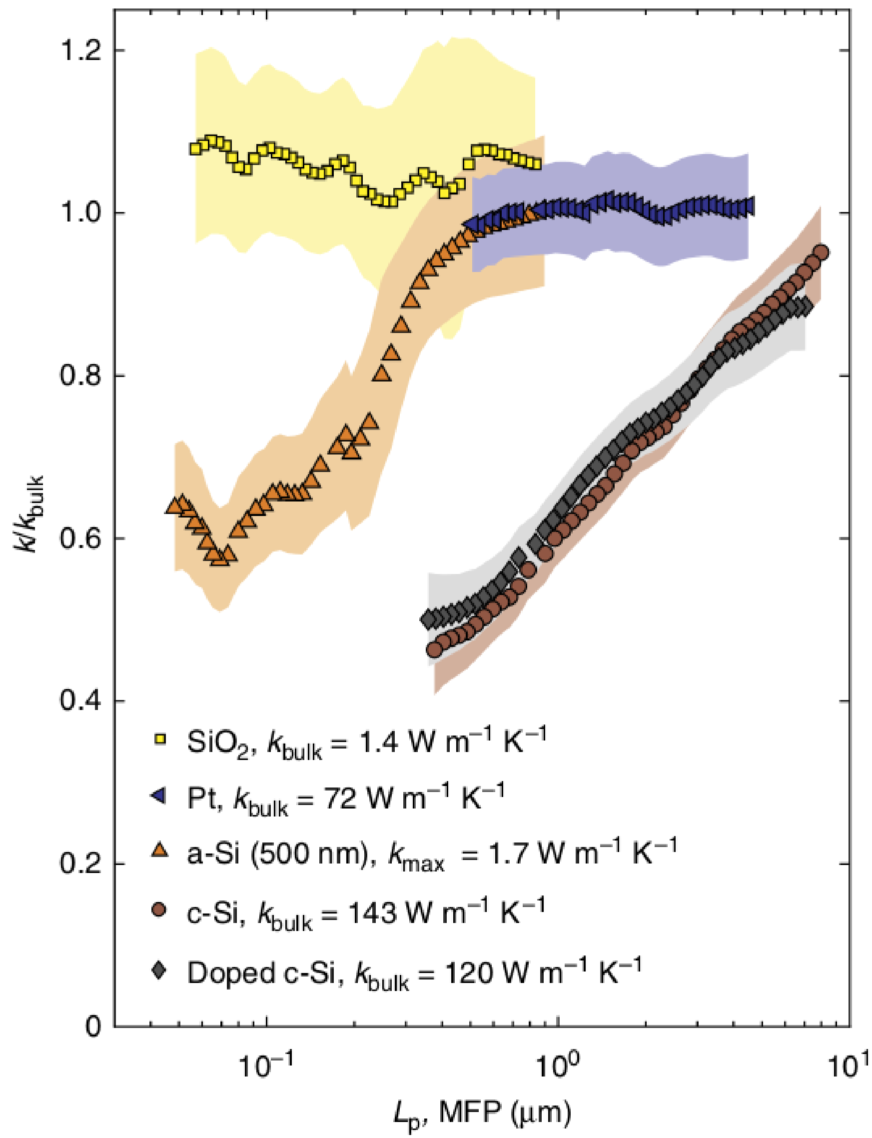
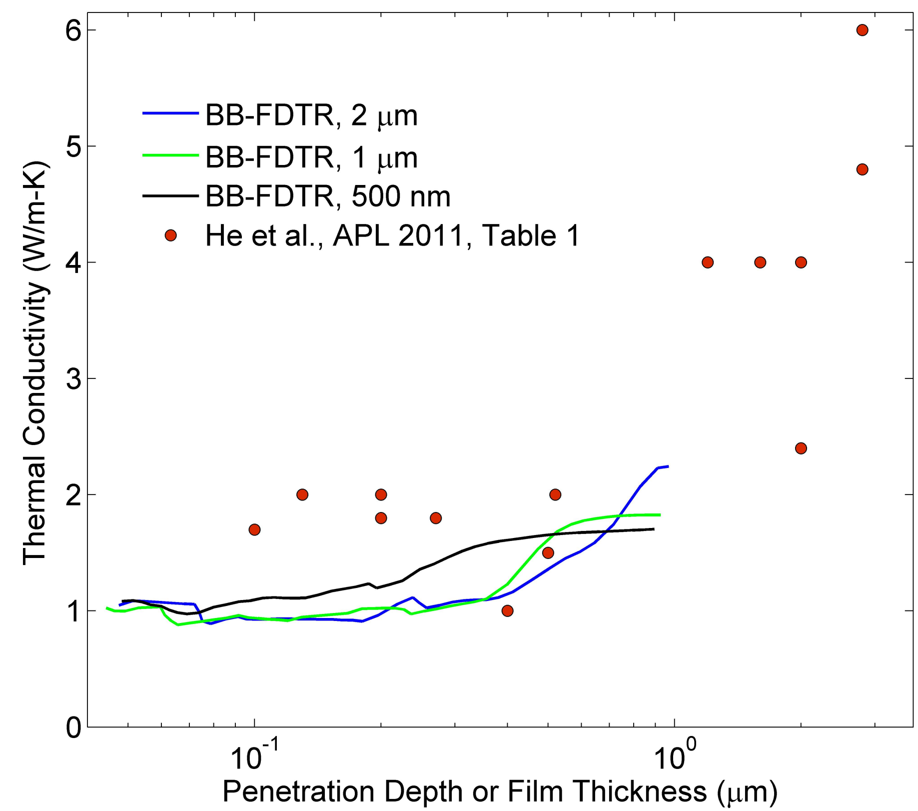
a-SiO2, a-Si: broadband experiments





Mechanical Engineering

vibrational thermal conductivity

$$k_{vib} = k_{ph} + k_{AF}$$

$$k_{ph} = \frac{1}{V}\int_0^{\omega_{cut}} d\omega DOS(\omega)C(\omega)D(\omega)$$

$$C(\omega) = k_{\mathrm{B}}$$

$$D(\omega) = \frac{1}{3}v_g^2(\omega)\tau(\omega)$$

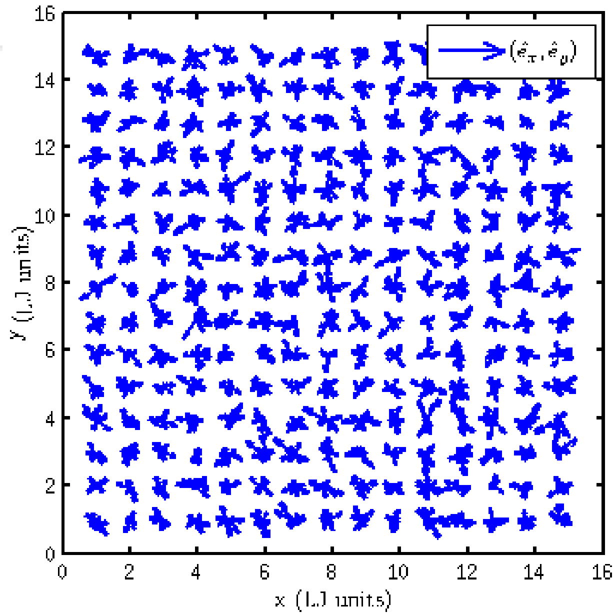
$$\Lambda(\omega) = v_g(\omega)\tau(\omega)$$

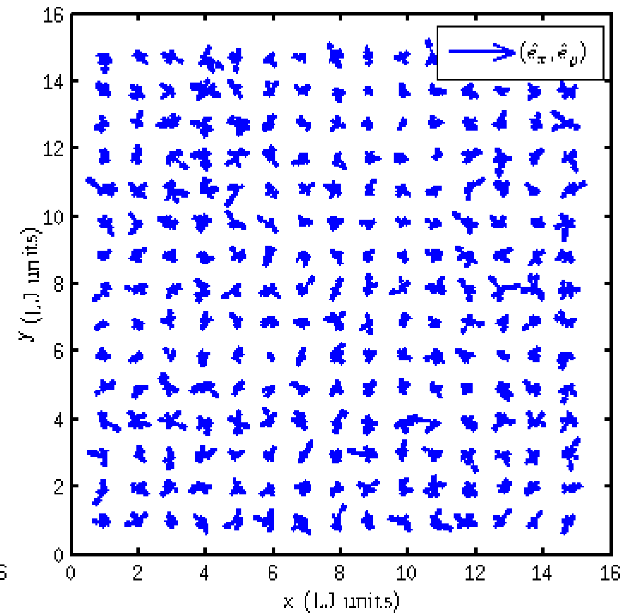
$$D(\omega) = \frac{1}{3}v_g(\omega)\Lambda(\omega)$$

Mechanical Engineering

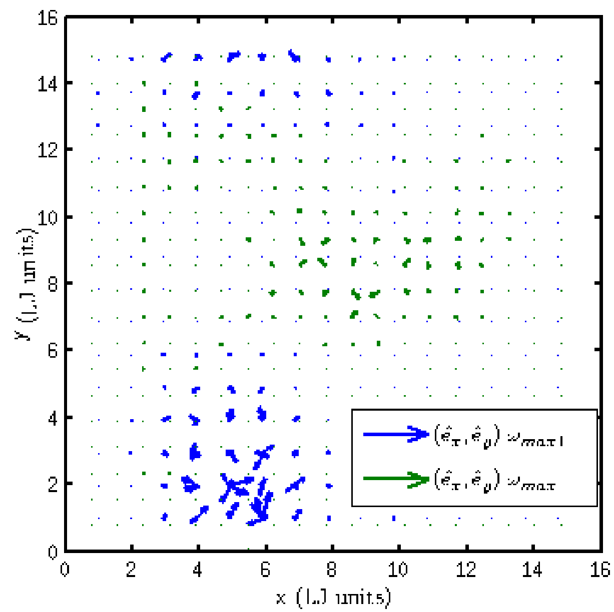
AF theory

$$k_{vib} = k_{ph} + k_{AF}$$





$$k_{AF} = \frac{1}{V} \sum_{\omega_i > \omega_{cut}} C_i(\omega) D_{AF,i}(\omega)$$

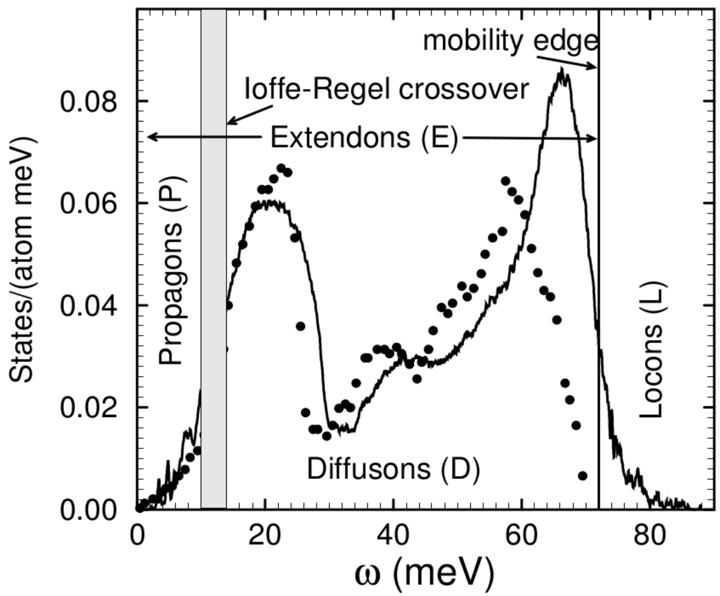


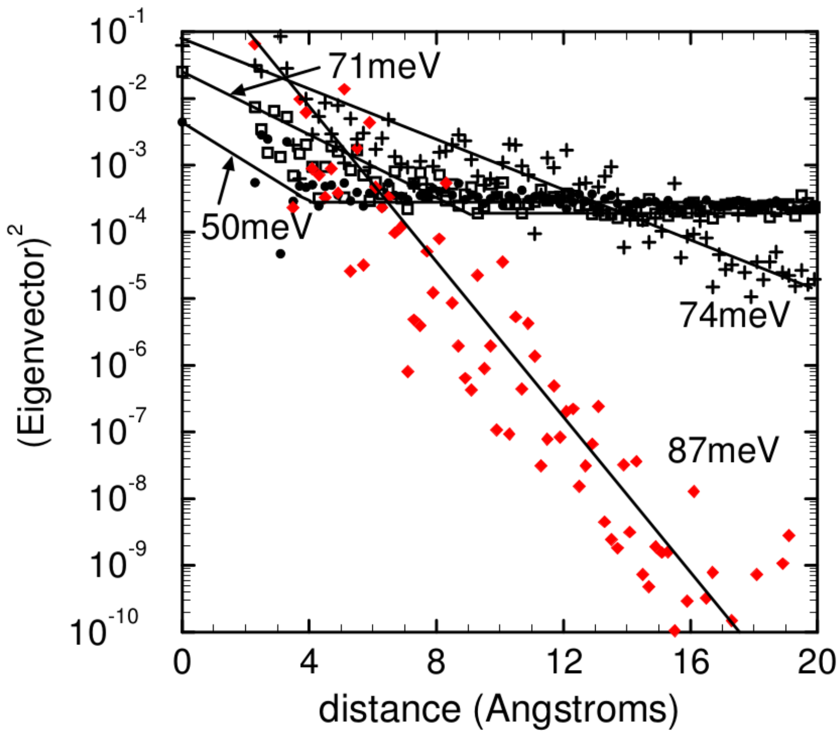
$$D_{AF,i} = \frac{\pi V^2}{\hbar^2 \omega_i^2} \sum_{j \neq i} |\langle i | J_{x,y,z} | j \rangle|^2 \delta(\omega_i - \omega_j)$$

Mechanical Engineering

vibrons: propagons, diffusons, locons

- vibrons
  - extendons
    - propagons
    - diffusons
  - locons





thermal diffusivity limits

$$D(\omega) = \frac{1}{3} v_g^2(\omega) \tau(\omega)$$

$$D(\omega) = B\omega^{-2}$$

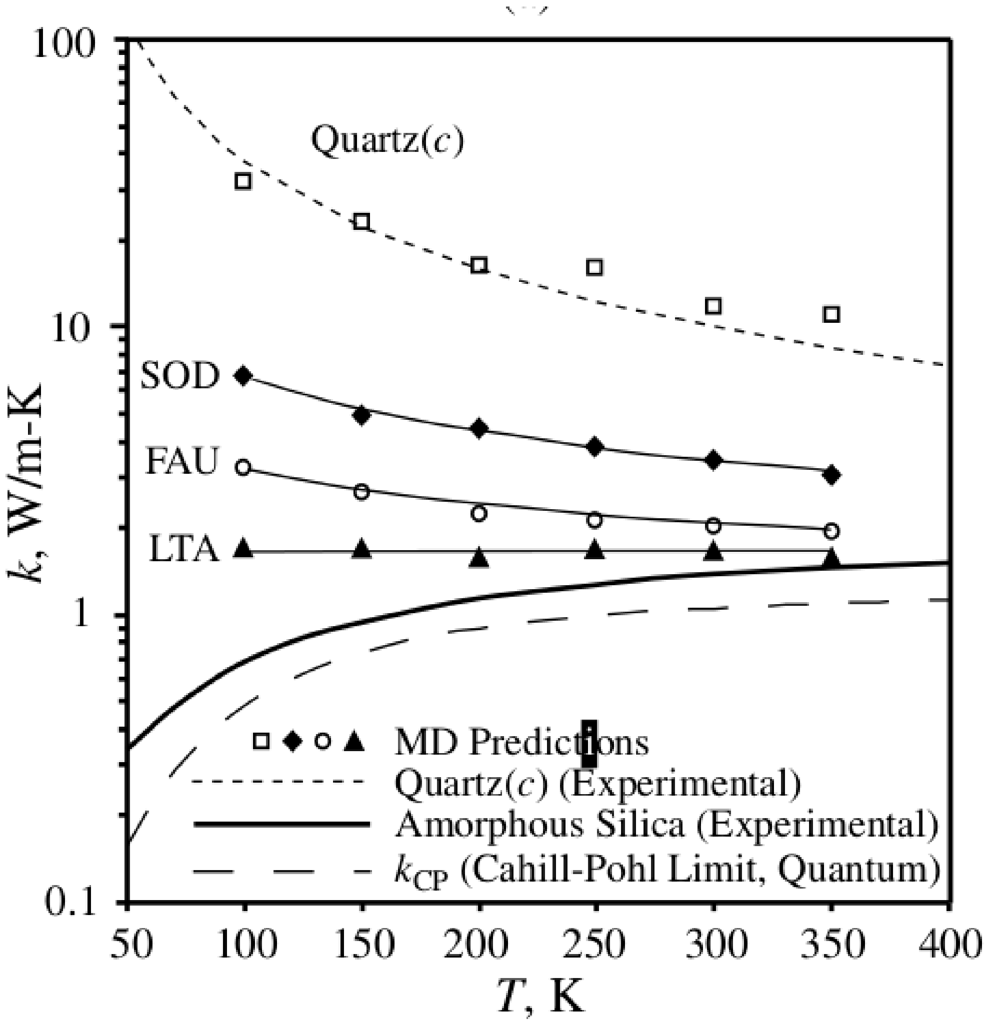
$$D(\omega) = B\omega^{-4}$$

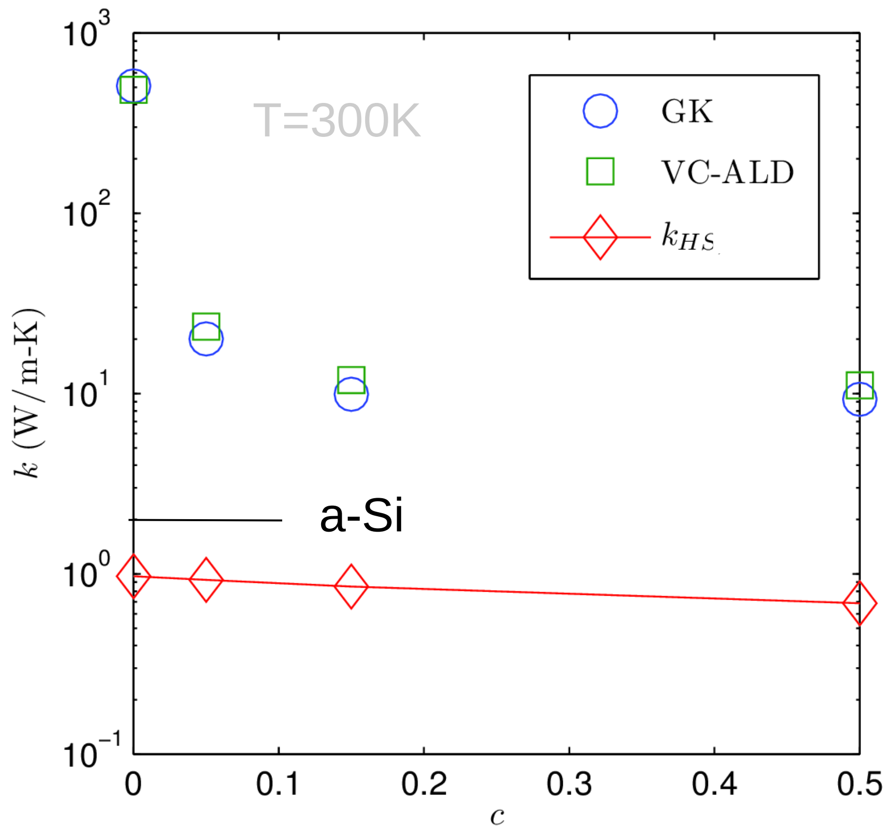
$$D_{HS} = \frac{1}{3} v_s a$$

$$k_{HS} = \frac{k_\mathrm{B}}{V_b} b v_s a$$

Mechanical Engineering

silica, silicon thermal conductivity





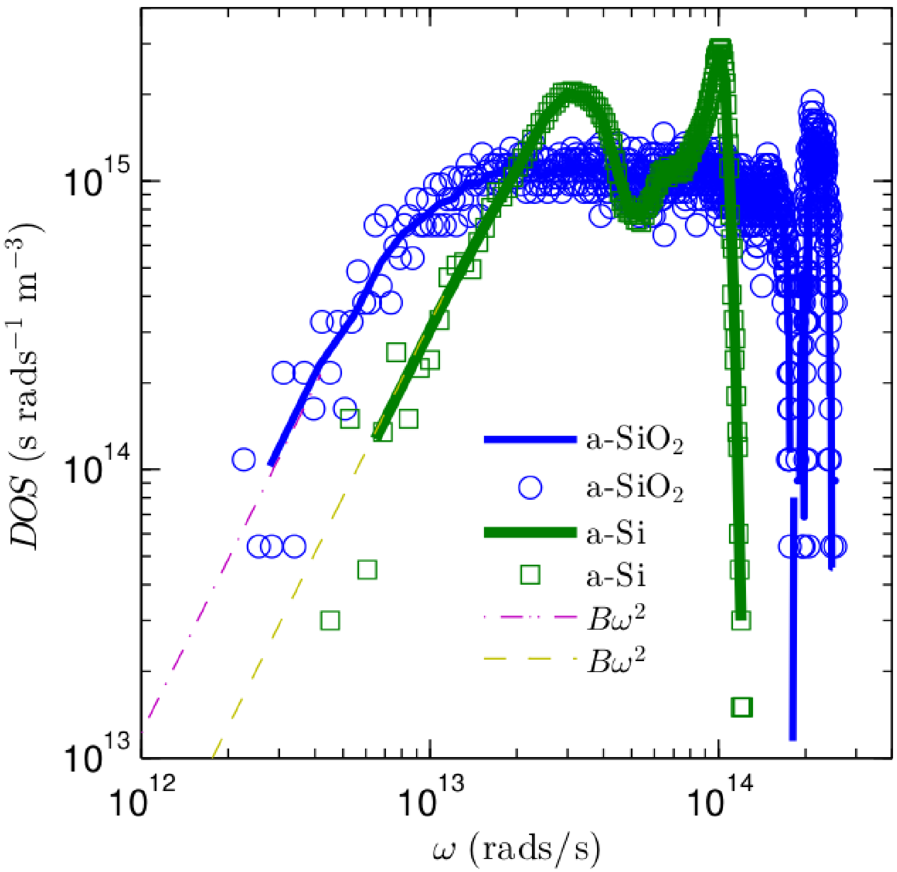
Mechanical Engineering

density of states

$$DOS(\omega) = \sum_i \delta(\omega_i - \omega)$$

$$DOS(\omega) = \frac{3\pi\omega^2}{2v_{s,DOS}^3}$$

$$v_s = \frac{2}{3}v_{s,L} + \frac{1}{3}v_{s,T}$$



method	Eqs. (17), (18)	Eqs. (20), (24)	DOS Eq. (10)
a-Si			
transverse	3,886	3,699	3,615
longitudinal	8,271	8,047	

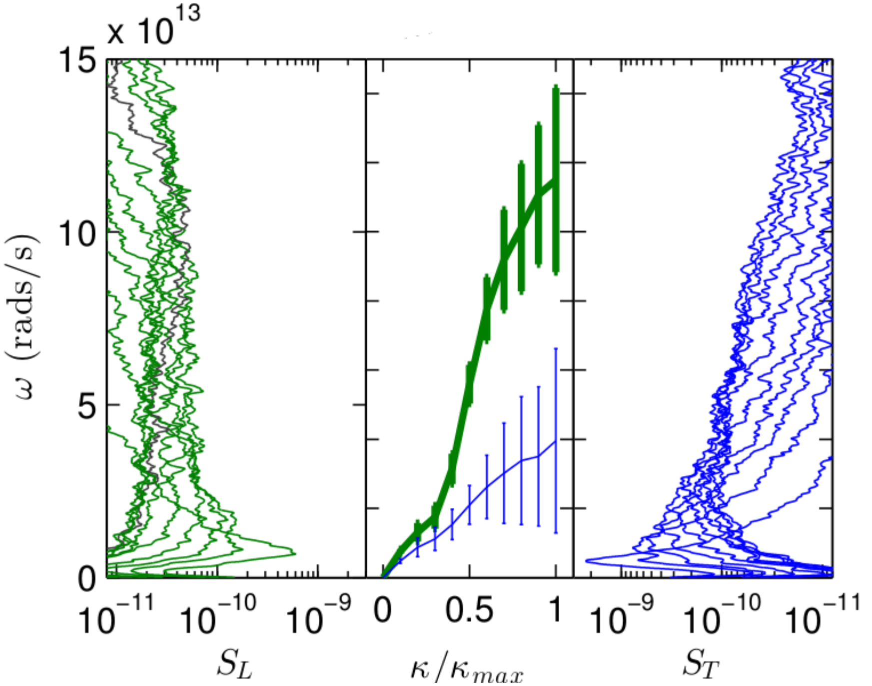
structure factor

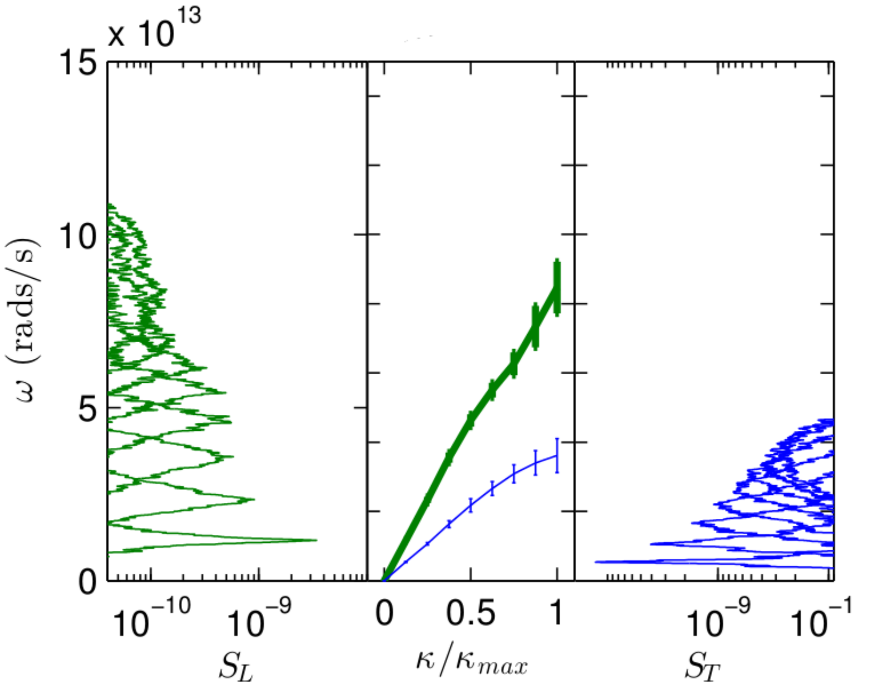
$$E^{L}\genfrac{(}{)}{0pt}{}{\boldsymbol{\kappa}}{\nu} = \left| \sum_{b} \hat{\boldsymbol{\kappa}} \cdot e\begin{pmatrix} \boldsymbol{\kappa}{=}\mathbf{0} & b \\ \nu & \alpha \end{pmatrix} \exp\!\left[i\boldsymbol{\kappa} \cdot \boldsymbol{r}_0\genfrac{(}{)}{0pt}{}{l{=}0}{b} \right] \right|^2$$

$$E^{T}\genfrac{(}{)}{0pt}{}{\boldsymbol{\kappa}}{\nu} = \left| \sum_{b} \hat{\boldsymbol{\kappa}} \times e\begin{pmatrix} \boldsymbol{\kappa}{=}\mathbf{0} & b \\ \nu & \alpha \end{pmatrix} \exp\!\left[i\boldsymbol{\kappa} \cdot \boldsymbol{r}_0\genfrac{(}{)}{0pt}{}{l{=}0}{b} \right] \right|^2$$

$$S^{L,T}\genfrac{(}{)}{0pt}{}{\boldsymbol{\kappa}}{\omega} = \sum_{\nu} E^{L,T}\genfrac{(}{)}{0pt}{}{\boldsymbol{\kappa}}{\nu}\, \delta\!\left(\omega - \omega\genfrac{(}{)}{0pt}{}{\boldsymbol{\kappa}{=}\mathbf{0}}{\nu}\right)$$

$$S^{L,T}\genfrac{(}{)}{0pt}{}{\boldsymbol{\kappa}}{\omega} = \frac{C_0(\boldsymbol{\kappa})}{[\omega_0(\boldsymbol{\kappa}) - \omega]^2 + \Gamma^2(\boldsymbol{\kappa})}$$





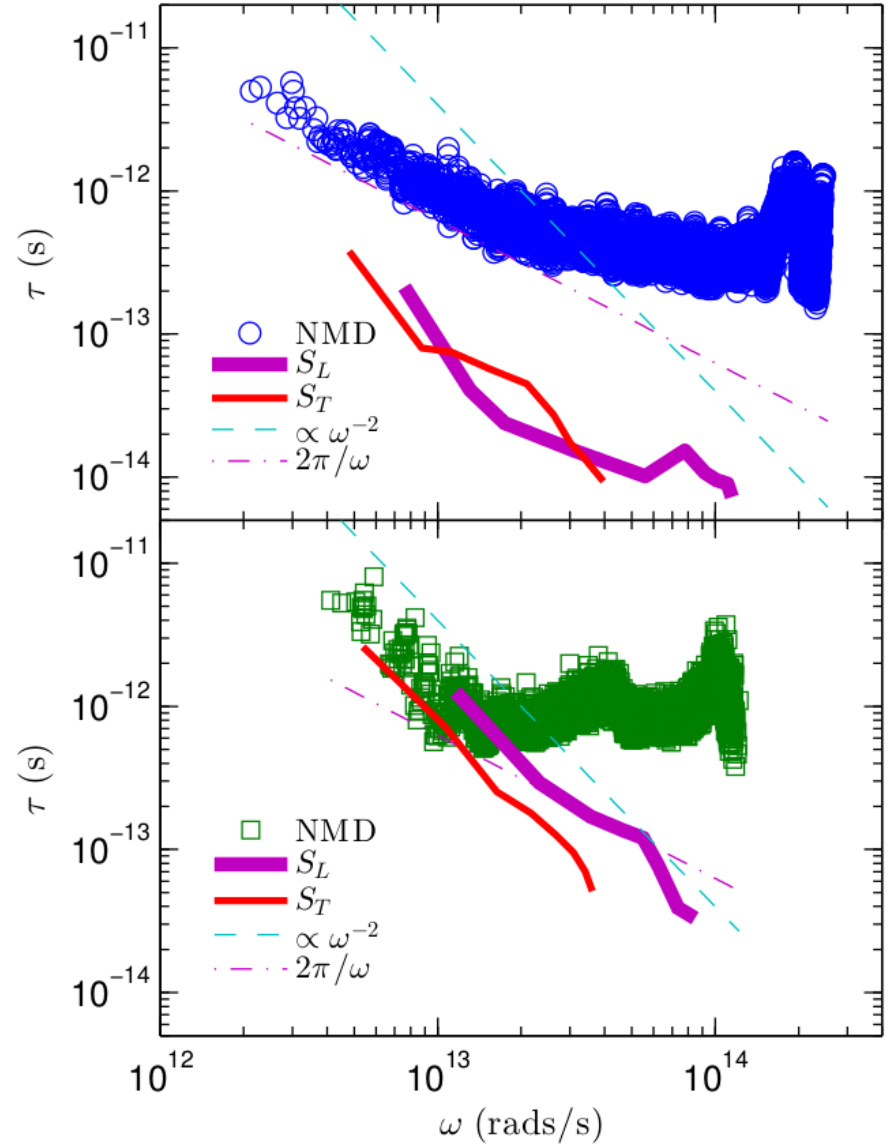
normal mode decomposition

$$\dot{q}\left(\begin{smallmatrix}\boldsymbol{\kappa}=\mathbf{0}\\ \nu\end{smallmatrix};t\right) = \sum_{\alpha,b,l}^{3,n,N} \sqrt{\frac{m_b}{N}}\,\dot{u}_\alpha\left(\begin{smallmatrix}l\\ b\end{smallmatrix};t\right)\, e^*\left(\begin{smallmatrix}\boldsymbol{\kappa}=\mathbf{0} & b\\ \nu & \alpha\end{smallmatrix}\right)\exp\left[i\left(\mathbf{0}\cdot\mathbf{r}_0\left(\begin{smallmatrix}l\\ 0\end{smallmatrix}\right)\right)\right]$$

$$\Phi(\nu,\omega) = \lim_{\tau_0\to\infty}\frac{1}{2\tau_0}\left|\frac{1}{\sqrt{2\pi}}\int_0^{\tau_0}\dot{q}\left(\begin{smallmatrix}\boldsymbol{\kappa}=\mathbf{0}\\ \nu\end{smallmatrix};t\right)\exp(-i\omega t)dt\right|^2$$

$$\Phi(\nu,\omega) = \frac{C_0(\nu)}{[\omega_0(\nu)-\omega]^2+\Gamma^2(\nu)}$$

$$\tau(\nu) = \frac{1}{2\Gamma(\nu)}$$



Mechanical Engineering

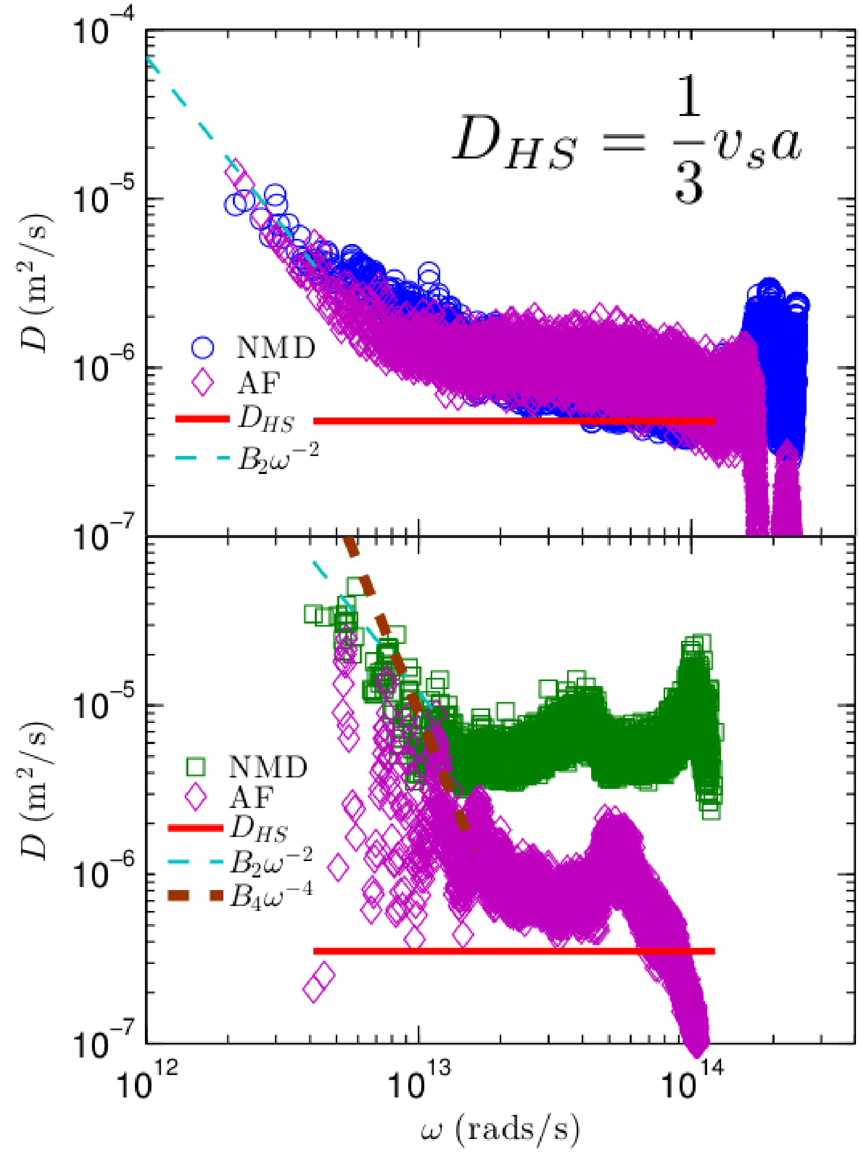
mode diffusivities

$$D(\omega) = \frac{1}{3} v_s \tau(\omega)$$

$$D_{AF,i} = \frac{\pi V^2}{\hbar^2 \omega_i^2} \sum_{j \neq i} | \langle i | J_{x,y,z} | j \rangle |^2 \delta(\omega_i - \omega_j)$$

$$D(\omega) = B\omega^{-2}$$

$$D(\omega) = B\omega^{-4}$$



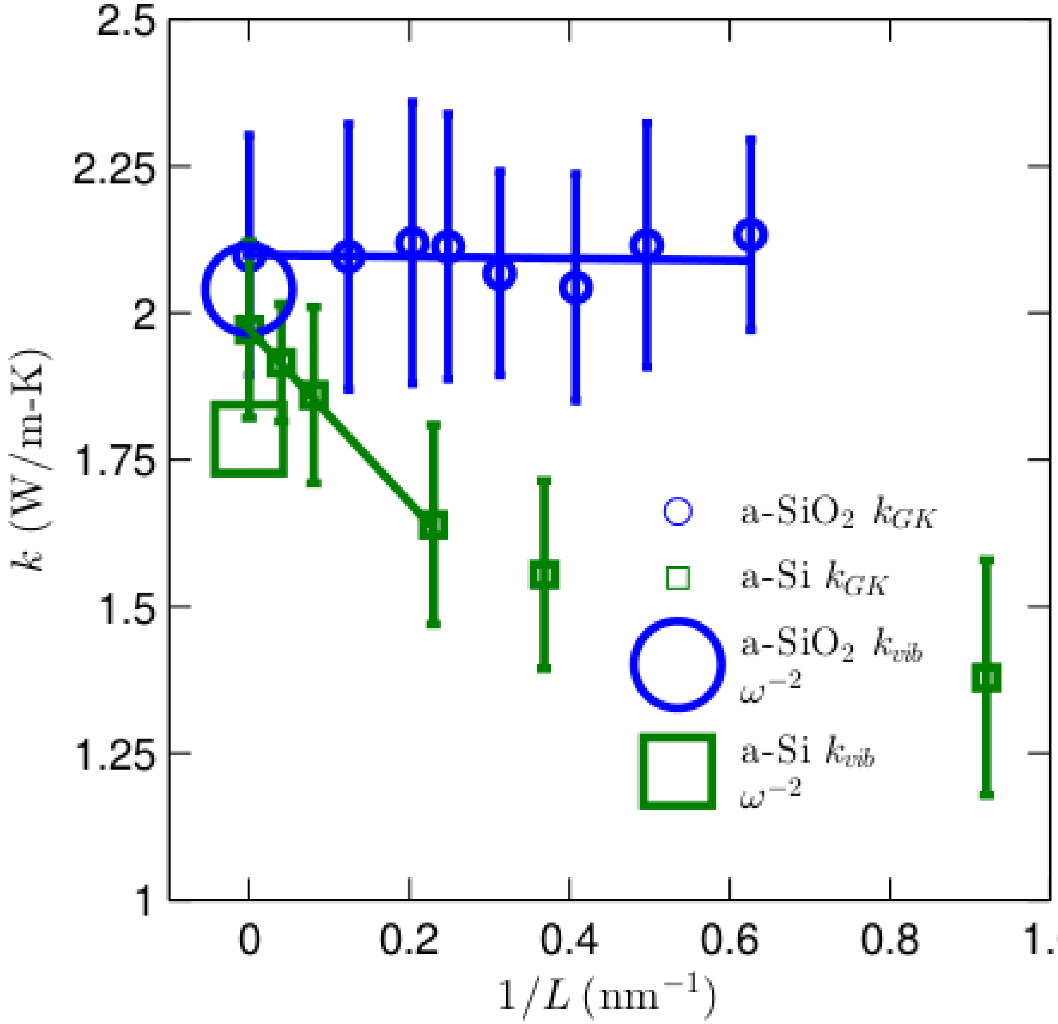
Mechanical Engineering

bulk thermal conductivity

$$k_{vib} = k_{ph} + k_{AF}$$

$$D(\omega) = B\omega^{-2}$$

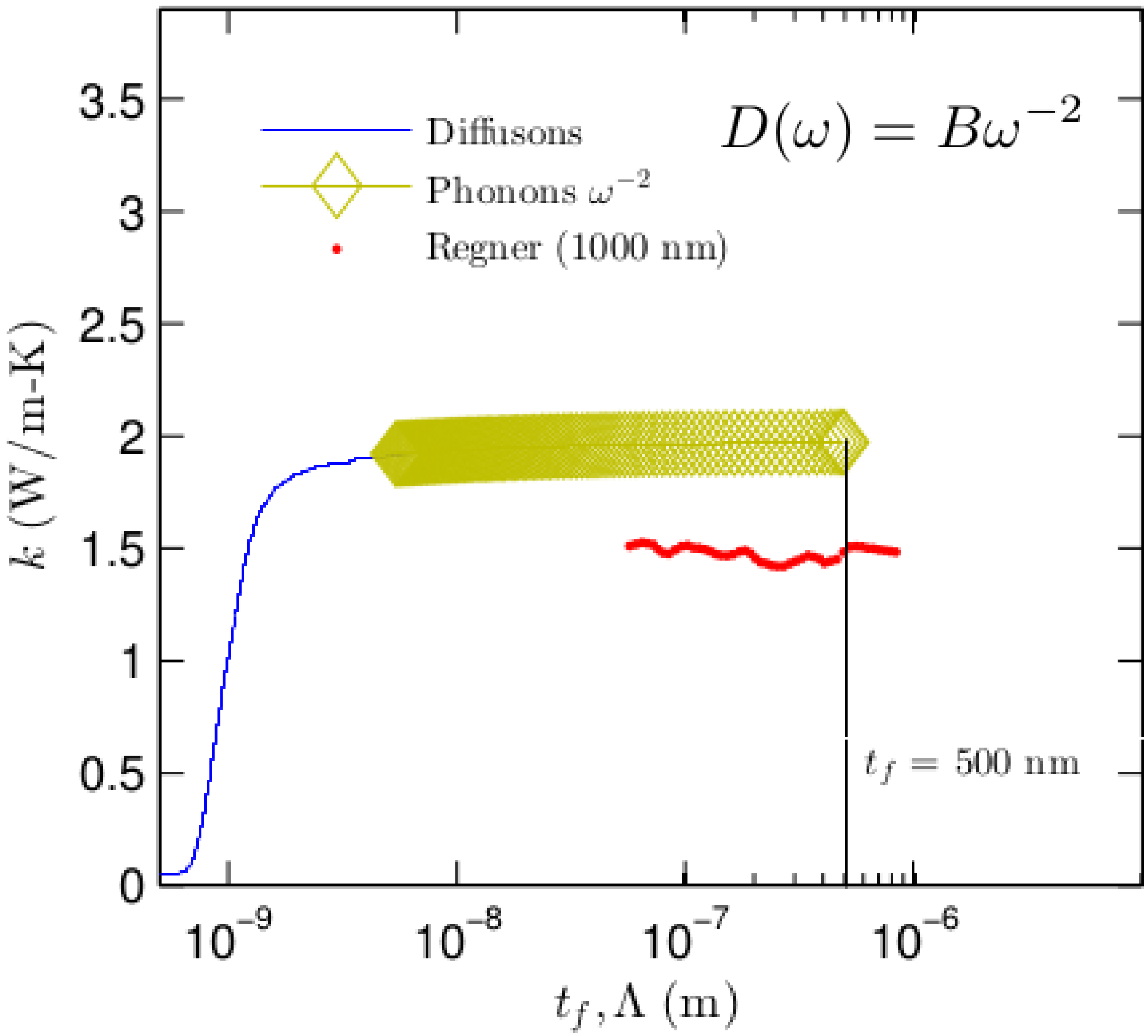
$$\frac{k(L)}{k_{bulk}} = 1 - \frac{c_0}{L}$$



Mechanical Engineering

accumulated thermal conductivity: a-SiO2

$$\frac{1}{\Lambda_{eff}(\omega)} = \frac{1}{\Lambda(\omega)} + \frac{1}{t_f}$$



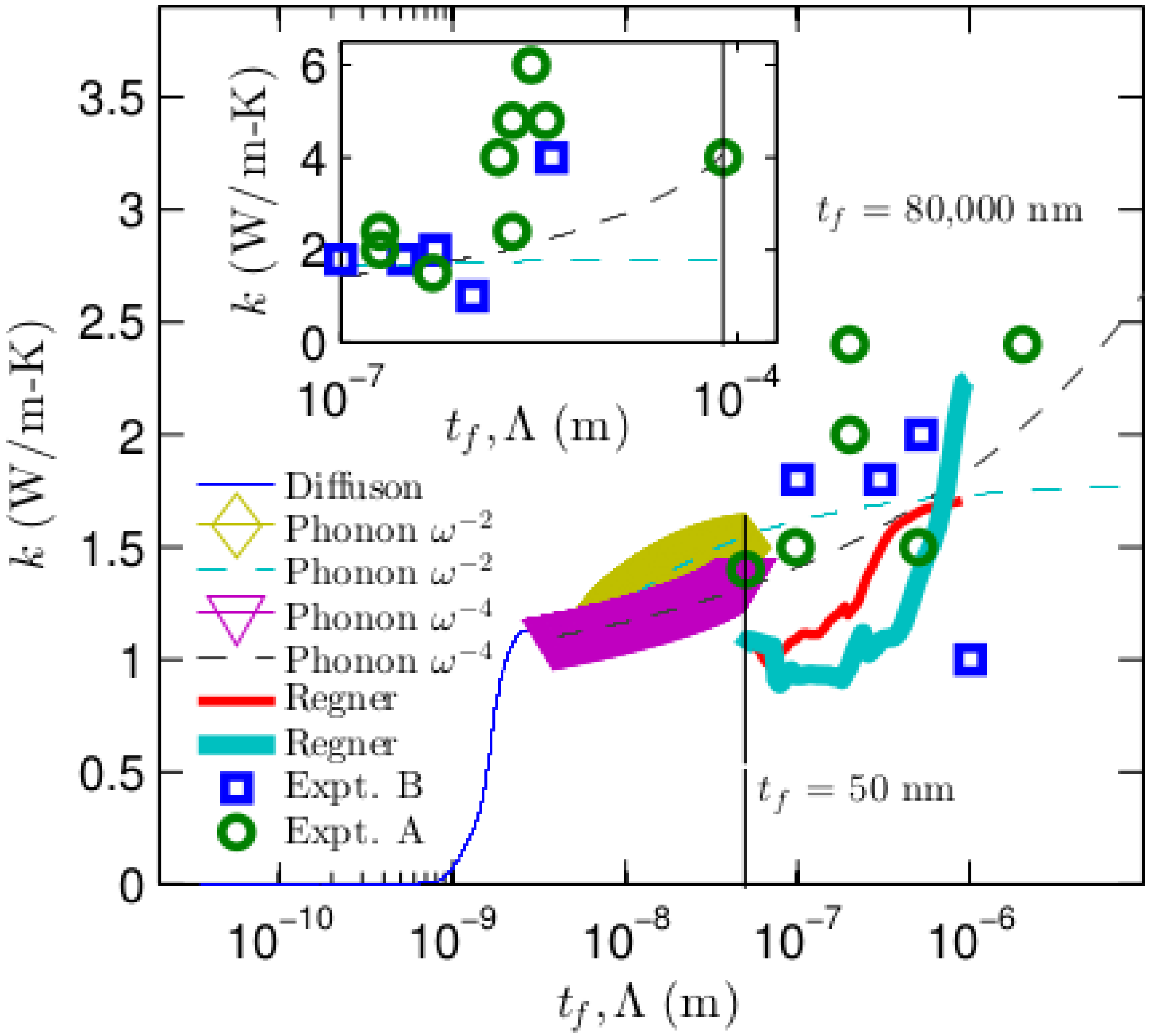
Mechanical Engineering

accumulated thermal conductivity: a-Si

$$\frac{1}{\Lambda_{eff}(\omega)} = \frac{1}{\Lambda(\omega)} + \frac{1}{t_f}$$

$$D(\omega) = B\omega^{-2}$$

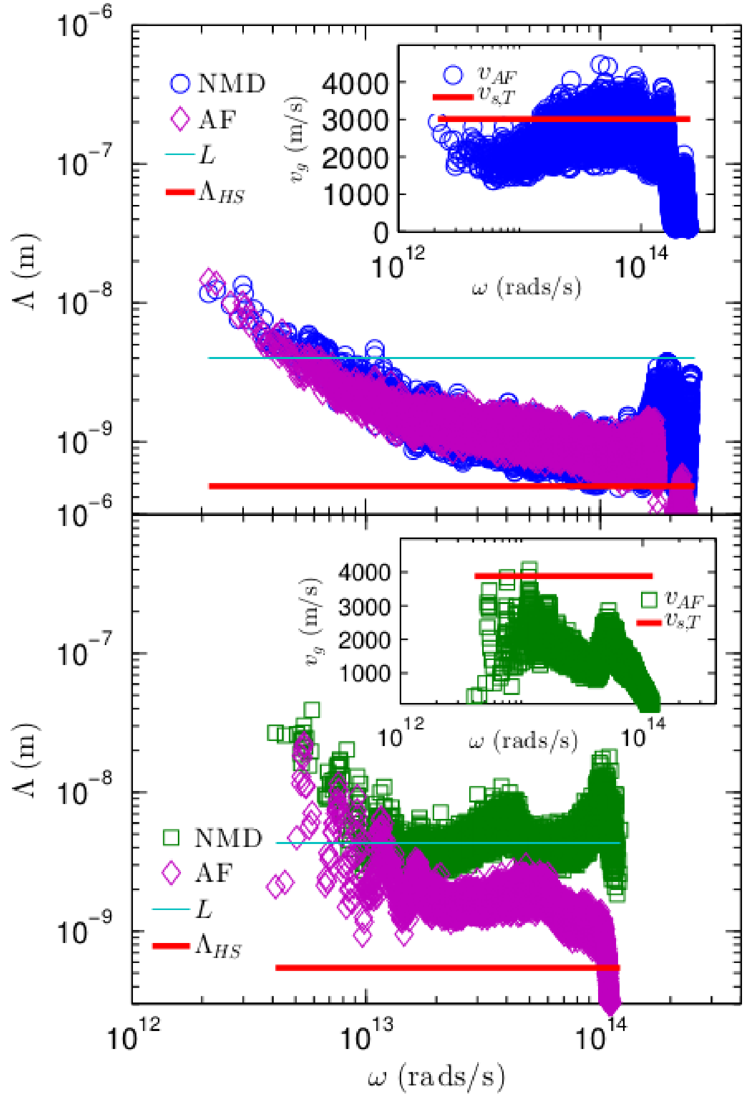
$$D(\omega) = B\omega^{-4}$$



Mechanical Engineering

$$v_{AF}(\omega) = \left(3\frac{D_{AF,i}(\omega)}{\tau(\omega)}\right)^{1/2}$$

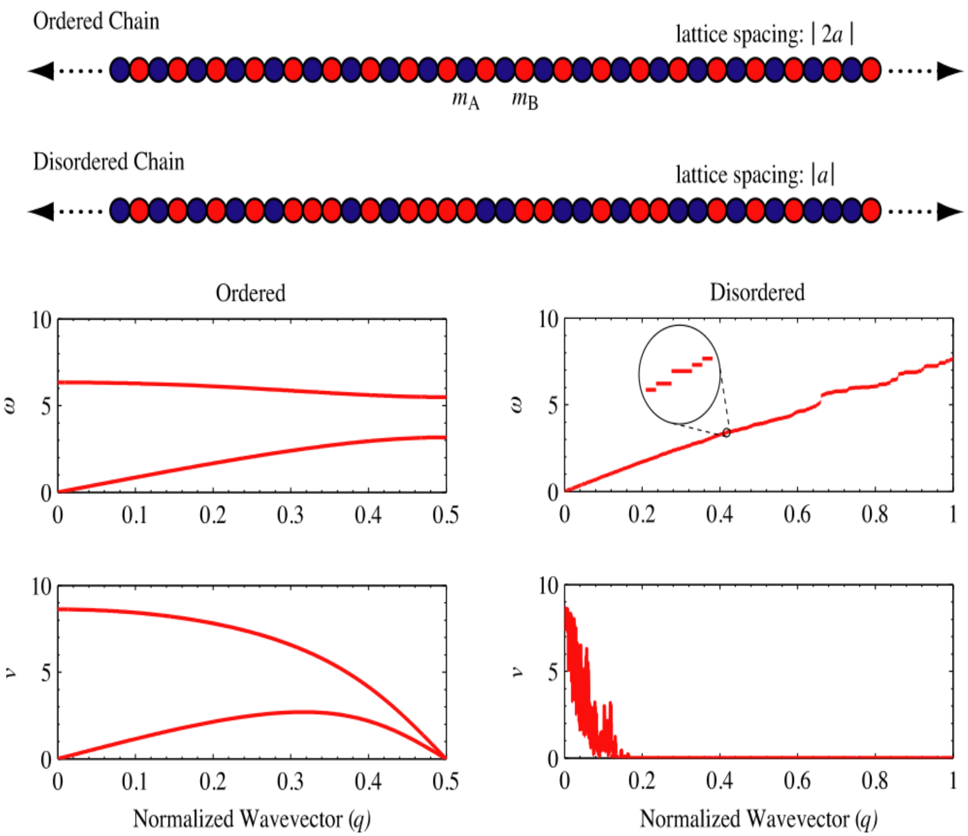
$$\Lambda_{AF}(\omega) = (3D_{AF,i}(\omega)\tau(\omega))^{1/2}$$



Mechanical Engineering

v_g from “zone-folding”:

http://iopscience.iop.org/0953-8984/23/20/205401



v_g from near [000]:

http://pubs.acs.org/doi/abs/10.1021/nn2003184

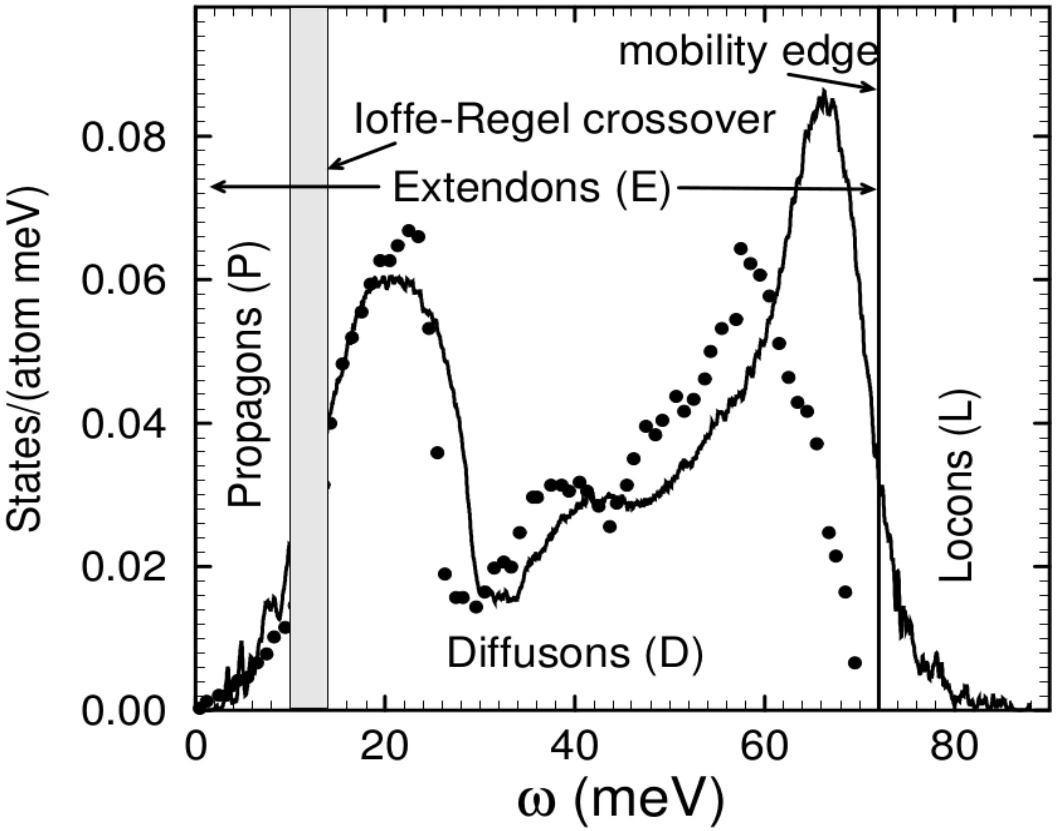
http://pubs.acs.org/doi/abs/10.1021/nl201359q

Mechanical Engineering

vibrons: propagons, diffusons, locons

Numerical studies of amorphous silicon show that the low-
est 4% of vibrational modes are plane-wave like (“propagons”) and the highest 3% of modes are localized (“locons”). The
rest are neither plane-wave like nor localized. We call them “diffusons.”

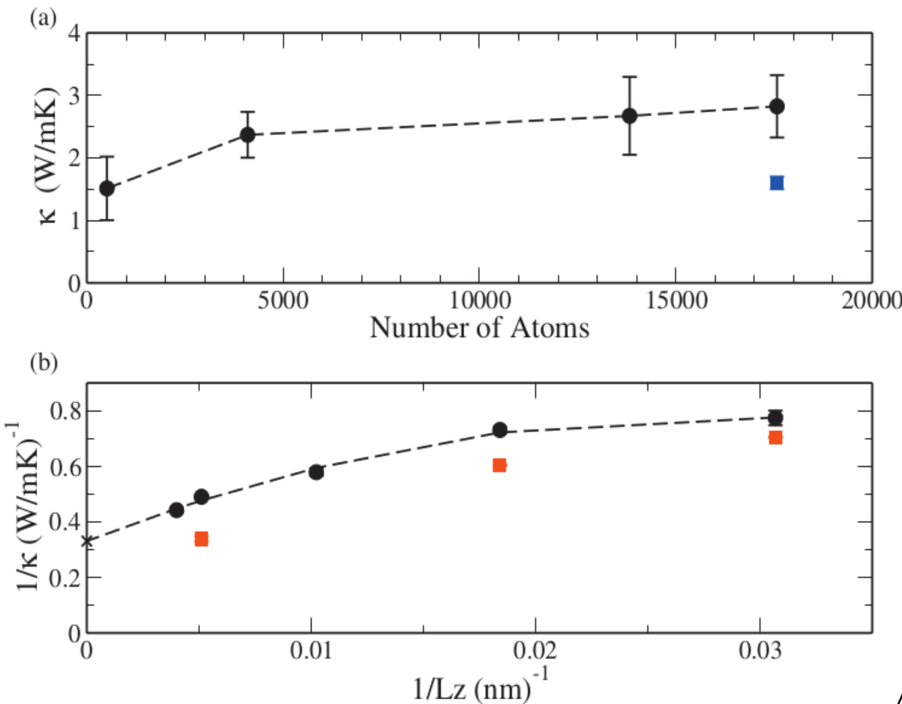
\cite{diffusons_allen_1999}

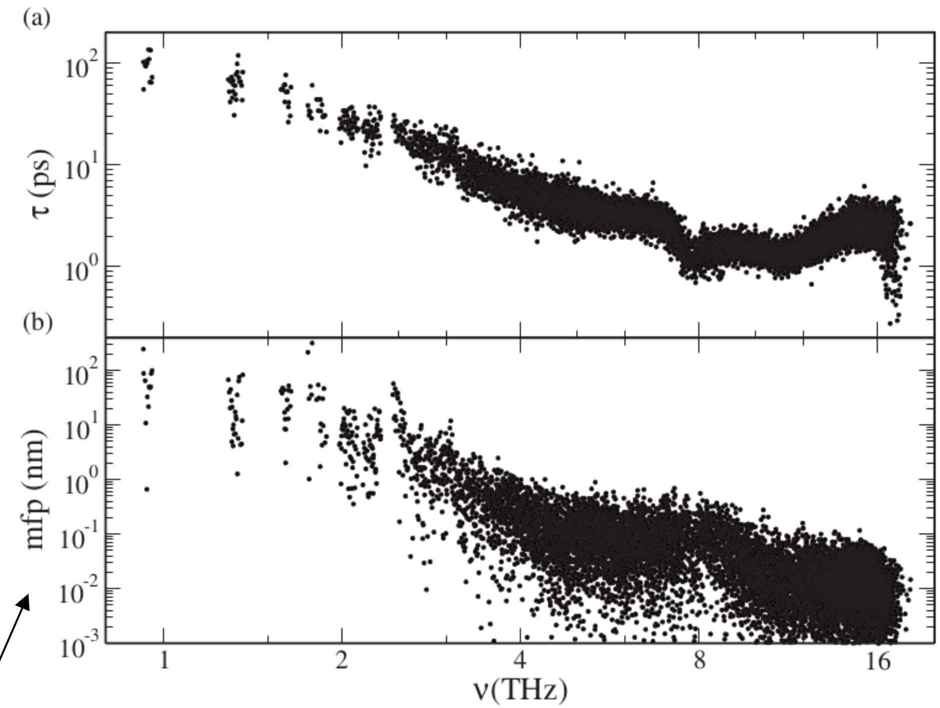


vibrons: extendons (propagons, diffusons); locons

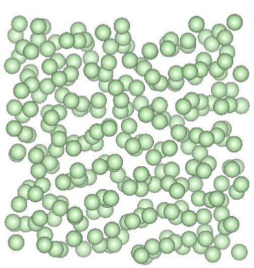
Mechanical Engineering

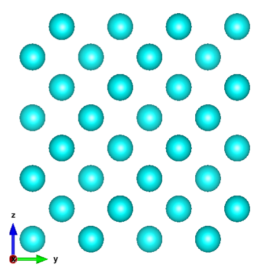
A-Si: Tersoff





MD-based: size of simulation cell=4.3 nm

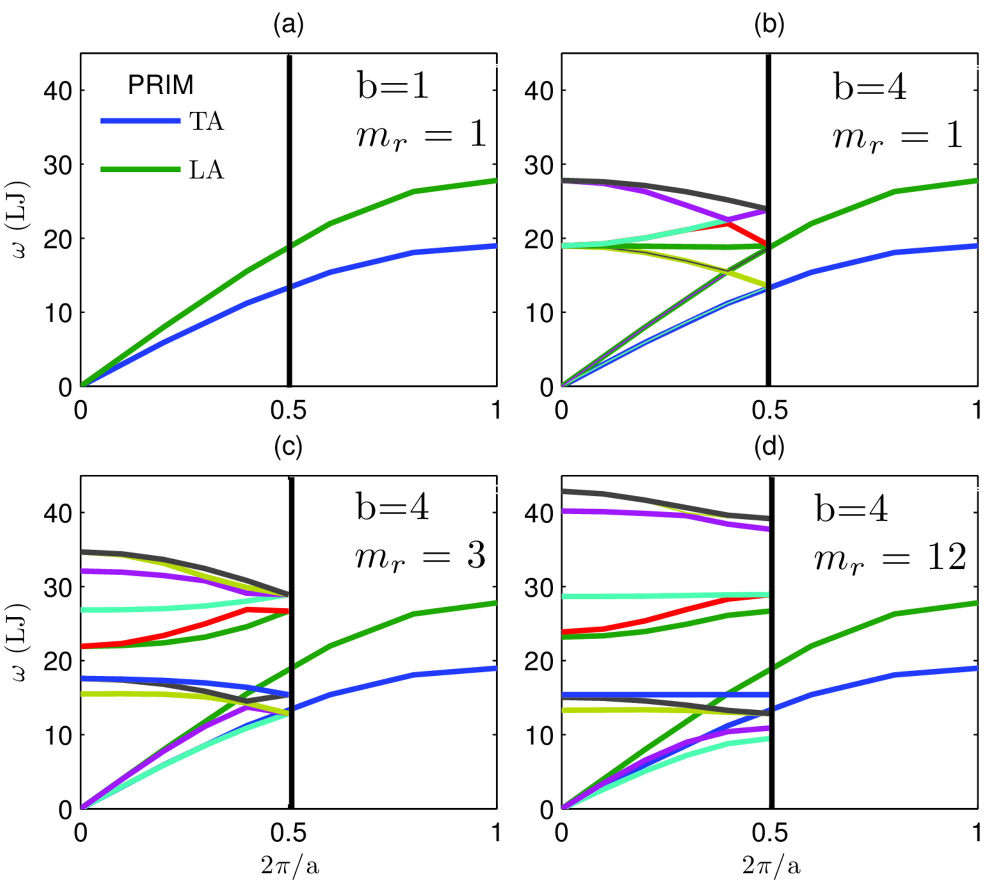




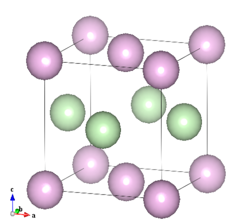
Appl. Phys. Lett. 98, 144101 (2011)

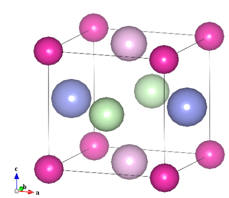
http://apl.aip.org/resource/1/applab/v98/i14/p144101_s1

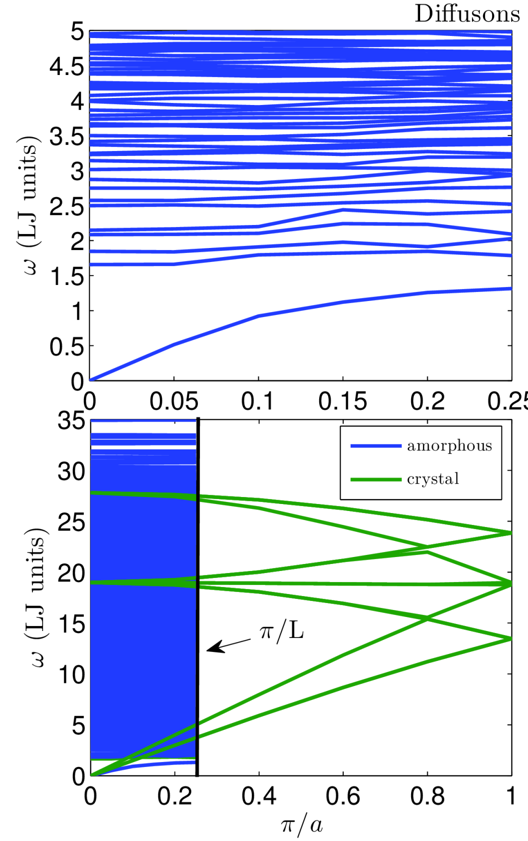
Mechanical Engineering



(a)
(b)
(c)
(d)
PRIM
TA
LA
b=1
$m_r = 1$
b=4
$m_r = 1$
b=4
$m_r = 3$
b=4
$m_r = 12$
ω (LJ)
$2\pi/a$







Diffusons
ω (LJ units)
amorphous
crystal
π/L
π/a