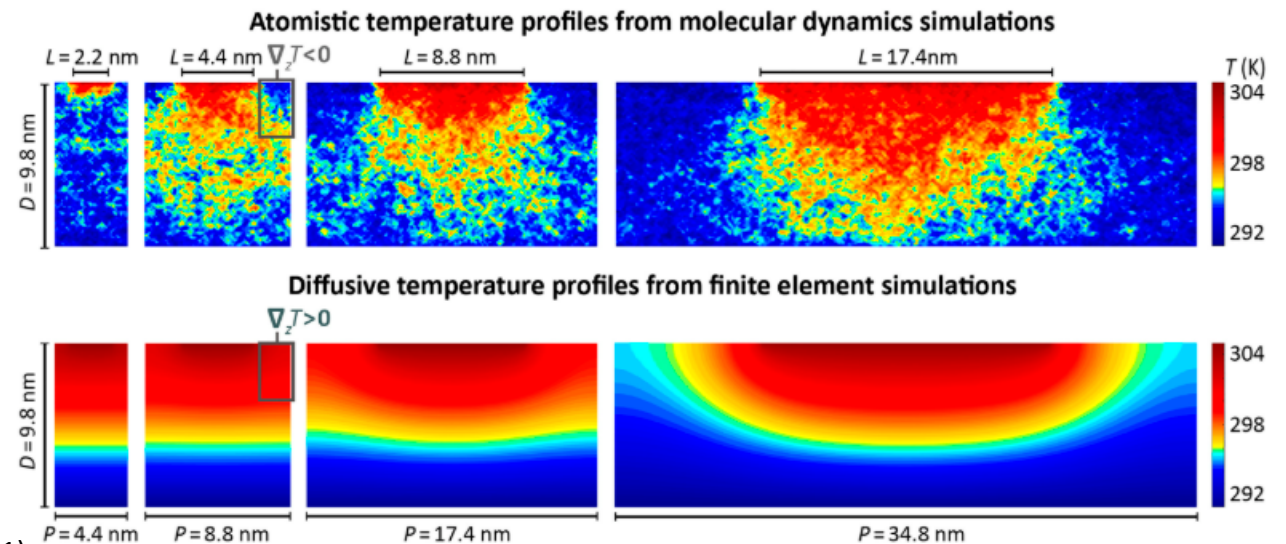
$$\kappa = \sum_k v_k \bar{\Lambda}_k c_k \quad \left\{ \begin{array}{l} \bar{\Lambda}_k = D \text{ if } \Lambda_k > D \\ \bar{\Lambda}_k = \Lambda_k \text{ if } \Lambda_k < D \end{array} \right.$$

Example: confinement

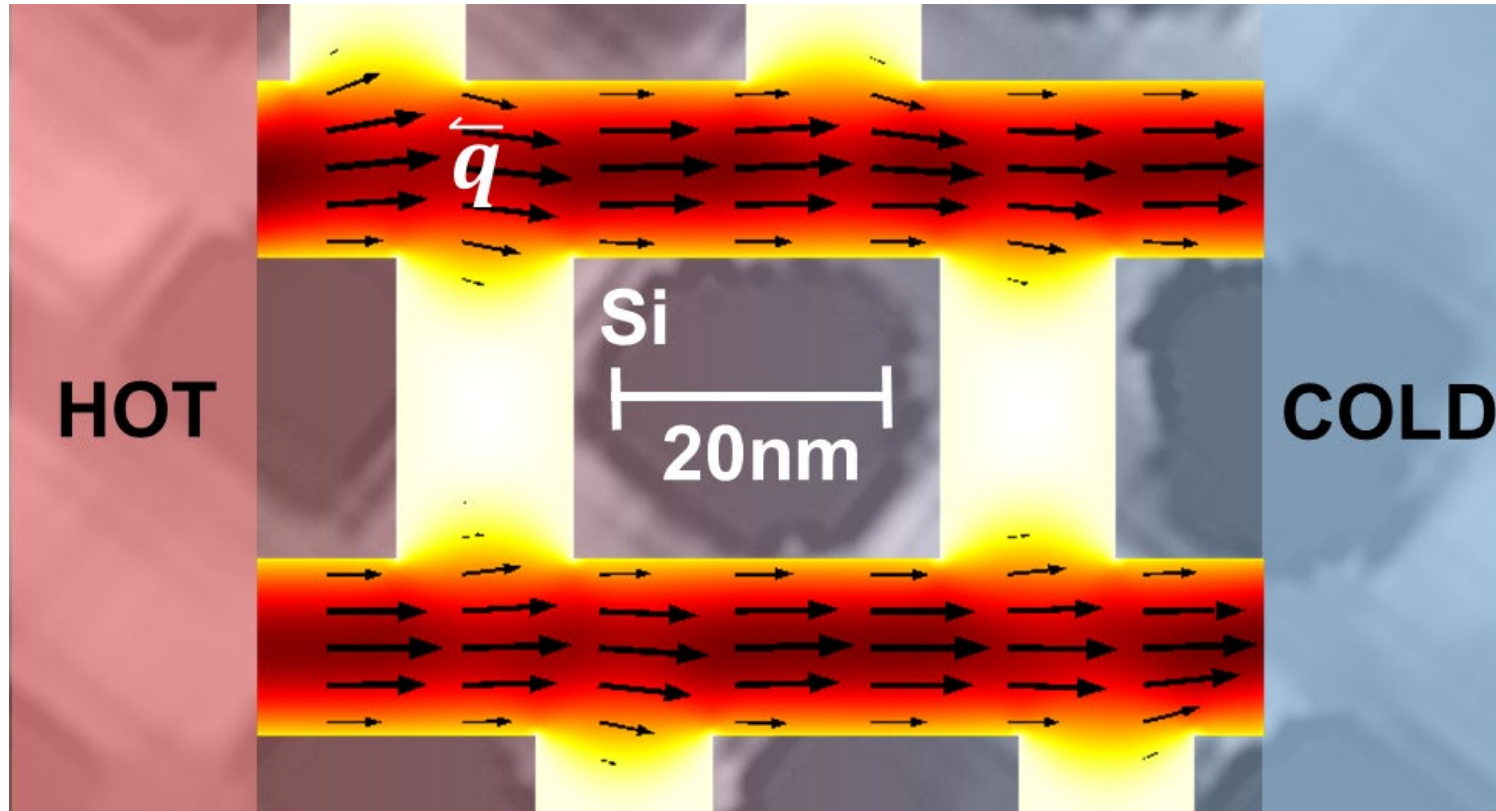


Heat flow across a film of similar thickness to the phonon mean free path

Sophisticated but (very) computationally intensive approach



Example: confinement



Nano Letters **23** 2129 (2023)

And what if your system looks like this?

Search for mesoscale theories: emergent phonon hydrodynamics

Phonon hydrodynamics

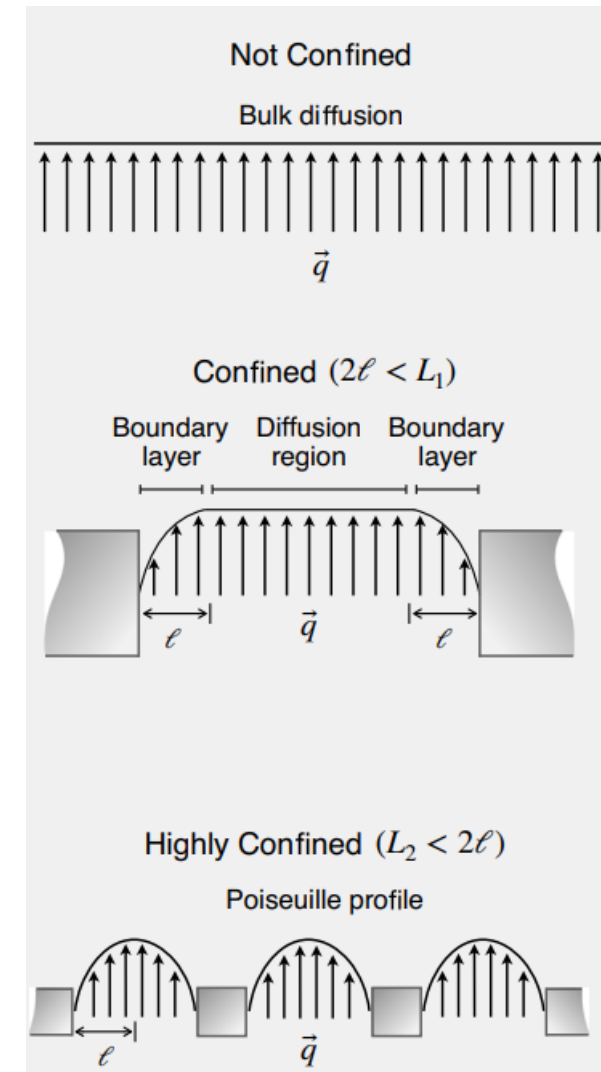
- Same process as before
- Thermodynamically-motivated distribution function at intermediate timescales

$$\mathbf{f}_\lambda = \mathbf{f}_\lambda^{\text{eq}} + \vec{\beta}_\lambda \cdot \vec{\mathbf{q}} + \vec{\mathbf{G}}_\lambda : \vec{\nabla} \vec{\mathbf{q}}$$

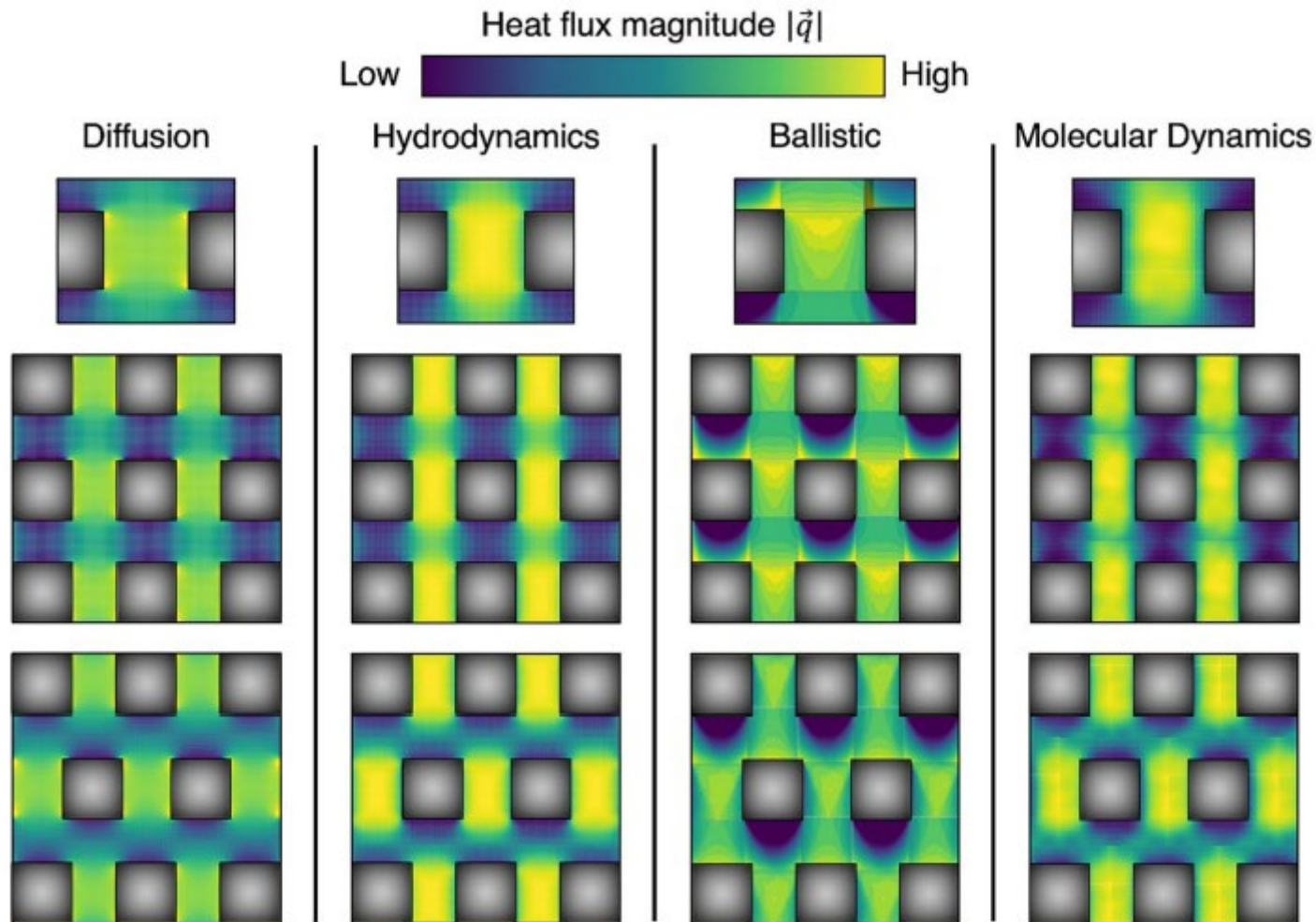
- Plug into the Boltzmann equation, arrive at an equation which looks like the Navier-Stokes Equation

$$\vec{\mathbf{q}} = -\kappa_{\text{GK}} \vec{\nabla} \mathbf{T} + \ell^2 \vec{\nabla}^2 \vec{\mathbf{q}}$$

viscous term



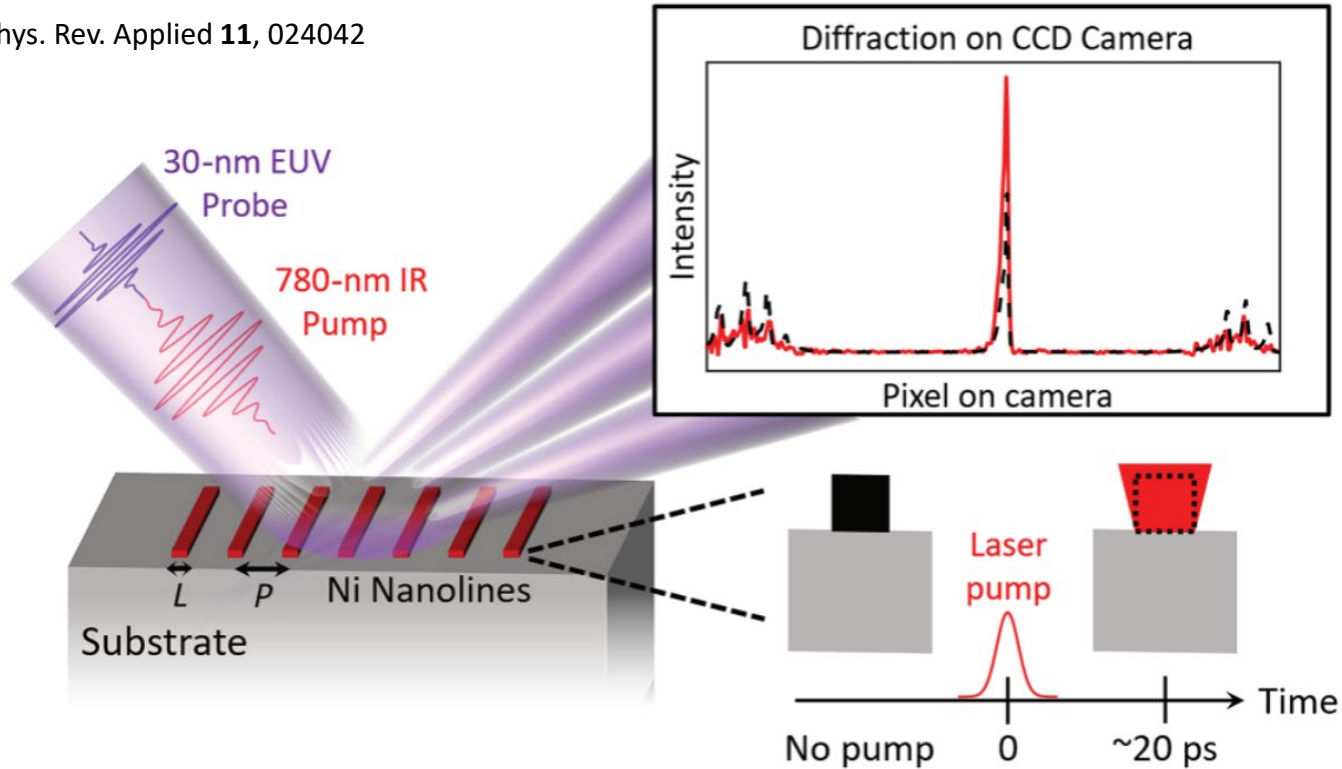
Phonon hydrodynamics (vs. other models)



How can we develop experimental tools to differentiate between these models?

Example: EUV scatterometry

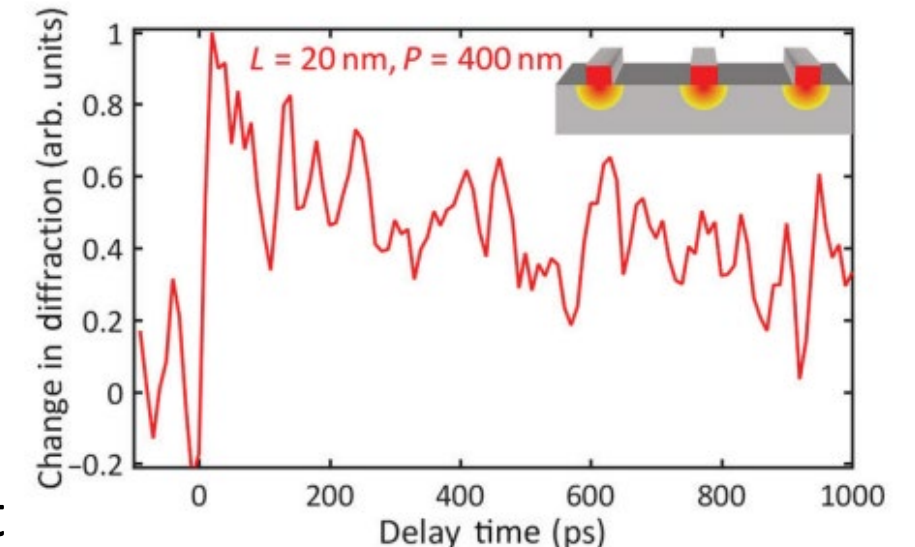
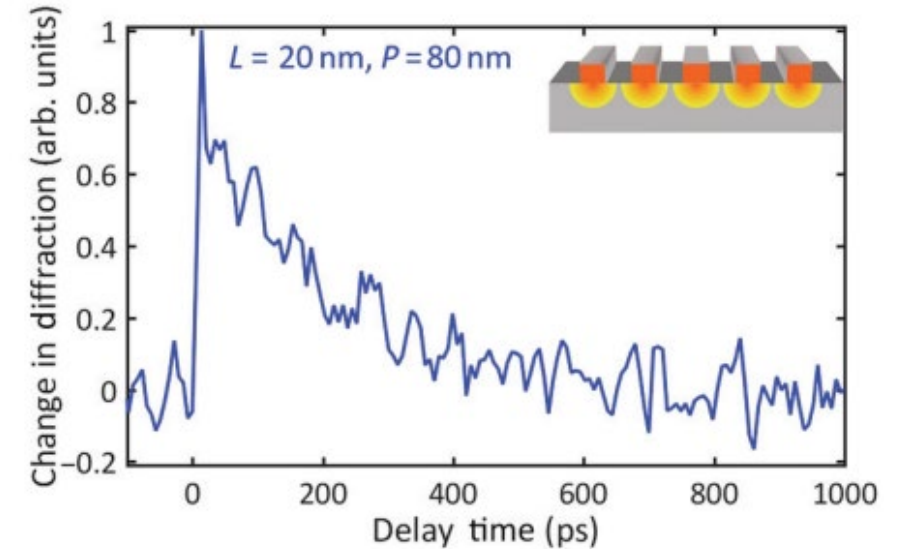
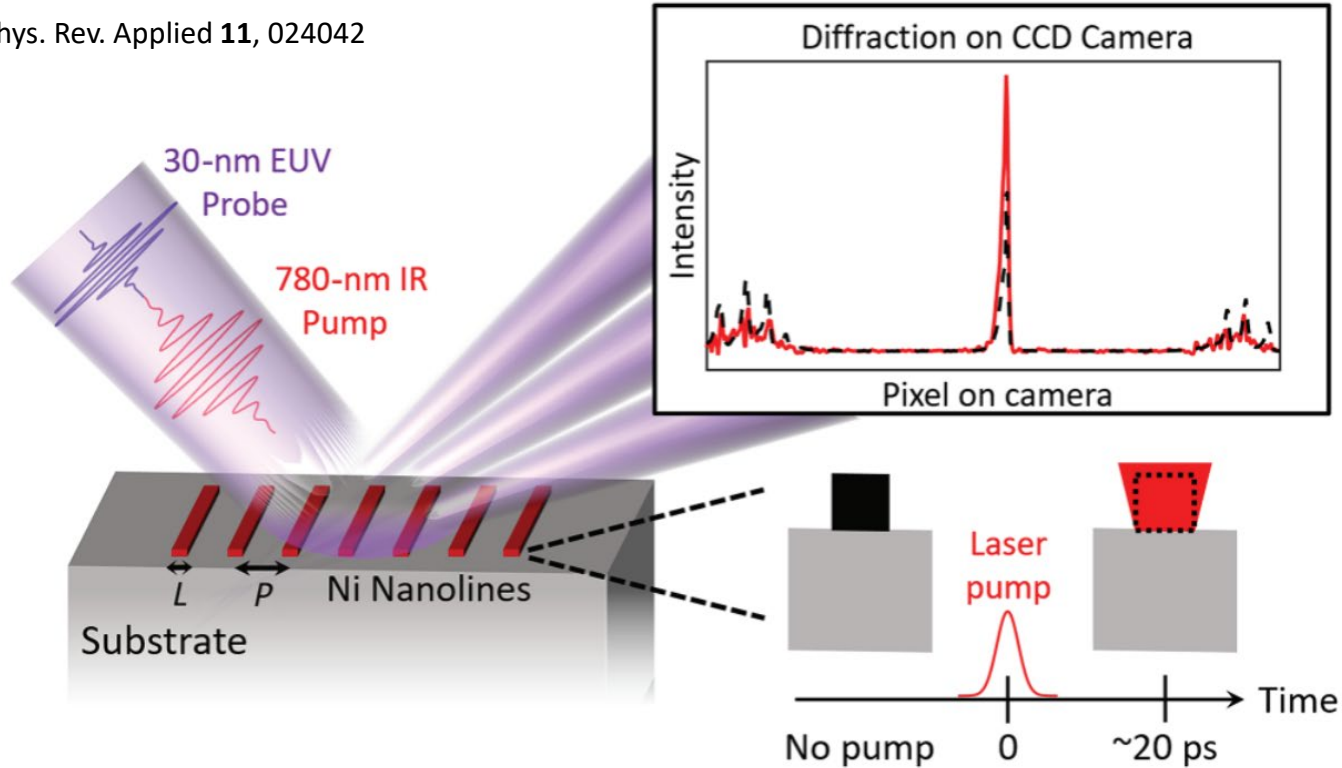
Phys. Rev. Applied **11**, 024042



1. Heat Ni nanowires on a silicon substrate with an infrared laser
2. Measure dynamic diffraction pattern (thermal expansion and contraction) using ultrafast EUV light

Example: EUV scatterometry

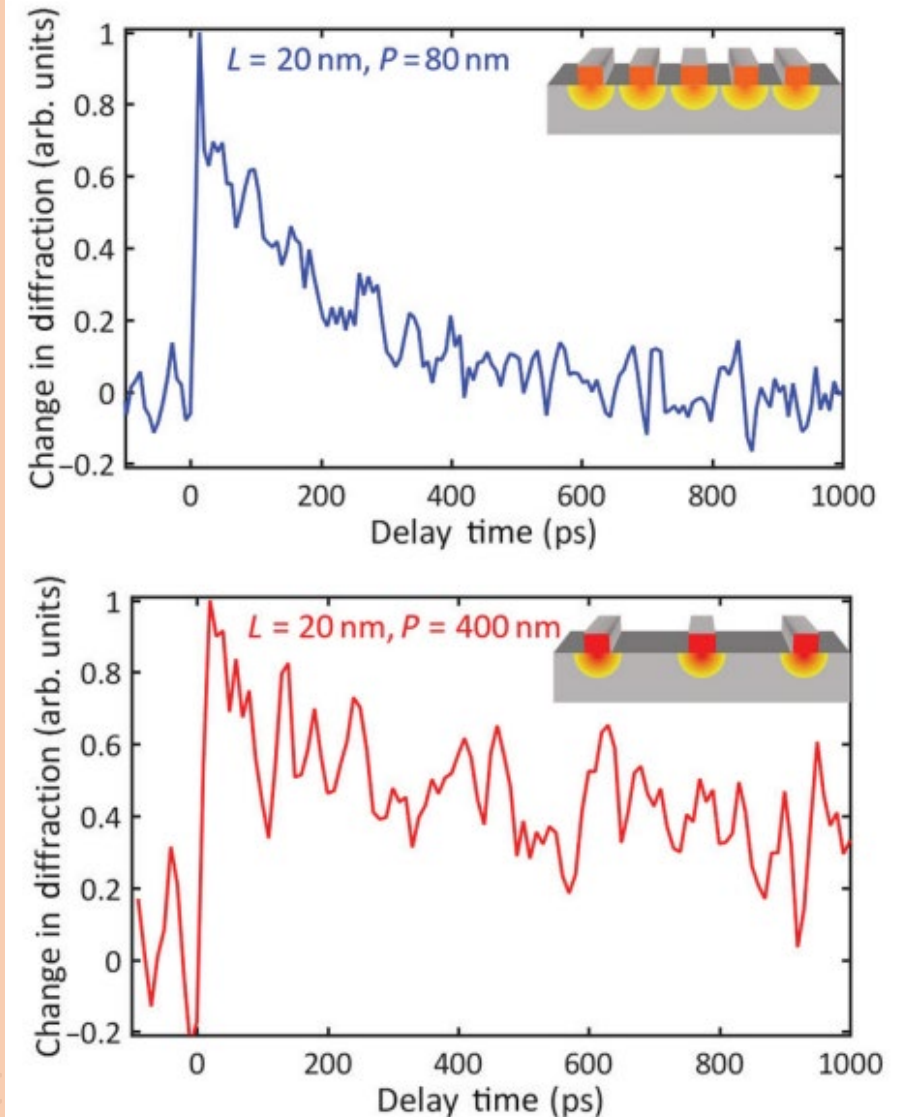
Phys. Rev. Applied 11, 024042



1. Heat Ni nanowires on a silicon substrate with an infrared laser
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Example: EUV scatterometry

Closely packed nanostructures cool faster than more isolated nanostructures under the same initial heat injection per unit volume!



Summary

1. Phonons appear everywhere in condensed matter physics and their behavior is highly material/system dependent
2. Our knowledge of phonon transport is decades behind electron transport because phonons cannot be as easily manipulated
3. Phonon transport is critical for semiconductors, energy efficiency, quantum technologies and much more

Thank you!

