NTPL: Nanoscale Transport Phenomena Laboratory

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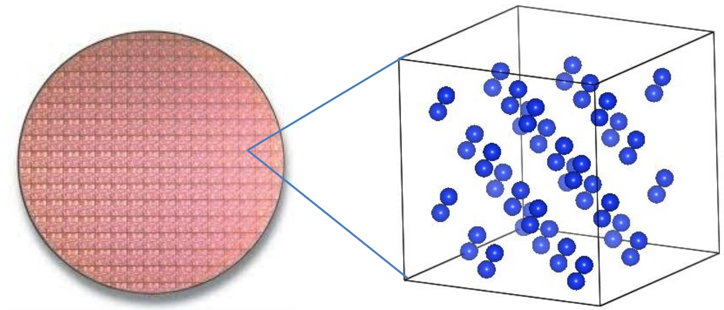
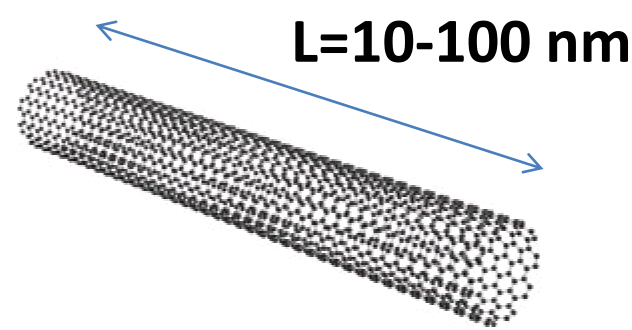
Nanoscale Transport Phenomena

- **Bulk Properties**



- **Transport Carriers: phonons,** electrons, photons, etc.
- **Statistical Properties:** classical vs. quantum

- **Nanoscale Behavior**



- **Transport**: continuum?
- **Carrier Properties**: Bulk?

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Predicting Thermal Conductivity of Defected Systems using Spectral Energy Density

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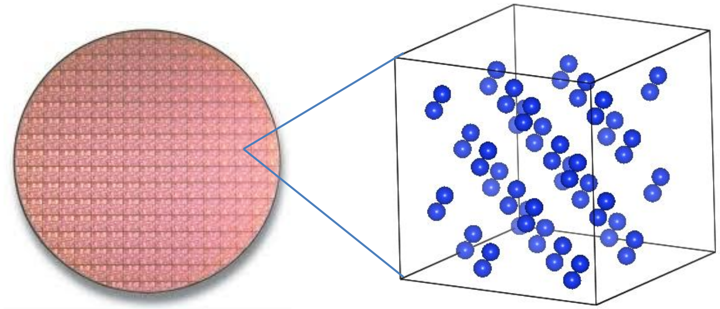
Dielectric Thermal Conductivity

- **<u>Dielectric crystal = Electrical Insulator</u>**



- Ex: Si, Ge

- **Bulk** dielectric: $\vec{q} = -\kappa \nabla T$

- **<u>Dielectric Thermal Conductivity:</u>**

$$\kappa_{total} = \kappa_{phonon} \cancel{+ \kappa_{elec}}$$

- **Phonons** are lattice vibrations…

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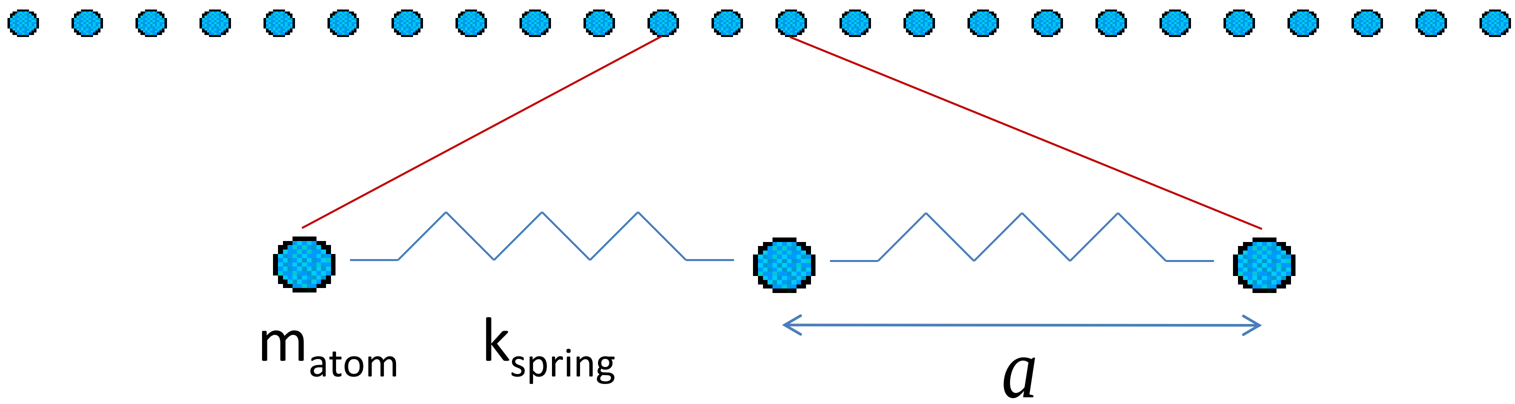
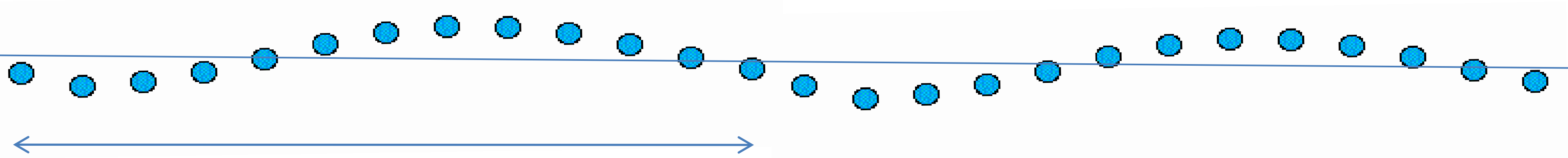
Phonons

1-D model of crystal:



Lattice vibrations (Phonons) are travelling waves:

$$u(x) \propto e^{i(kx-\omega t)} \longrightarrow v_g$$



$$k = \frac{2\pi}{\lambda}, \omega$$

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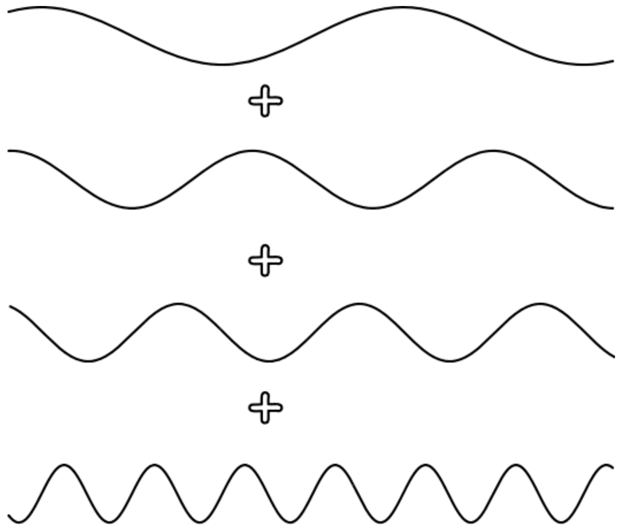
Phonon Gas

$$E_{phonon} = \hbar\omega$$



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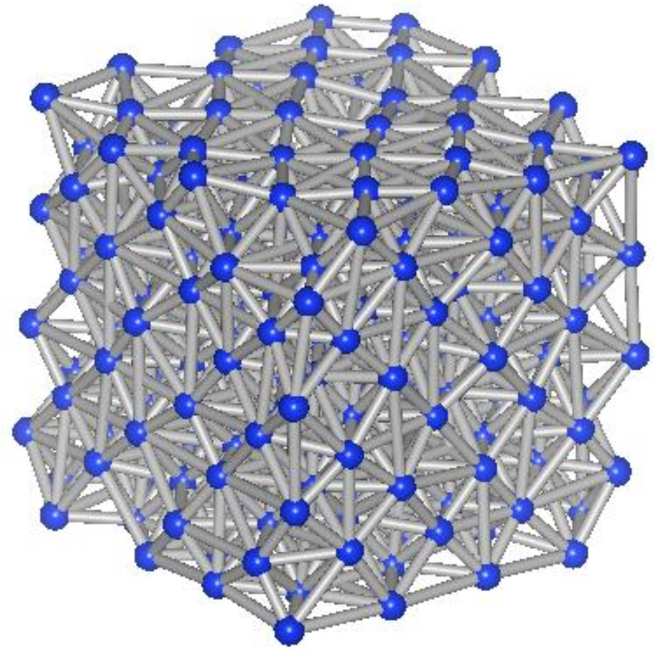
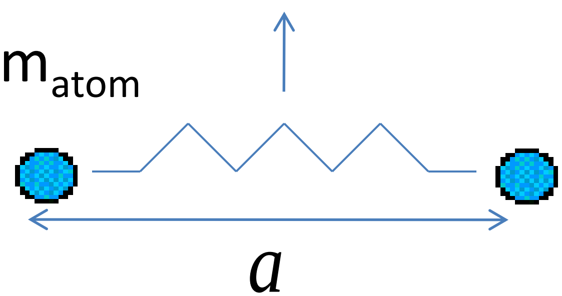


Phonons Interact:

$$F \propto kx + \varepsilon x^3 + \ldots$$

m_{atom}



- Non-linear springs make an **Interacting Gas…**

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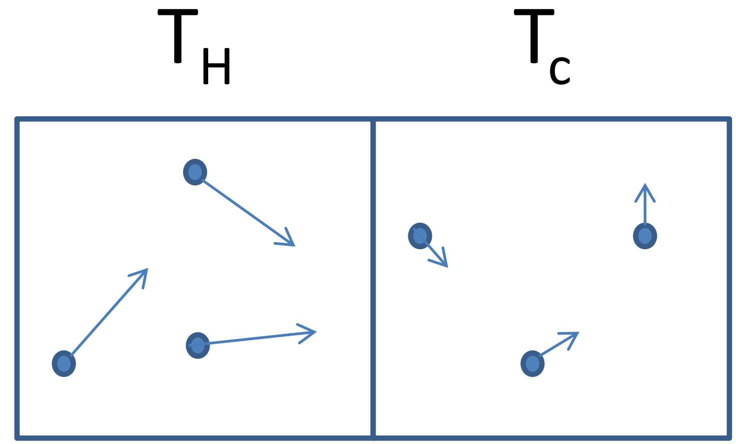
Thermal Conductivity Phonon Gas

Kinetic Theory:

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



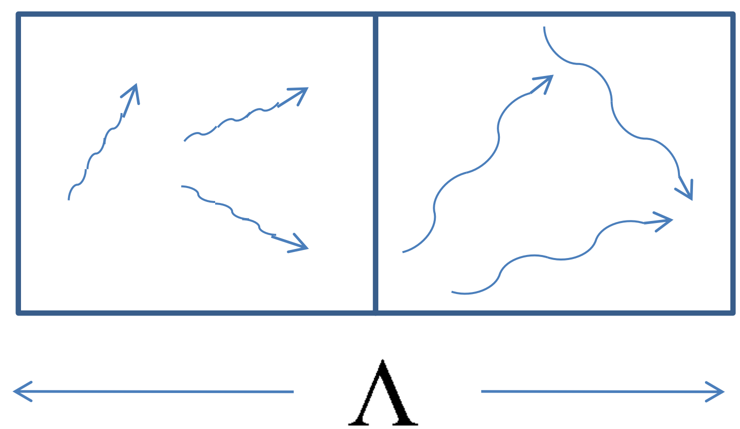
Ideal Gas:

$$\kappa = \frac{1}{3} \rho c_v \langle v \rangle \Lambda$$

Phonon Gas:

- If system L >> Λ :

$$\kappa = \frac{1}{3} \rho c_v v_g \Lambda$$



-**Phonons interact**: with each other, impurities, defects, etc.

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Thermal Conductivity Phonon Gas

Phonons interact

$$\kappa = \frac{1}{3}\rho c_v v_g \Lambda \quad \Rightarrow \quad \kappa = \frac{1}{V}\sum_i c_v(\omega_i) v_g^2(\omega_i)\tau_i(\omega_i)$$

Phonon Lifetime:

$$\Lambda_i(\omega_i) = \tau_i(\omega_i) v_g(\omega_i)$$

Properties needed for κ prediction:

$$\omega_i, \tau_i(\omega_i), v_g(\omega_i)$$

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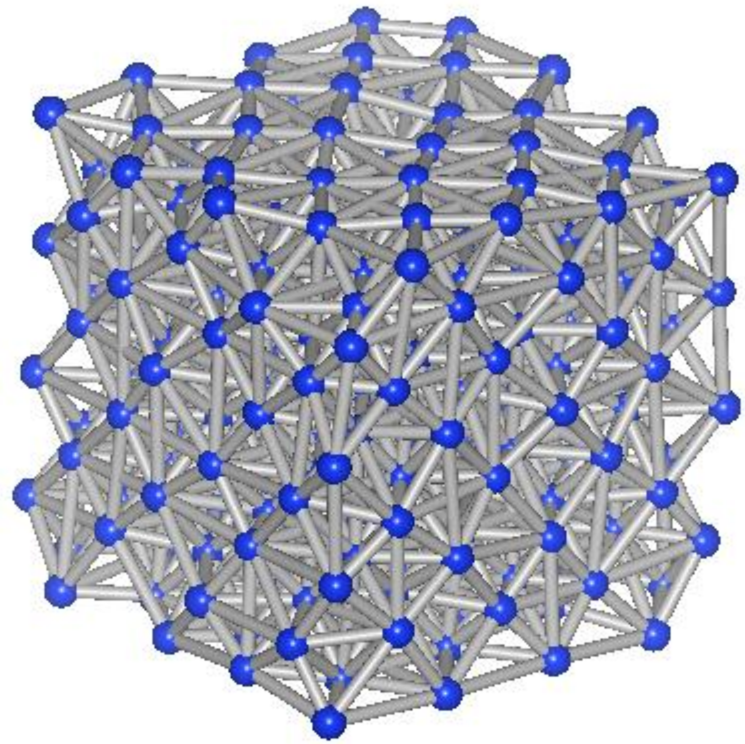
Molecular Dynamics and Spectral Energy Density

- **Molecular Dynamics**

$$\vec{F} = m\vec{a}$$

- Equilibrium/non-equlibrium properties:

$$\vec{r}(t), \vec{p}(t)$$



- **Spectral Energy Density**

- **Frequency, group velocity** and **lifetimes** of phonons from Molecular Dynamics.

$$\omega_i, \tau_i(\omega_i), v_g(\omega_i)$$

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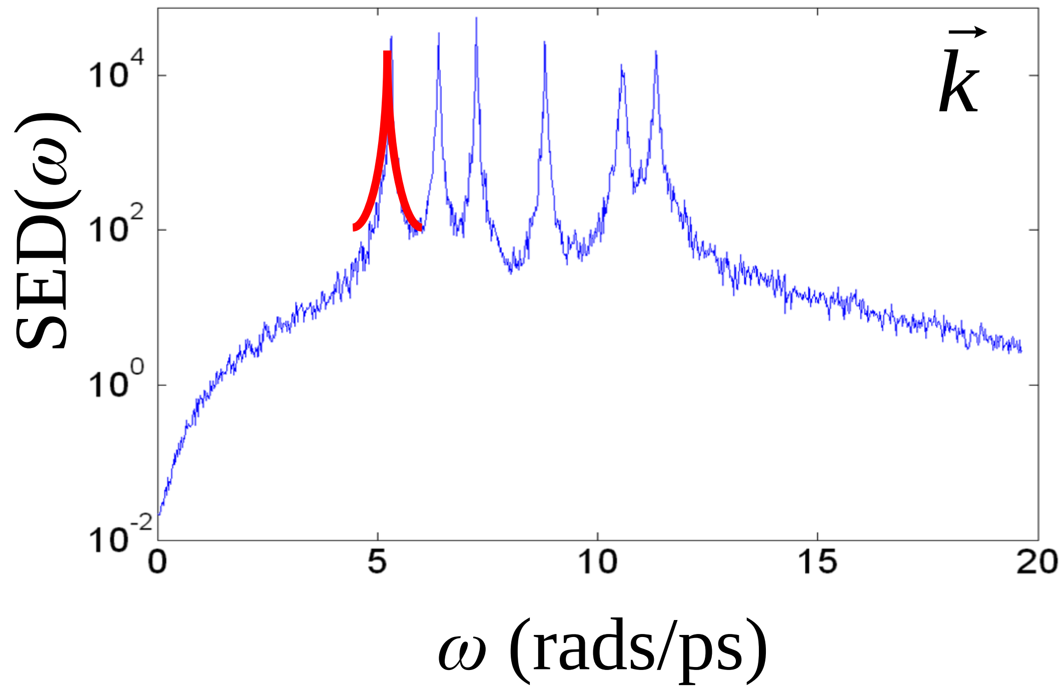
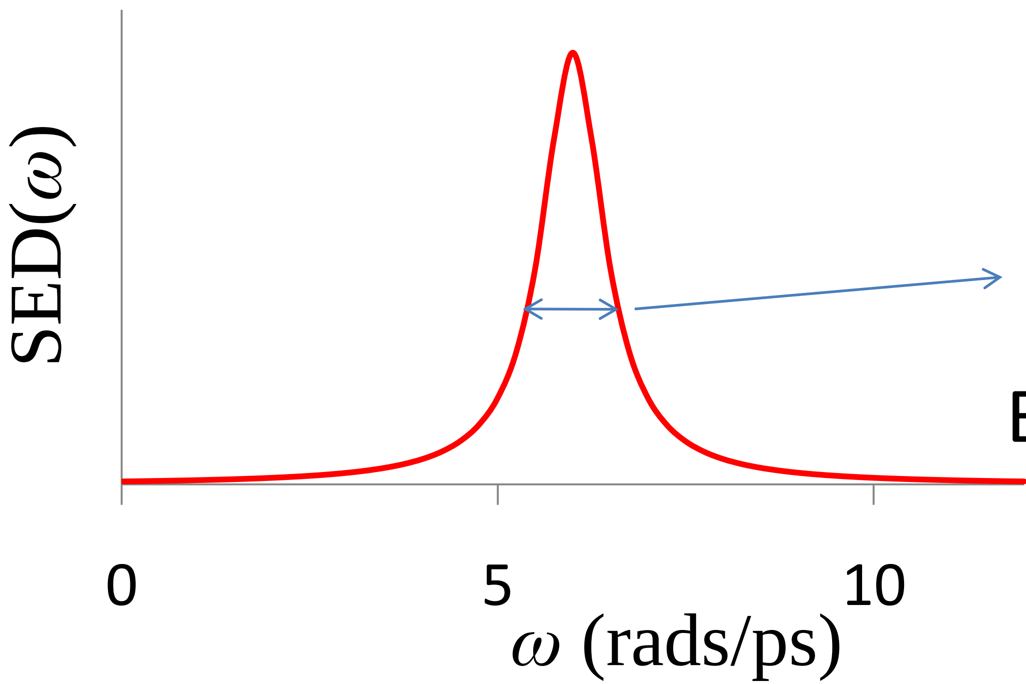
Spectral Energy Density

- **Spectral Energy Density:** **(SED)** system energy in frequency space.

$$\omega_i, \tau_i(\omega_i), v_g(\omega_i)$$





$$\Gamma \rightarrow \quad \tau_i(\omega_i) = 1/\Gamma$$

Broad peak = short **lifetime**

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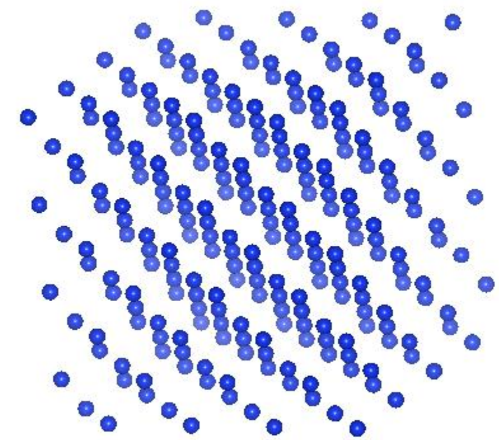
Thermal Conductivity Disordered Materials

Disorder = non-periodic

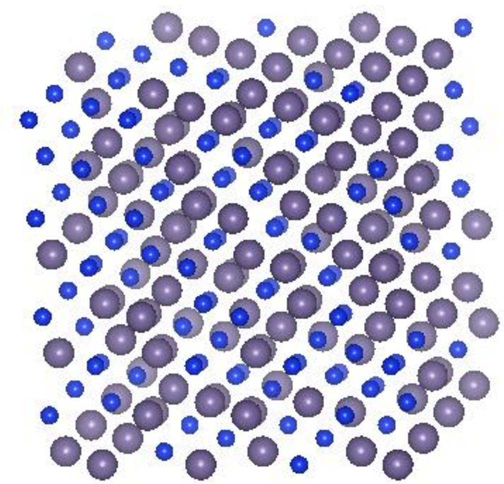
$c = 0.0$



Blue => mass=1.0

Purple => mass=3.0

$c = 0.5$



Phonon picture still valid?

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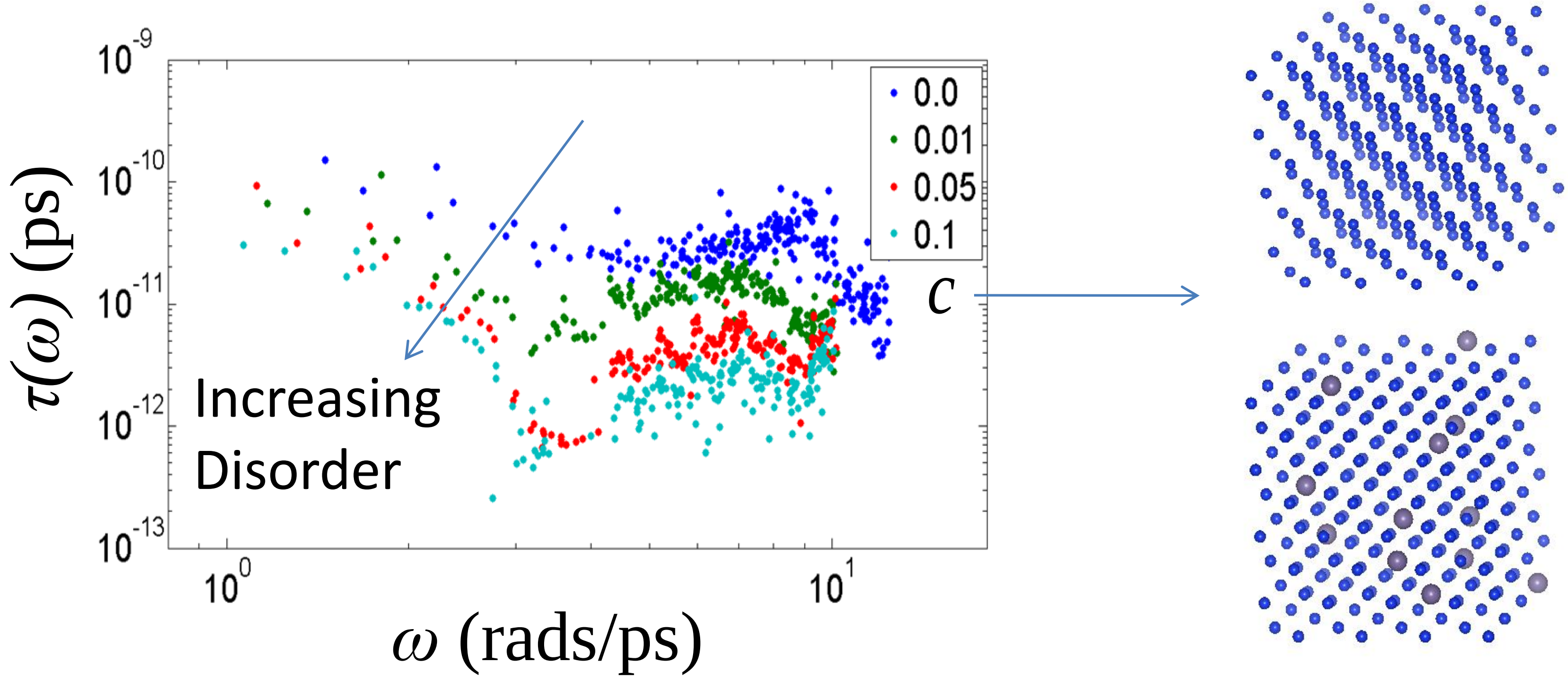
Phonon Lifetimes (Mean Free Path)



Pure

Defected

$$\Lambda^{0.0} = 74 - 0.5 \text{ nm}$$

$$\Lambda^{0.1} = 11 - 0.1 \text{ nm}$$

$$L \approx \Lambda$$

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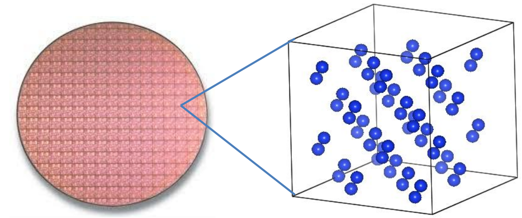
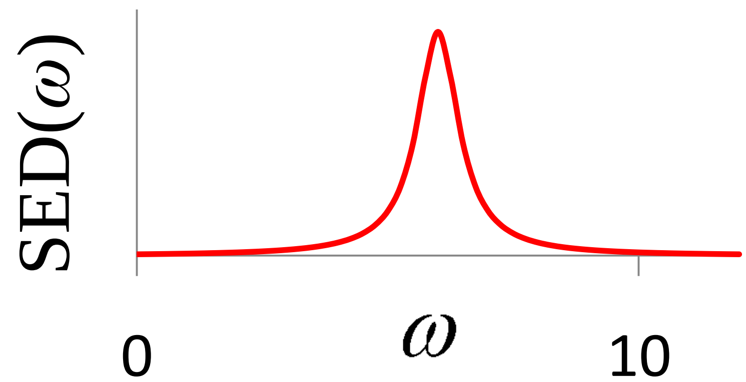
Discussion

- Dielectric thermal conductivity can be described by Kinetic Theory (bulk system).



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

- Molecular Dynamics and Spectral Energy Density can measure phonon properties.



- Phonon properties can be predicted for “weakly” perturbed systems, analyzed on mode by mode basis.

$$\omega_i, \tau_i(\omega_i), v_g(\omega_i)$$

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Questions

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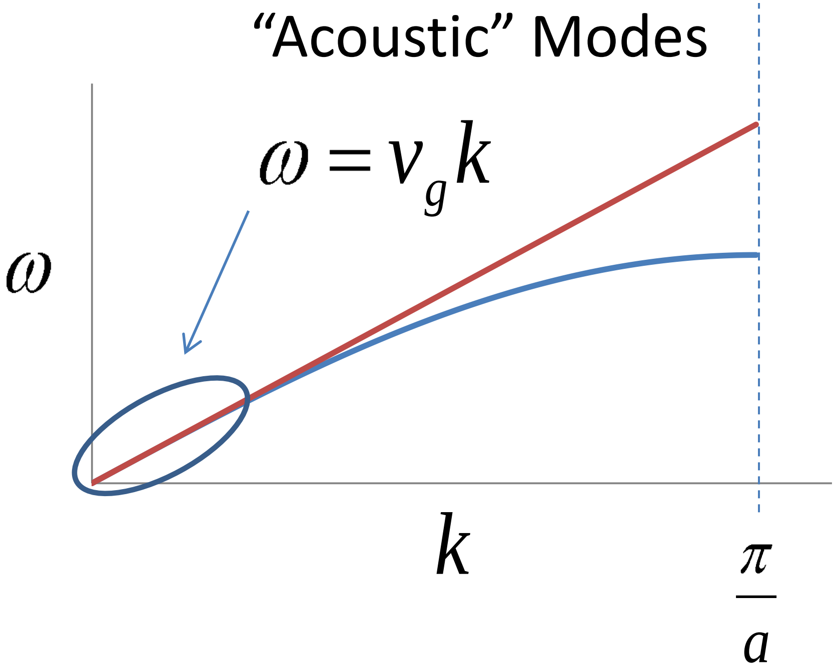
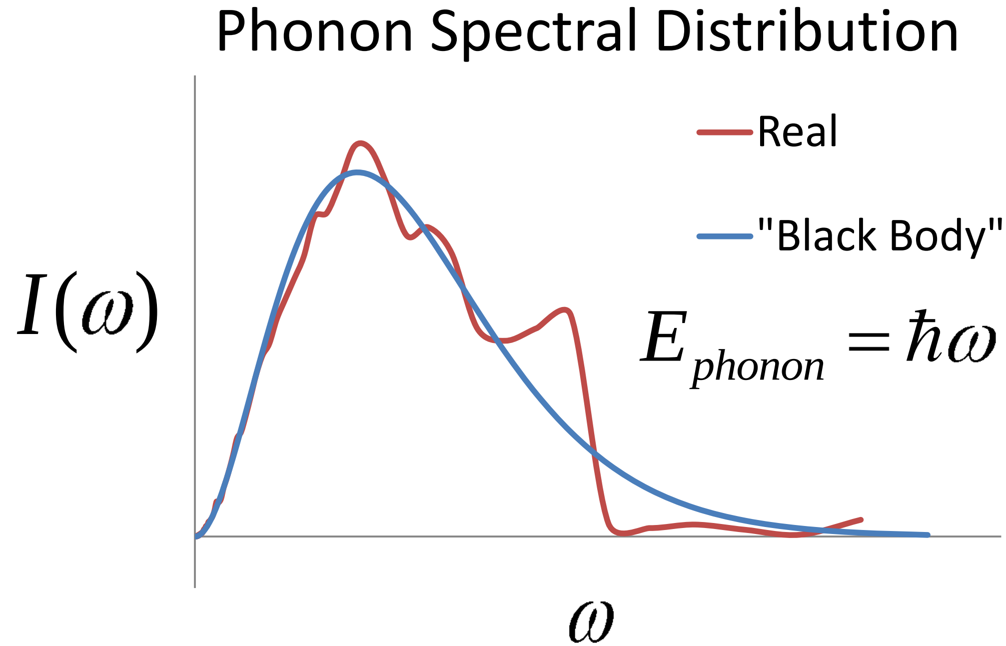
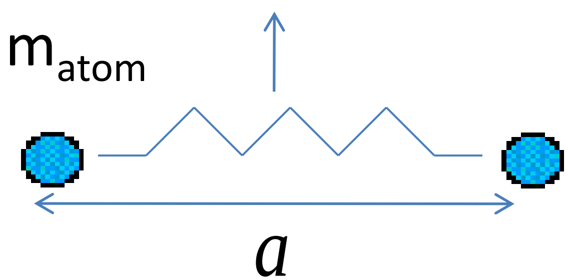
Phonon Gas





Phonons vs. Photons:

$$F \propto kx + \varepsilon x^3 + \ldots$$



- Non-linear springs
- Phonons interact with each other
- **Interacting Gas…**

$$\Phi(\omega, \boldsymbol{\kappa}) = 2\sum_{\nu}^{3n}\sum_{\alpha,b}^{3,n}\left\langle T\left(\begin{smallmatrix}\boldsymbol{\kappa} & b \\ \nu & \alpha\end{smallmatrix}; \omega\right)\right\rangle$$

$$= \frac{1}{4\pi\tau_0 N}\sum_{b}^{n} m_b \sum_{\alpha}^{3}\left|\int_{-\tau_0}^{\tau_0}\sum_{l}^{N}\dot{u}_\alpha\left(\begin{smallmatrix}l \\ b\end{smallmatrix}; t\right)\exp\left[i\boldsymbol{\kappa}\cdot\mathbf{r}_0\left(\begin{smallmatrix}l \\ 0\end{smallmatrix}\right) - i\omega t\right]dt\right|^2$$

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