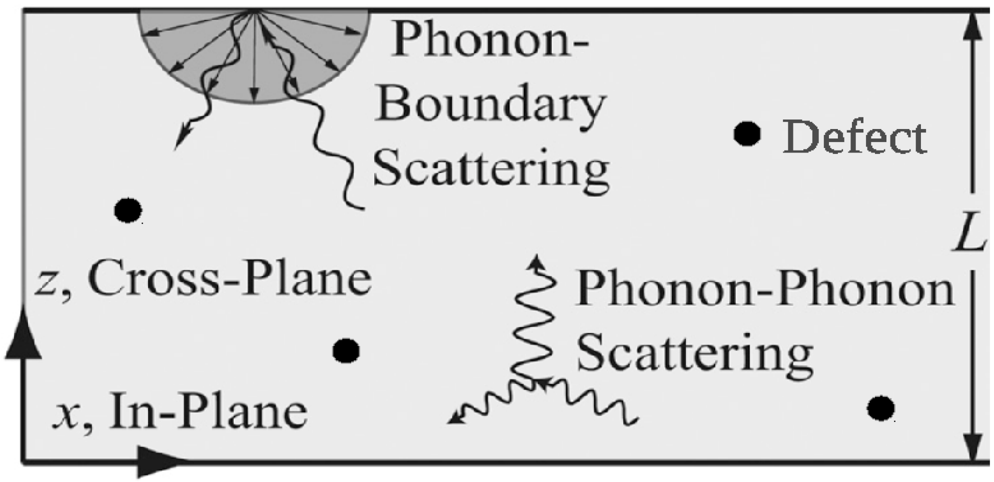
phonon scattering mechanisms

- Matthiessen rule:

$$\frac{1}{\tau} = \frac{1}{\tau_{p-p}} + \frac{1}{\tau_b} + \frac{1}{\tau_d}$$



ALD + Debye->

$$\tau_{p-p} = \frac{(6\pi^2)^{1/3}\bar{m}v_g v_p^2}{2V^{1/3}\omega^2\gamma^2 T}$$

$$\frac{1}{\tau_d} = \frac{V\omega^4}{4\pi v_p^2 v_g}\sum_i c_i(1 - m_i/\bar{m})^2$$

[1] P. G. Klemens, ed. R. P. Tye, 1969, Vol. 1, Academic Press, London.
[2] Alan J. H. McGaughey and Ankit Jain, Applied Physics Letters, 100(6):061911, 2012.
[3] P. G. Klemens, Proc. Phys. Soc., London, Sect. A, 1955, 68, 1113.
[4] David G. Cahill, Fumiya Watanabe, Angus Rockett, and Cronin B. Vining, Phys. Rev. B, 71:235202, Jun 2005.

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normal mode decomposition (nmd)

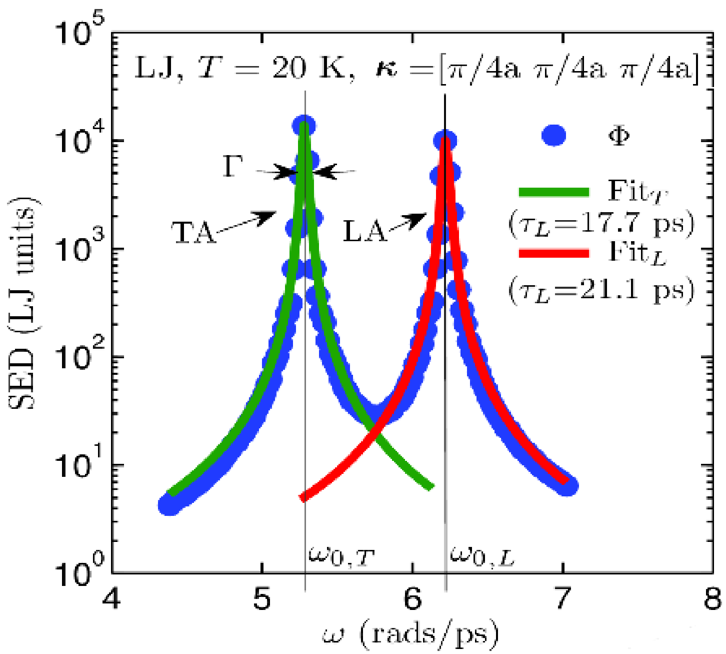
- Phonon Normal Mode Coordinate:

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

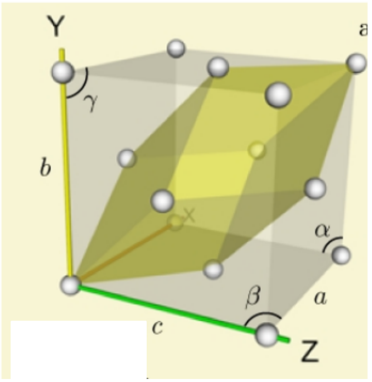
MD (anharmonic)

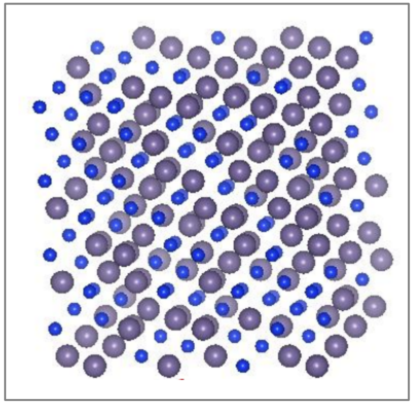
Lattice Dynamics (harmonic)

$$\Phi(\boldsymbol{\kappa},\omega) = \sum_{\nu}^{3n} C_0\left(\begin{smallmatrix}\boldsymbol{\kappa}\\ \nu\end{smallmatrix}\right) \frac{\Gamma\left(\begin{smallmatrix}\boldsymbol{\kappa}\\ \nu\end{smallmatrix}\right)/\pi}{\left[\omega_0\left(\begin{smallmatrix}\boldsymbol{\kappa}\\ \nu\end{smallmatrix}\right)-\omega\right]^2 + \Gamma^2\left(\begin{smallmatrix}\boldsymbol{\kappa}\\ \nu\end{smallmatrix}\right)} \qquad \tau\left(\begin{smallmatrix}\boldsymbol{\kappa}\\ \nu\end{smallmatrix}\right) = \frac{1}{2\Gamma\left(\begin{smallmatrix}\boldsymbol{\kappa}\\ \nu\end{smallmatrix}\right)}$$



vc vs gamma





Unit cell?

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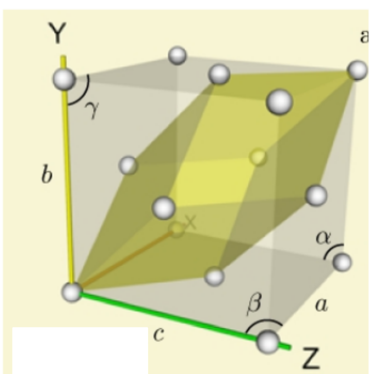
normal mode decomposition (NMD)

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

- Phonon Normal Mode Coordinate:

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

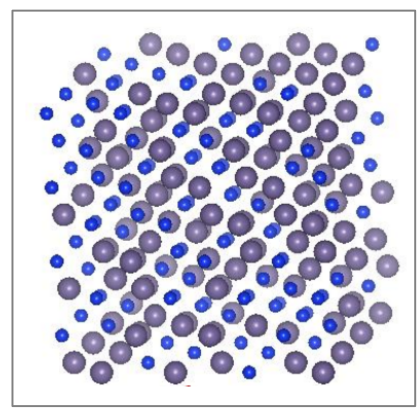
VC



$$\tau\left(\begin{smallmatrix}\boldsymbol{\kappa}\\ \nu\end{smallmatrix}\right)$$

vs

Gamma



$$\tau\left(\begin{smallmatrix}\boldsymbol{\kappa}=0\\ \omega\end{smallmatrix}\right)$$

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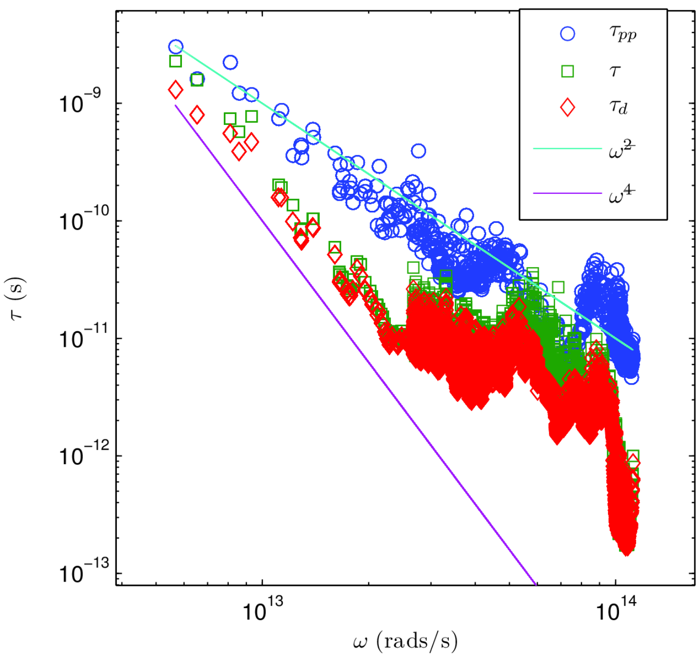
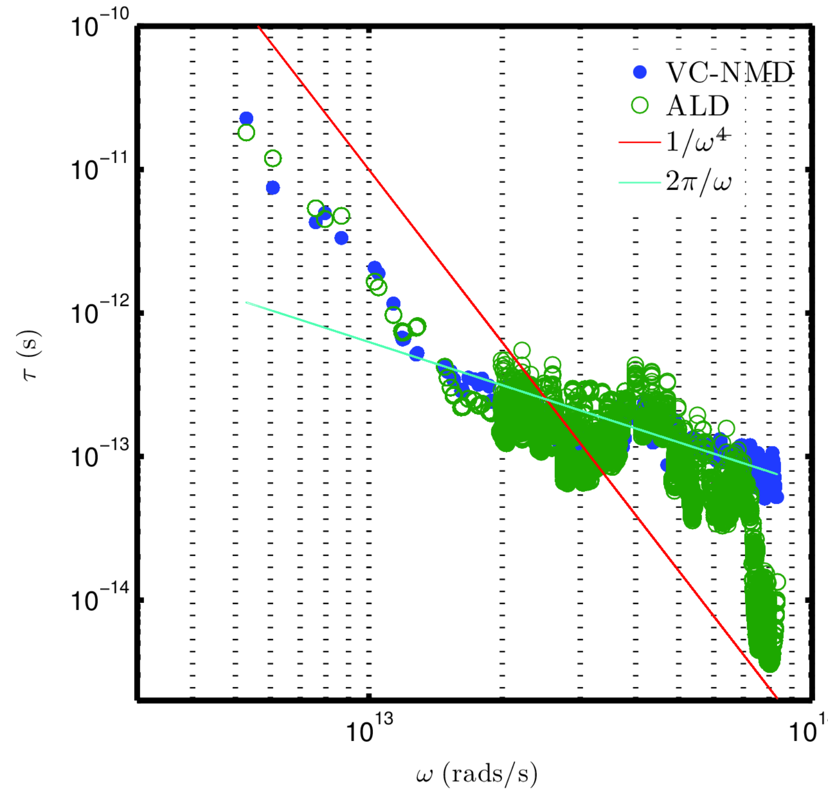
nmd vc vs ald lifetimes

SW:

- ALD+taud agrees with VC-NMD.





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phonon scattering mechanisms

- Matthiessen rule: $$\frac{1}{\tau} = \frac{1}{\tau_{p-p}} + \frac{1}{\tau_b} + \frac{1}{\tau_d}$$

- phonon-phonon scattering [1] (ald):

$$1/\tau_{p-p}\begin{pmatrix}\boldsymbol{\kappa}\\ \nu\end{pmatrix} = \frac{\pi\hbar}{16N}\sum_{\boldsymbol{\kappa}',\nu'}^{N,3n}\sum_{\boldsymbol{\kappa}'',\nu''}^{N,3n}\left|\Phi\begin{pmatrix}\boldsymbol{\kappa} & \boldsymbol{\kappa}' & \boldsymbol{\kappa}''\\ \nu & \nu' & \nu''\end{pmatrix}\right|^2\left\{\left[f\begin{pmatrix}\boldsymbol{\kappa}'\\ \nu'\end{pmatrix} + f\begin{pmatrix}\boldsymbol{\kappa}''\\ \nu''\end{pmatrix} + 1\right]\left[\delta\left(\omega\begin{pmatrix}\boldsymbol{\kappa}\\ \nu\end{pmatrix} - \omega\begin{pmatrix}\boldsymbol{\kappa}'\\ \nu'\end{pmatrix} - \omega\begin{pmatrix}\boldsymbol{\kappa}''\\ \nu''\end{pmatrix}\right)\right] + \left[f\begin{pmatrix}\boldsymbol{\kappa}'\\ \nu'\end{pmatrix} - f\begin{pmatrix}\boldsymbol{\kappa}''\\ \nu''\end{pmatrix}\right]\right.$$
$$\left.\times\left[\delta\left(\omega\begin{pmatrix}\boldsymbol{\kappa}\\ \nu\end{pmatrix} + \omega\begin{pmatrix}\boldsymbol{\kappa}'\\ \nu'\end{pmatrix} - \omega\begin{pmatrix}\boldsymbol{\kappa}''\\ \nu''\end{pmatrix}\right) - \delta\left(\omega\begin{pmatrix}\boldsymbol{\kappa}\\ \nu\end{pmatrix} - \omega\begin{pmatrix}\boldsymbol{\kappa}'\\ \nu'\end{pmatrix} + \omega\begin{pmatrix}\boldsymbol{\kappa}''\\ \nu''\end{pmatrix}\right)\right]\right\}. \quad (16)$$

- f(freq_hld,eigvec_hld,fc_3)
  freq_hld, eigvec_hld = easy
  fc_3 = hard

Debye-> $$\tau_{p-p} = \frac{(6\pi^2)^{1/3}\bar{m}v_g v_p^2}{2V^{1/3}\omega^2\gamma^2 T}$$

phonon scattering mechanisms

- Defect scattering [3]:

$$\frac{1}{\tau_d\binom{\boldsymbol{\kappa}}{\nu}} = \frac{\pi}{2N}\omega_{\mathbf{q}s}^2 \sum_{\mathbf{q}'s'} \delta(\omega_{\mathbf{q}s} - \omega_{\mathbf{q}'s'}) \sum_b g(b) |e^*_{\mathbf{q}'s'}(b) \cdot e_{\mathbf{q}s}(b)|^2$$

$$g(b) = \sum_i c_i(b)(1 - m_i(b)/\bar{m}(b))^2$$

- f(freq_hld,eigvec_hld)
  freq_hld, eigvec_hld = easy

Debye-> $$\frac{1}{\tau_d} = \frac{V\omega^4}{4\pi v_p^2 v_g} \sum_i c_i(1 - m_i/\bar{m})^2$$

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Diffuson Theory

- Allen Feldman theory of diffusons [1]:

$$k_{AF} = \sum_i C(\omega_i) D_{AF}(\omega_i)$$

$$D_{AF}(\omega_i) = \frac{\pi V^2}{3\hbar^2\omega_i^2} \sum_j^{\neq i} |S_{ij}|^2 \delta(\omega_i - \omega_j)$$

- Conservation of energy:

$$\delta(\omega_i - \omega_j)$$

- Heat current operator:

$$|S_{ij}|^2$$

- Ingredients: **harmonic** Lattice Dynamics

[1] Philip B. Allen and Joseph L. Feldman. Thermal conductivity of disordered harmonic solids. Physical Review B, 48(17):12581–12588, Nov 1993.

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