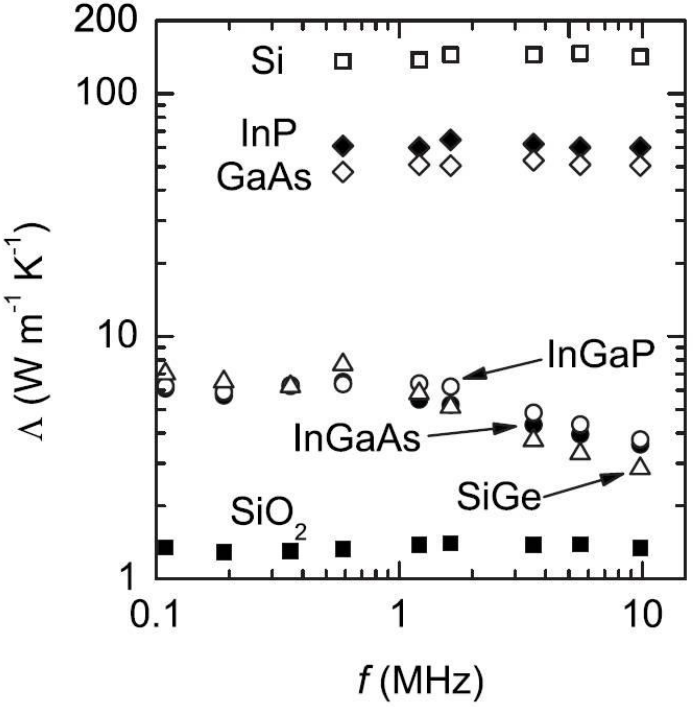
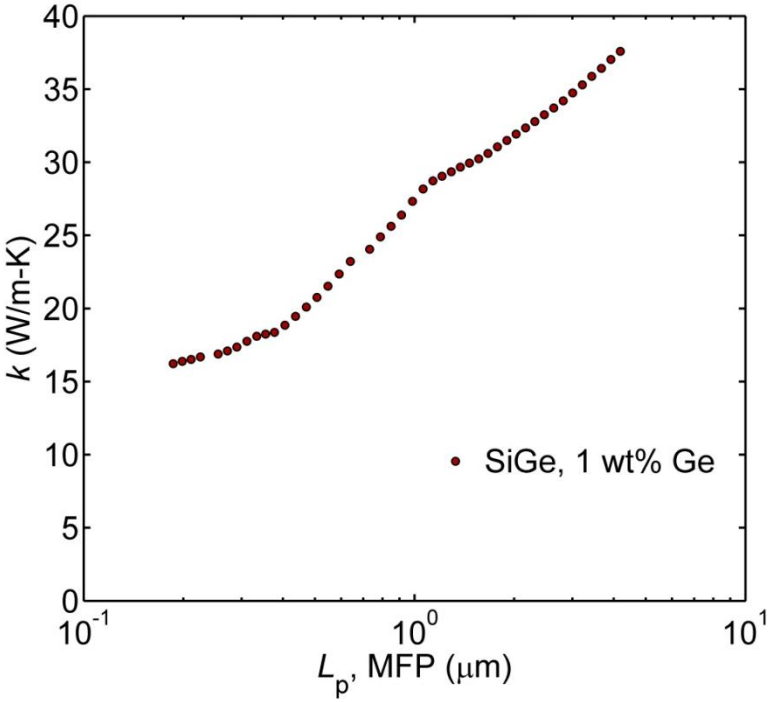
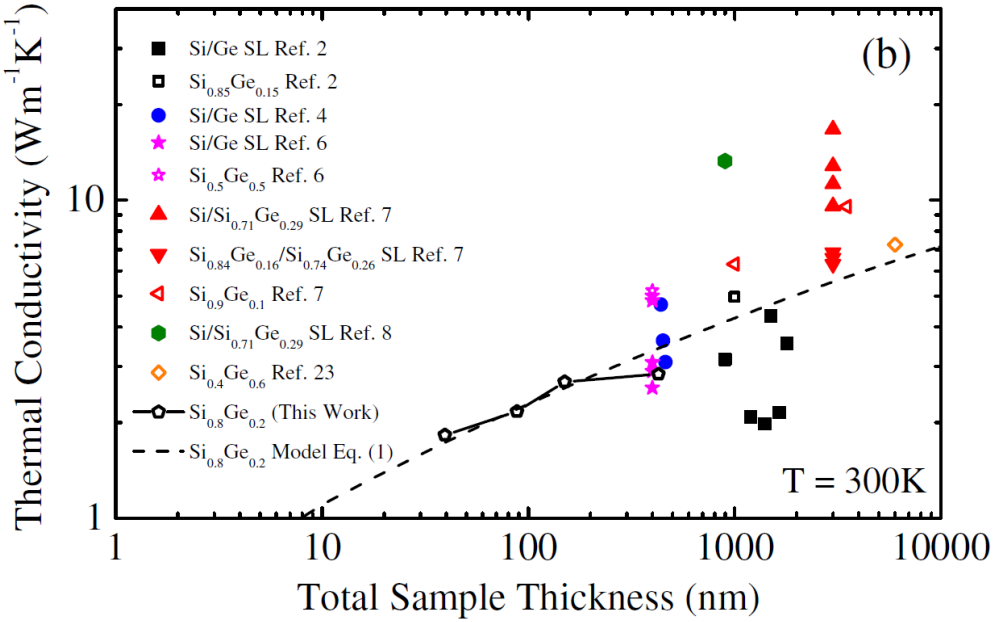
Evidence for propagating modes in alloys and amorphous solids

Discussion with Jason and Keith
February 8, 2013

SiGe measurements



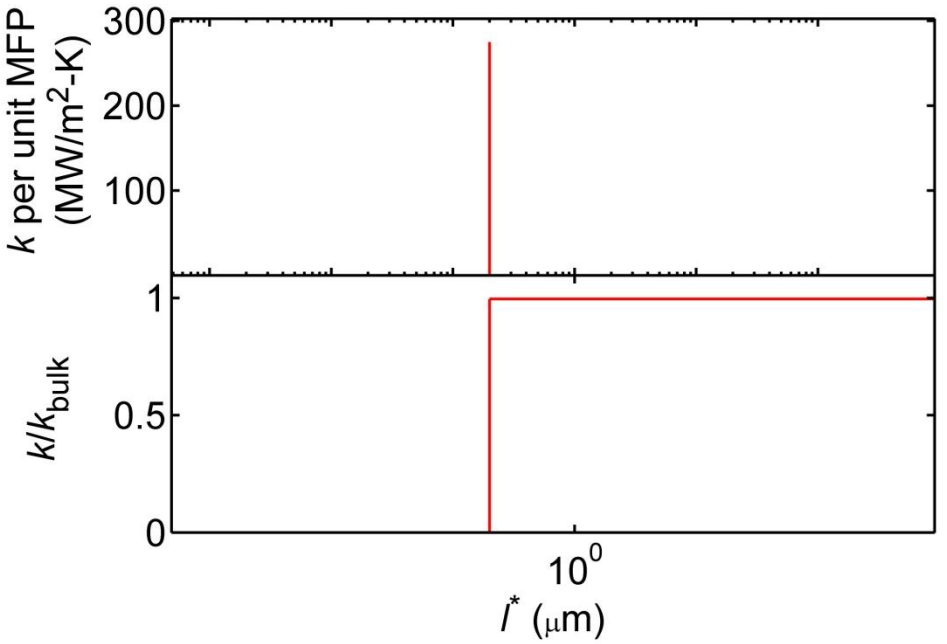




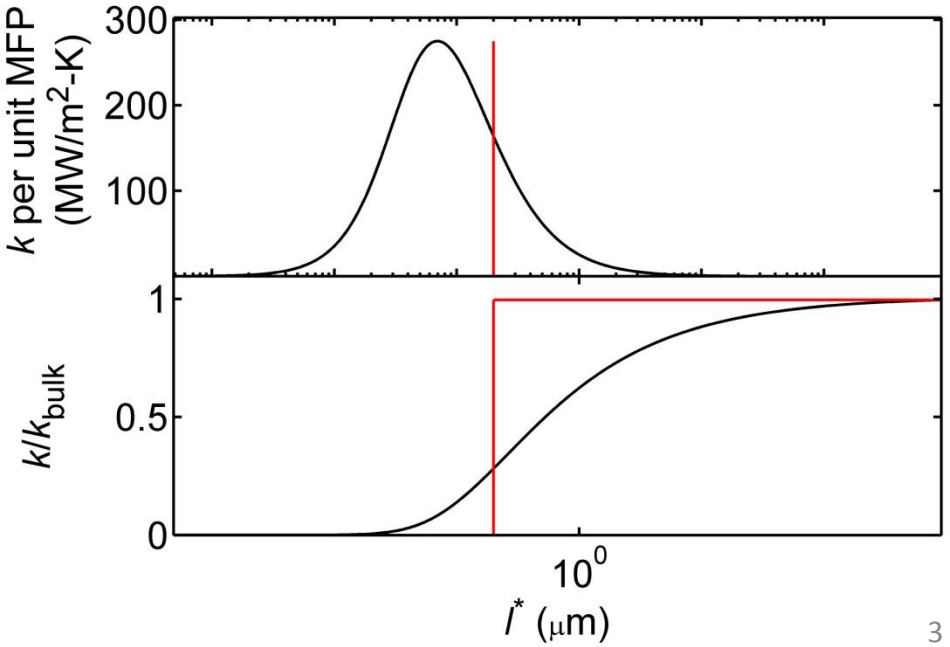
Koh and Cahill, PRB 2007
Cheaito et al., PRL 2012

accumulation function

$$l_{\text{bulk, Si}} = \frac{3k}{\int Cv\,\mathrm{d}\omega} = 225\ \text{nm}$$

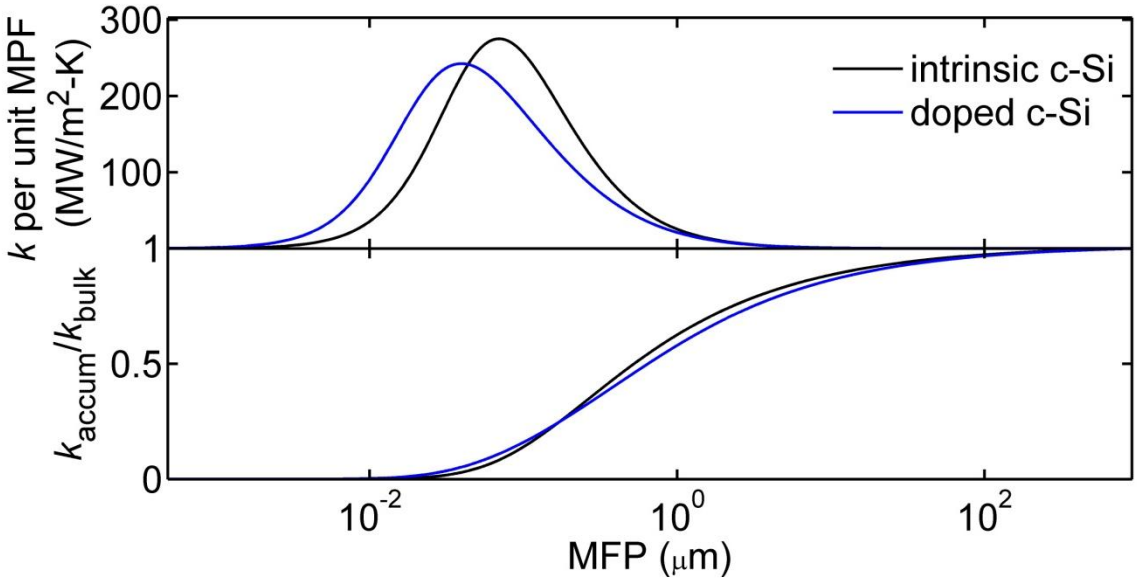


Distribution from the ω dependence of phonon scattering



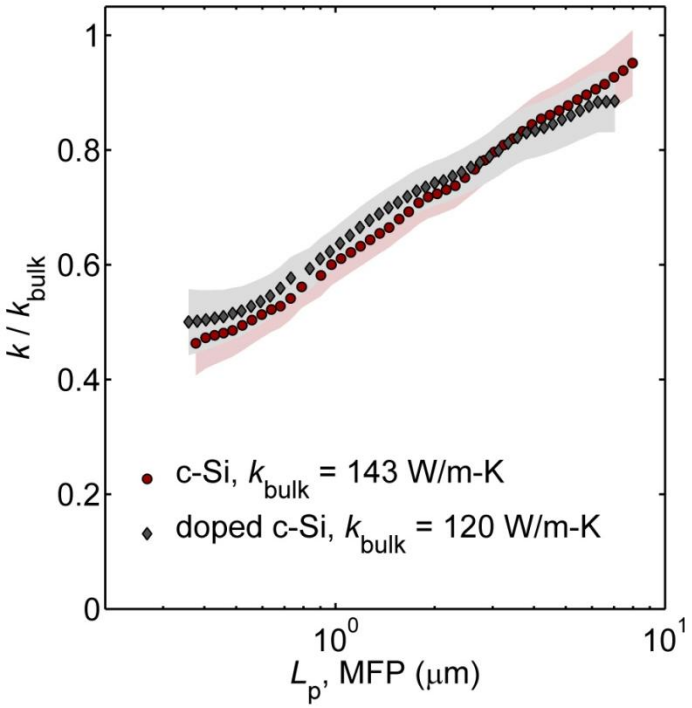
Torberer et al., Annu. Rev. Mater. Res. 2012

intrinsic vs. doped Si



We would expect that impurity scattering should reduce MFPs

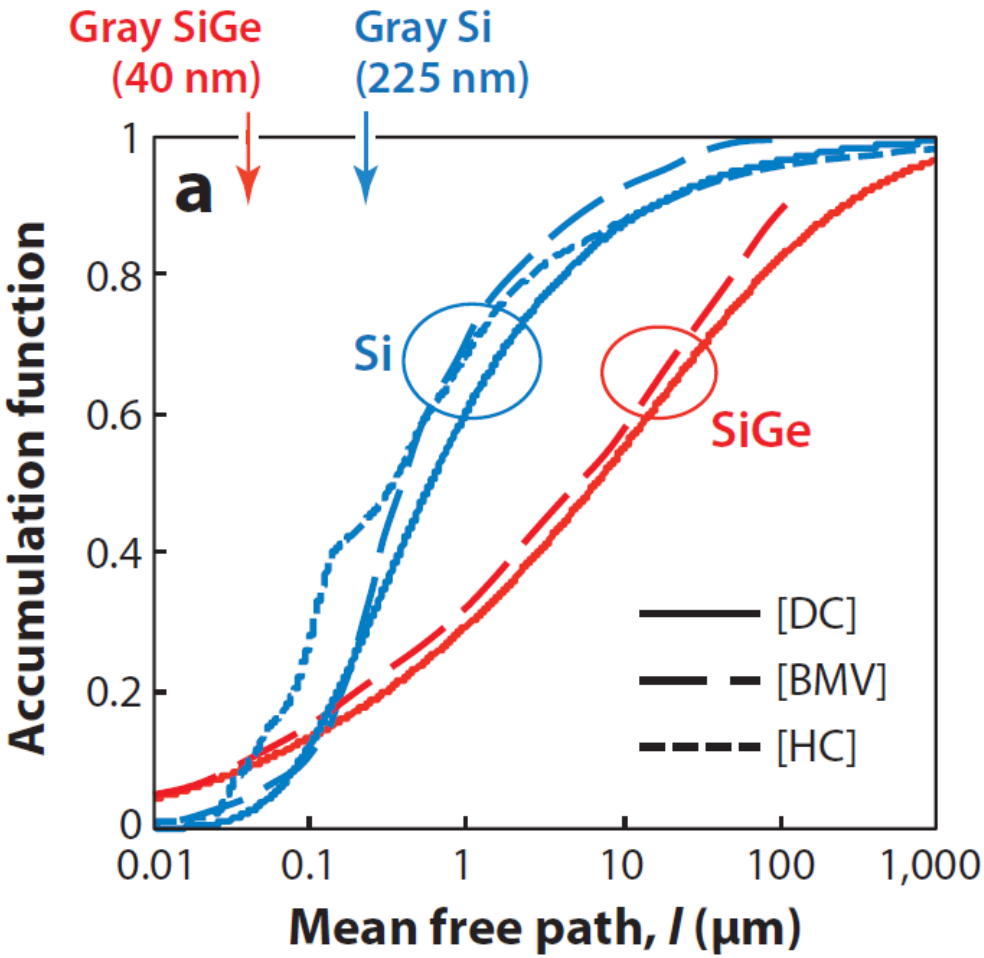
MFP spectrum in doped Si is broader than that of crystalline Si???



SiGe alloy

$$l_{\text{bulk, Si}} = \frac{3k}{\int Cv\,\mathrm{d}\omega} = 225\ \text{nm}$$

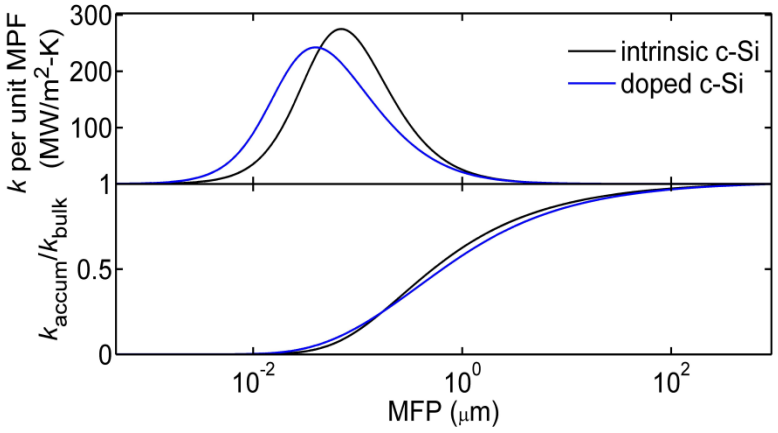
$$l_{\text{bulk,SiGe}} = \frac{3k}{\int Cv\,\mathrm{d}\omega} = 40\ \text{nm}$$

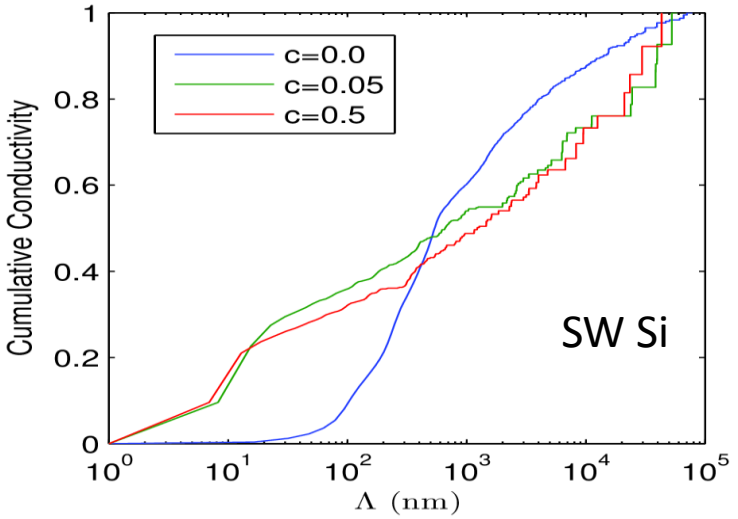


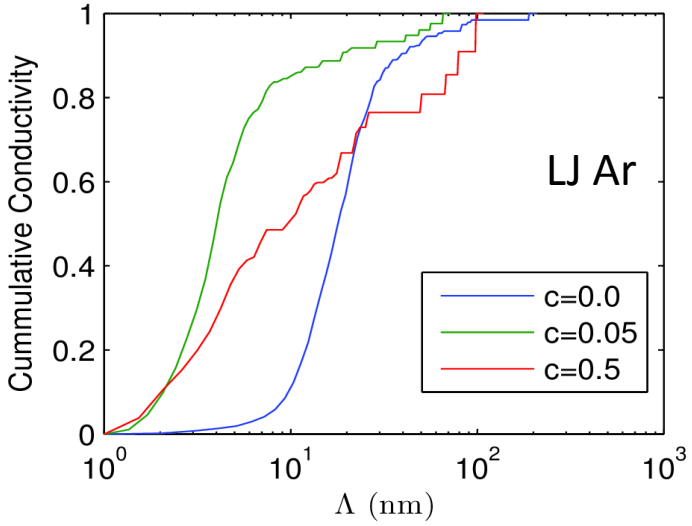
Defects strongly suppress short λ phonons (high ω), the phonons remaining to contribute to *k* are now biased towards longer λ (lower ω), which skews the distribution towards longer MFP phonons

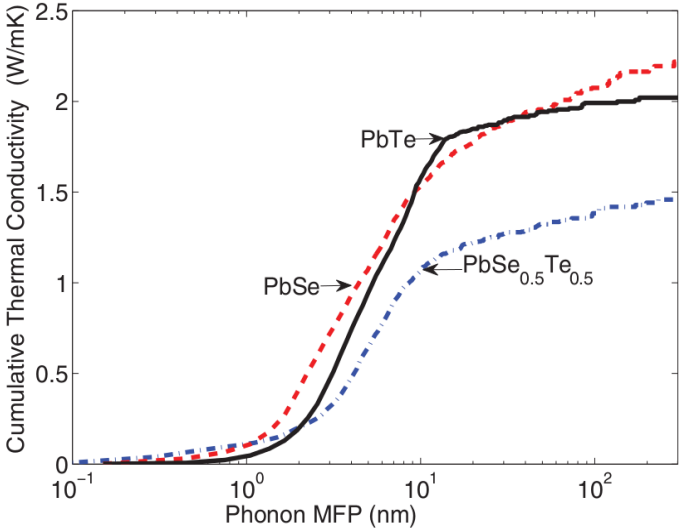
Torberer et al., Annu. Rev. Mater. Res. 2012

conductivity accumulation



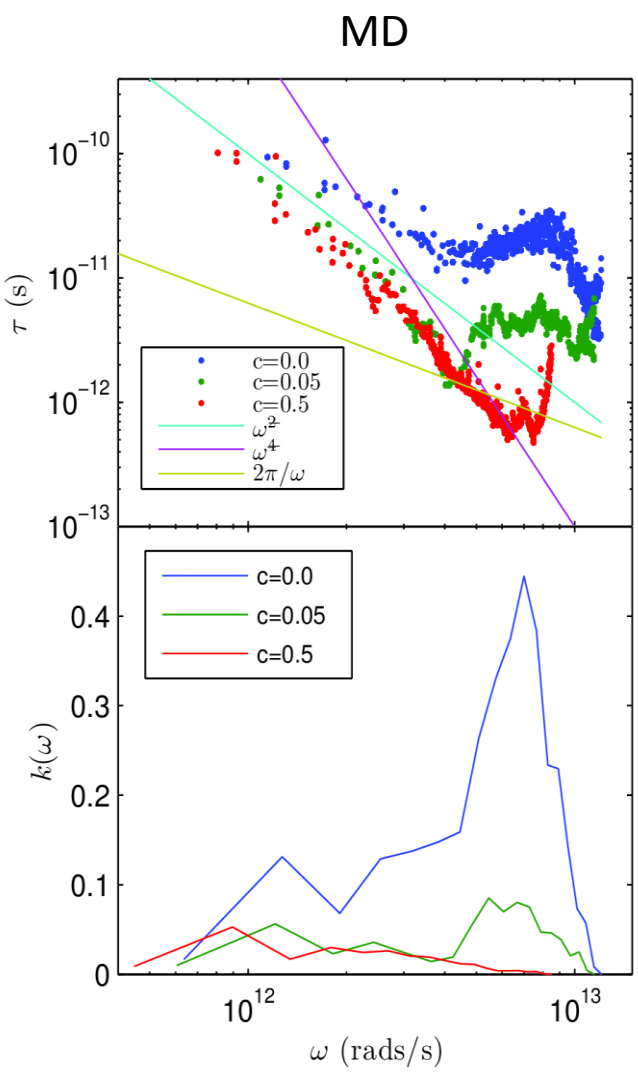


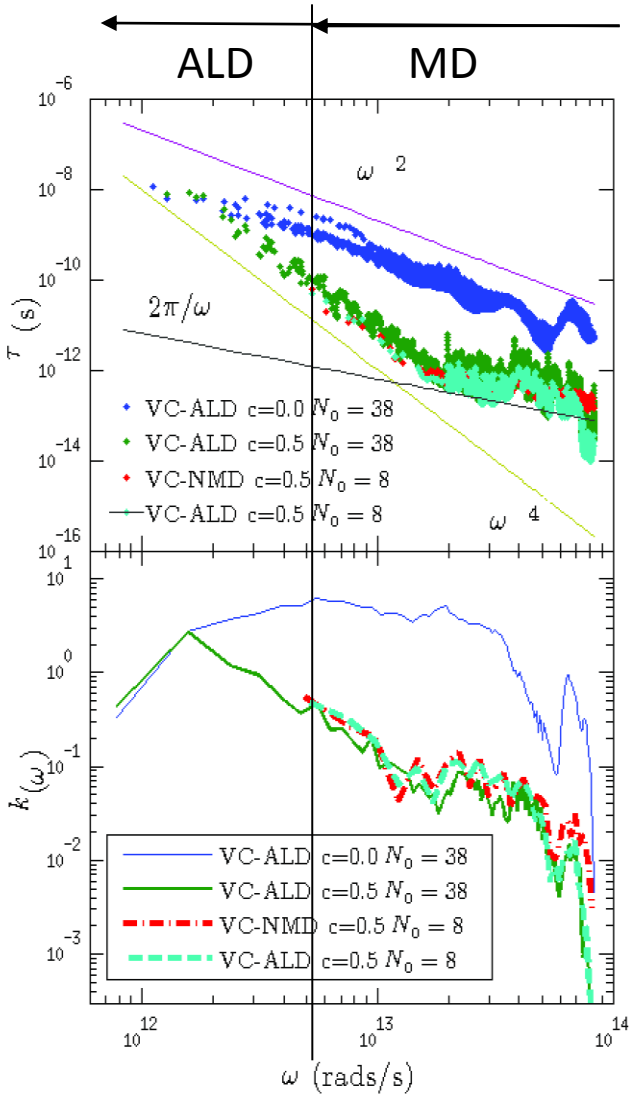




PRB 85, 184303 (2012)

Phonon spectrum: LJ Ar vs. SW Si





MD-based:

1E4 modes

(7 days)*(100 cpu)

ALD:

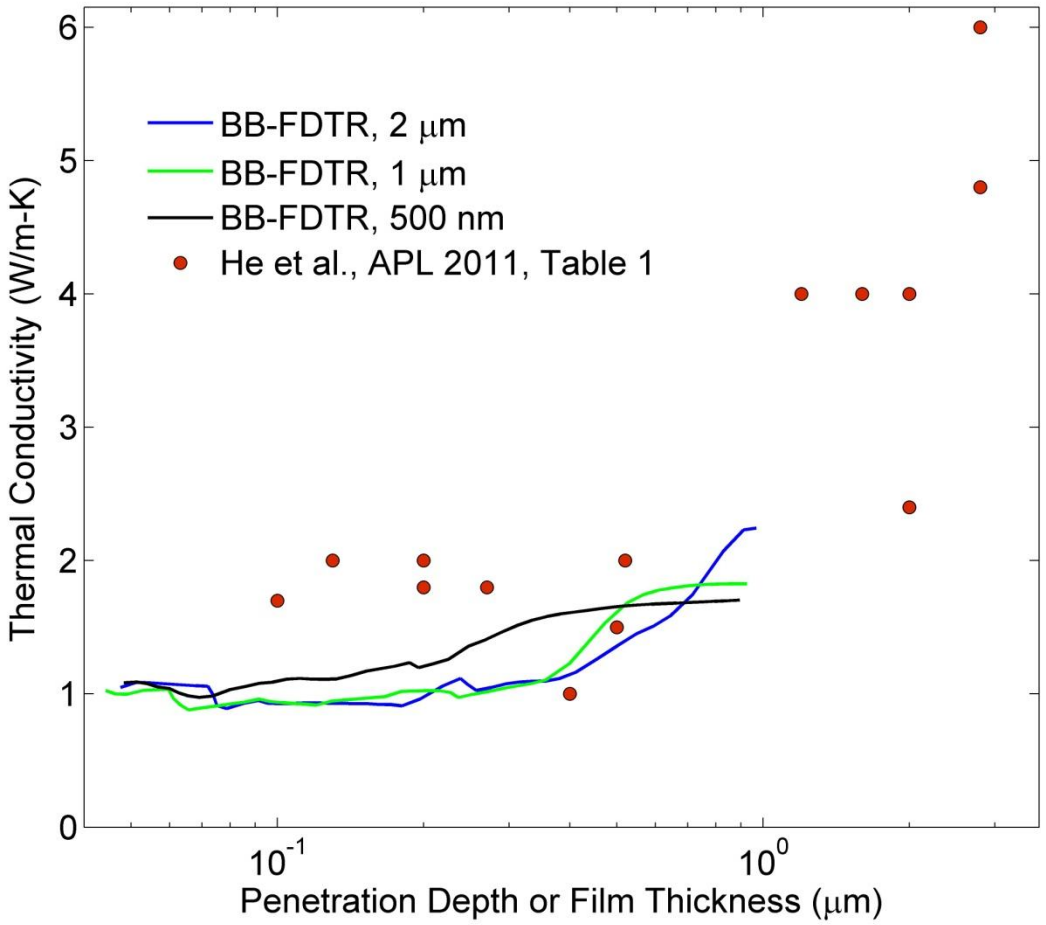
1E6 modes

(7 days)*(12 cpu)

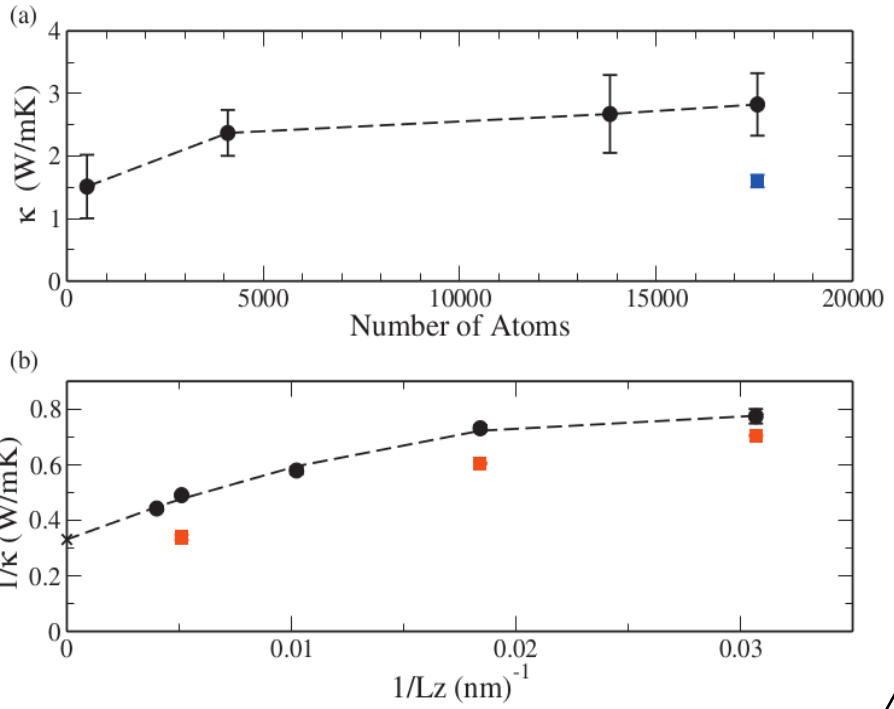
amorphous Si measurements

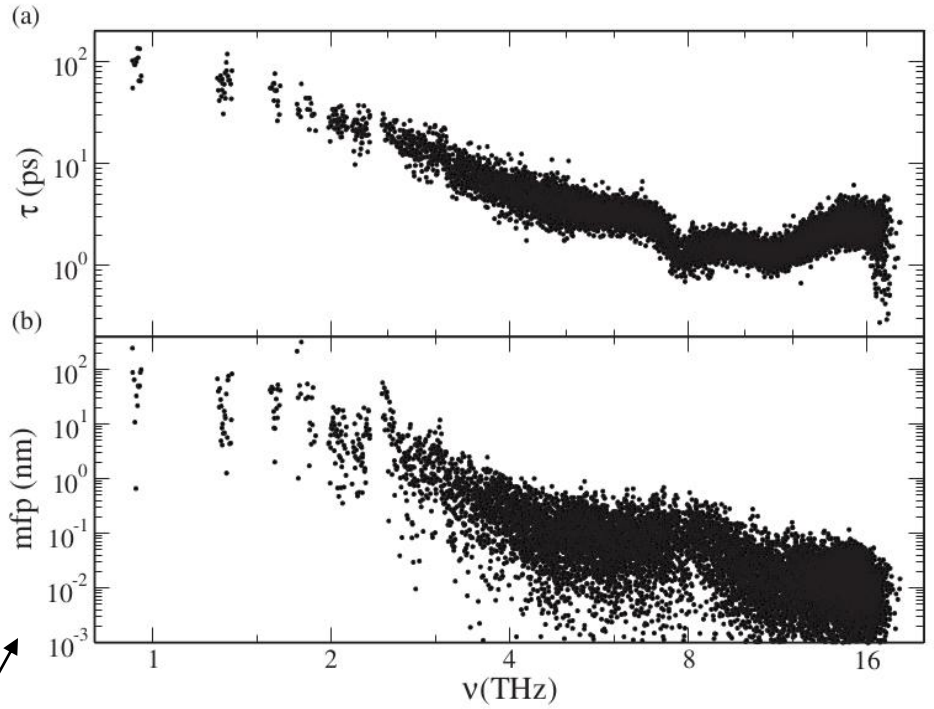
Is there some inherent lower limit on the MFP that is greater than zero?

Does it even make sense to talk about MFP within this plateau?

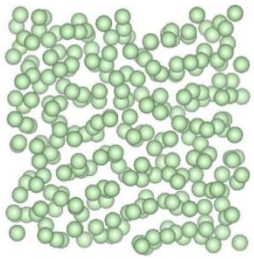


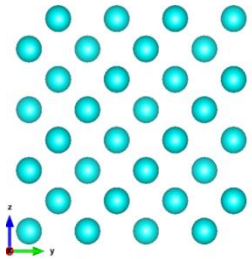
MFP in a-Si from Tersoff and MD





MD-based: size of simulation cell=4.3 nm





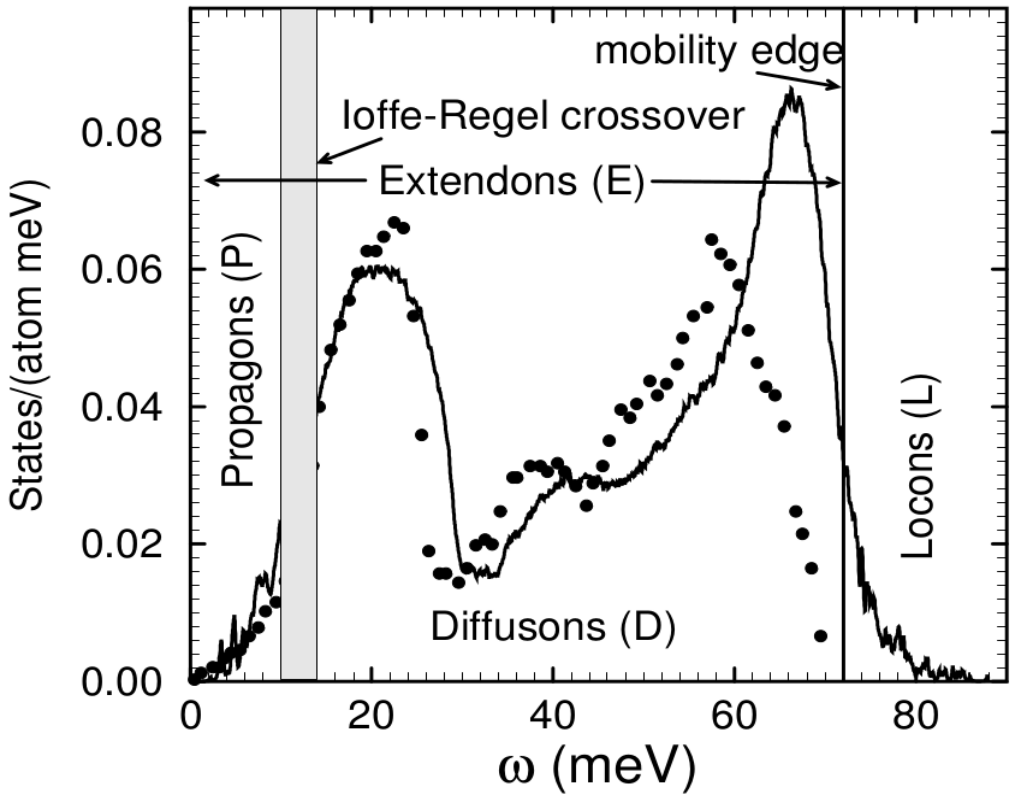
APL 98, 144101 (2011)

propagons, locons, diffusons

Numerical studies of amorphous silicon show that the lowest 4% of, vibrational modes are plane-wave like, “propagons”

the highest 3% of modes are localized, “locons”

The rest are neither plane-wave like nor localized, “diffusons”



vibrons { extendons { propagons, diffusons; locons }

Allen, PRB 1993

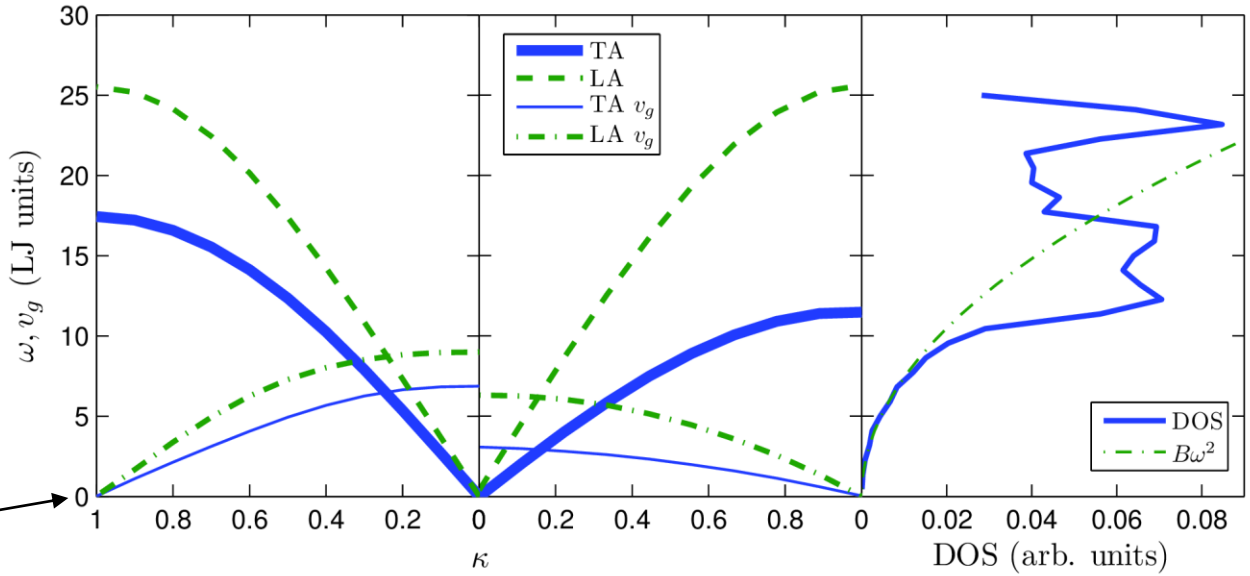
ordered and disordered

$$k_{ph,\mathbf{n}} = \sum_{\boldsymbol{\kappa}} \sum_{\nu} \frac{k_B}{V} \boldsymbol{v}^2_{g,\mathbf{n}}\left(\begin{smallmatrix}\boldsymbol{\kappa}\\ \nu\end{smallmatrix}\right) \tau\left(\begin{smallmatrix}\boldsymbol{\kappa}\\ \nu\end{smallmatrix}\right) \qquad v_{g,\mathbf{n}}\left(\begin{smallmatrix}\boldsymbol{\kappa}\\ \nu\end{smallmatrix}\right) = \partial\omega\left(\begin{smallmatrix}\boldsymbol{\kappa}\\ \nu\end{smallmatrix}\right) / \partial\boldsymbol{\kappa}$$

$$D_{ph}\left(\begin{smallmatrix}\boldsymbol{\kappa}\\ \nu\end{smallmatrix}\right) = \boldsymbol{v}^2_g\left(\begin{smallmatrix}\boldsymbol{\kappa}\\ \nu\end{smallmatrix}\right) \tau\left(\begin{smallmatrix}\boldsymbol{\kappa}\\ \nu\end{smallmatrix}\right)$$

$$\Lambda\left(\begin{smallmatrix}\boldsymbol{\kappa}\\ \nu\end{smallmatrix}\right) = \left|\boldsymbol{v}_g\right| \tau\left(\begin{smallmatrix}\boldsymbol{\kappa}\\ \nu\end{smallmatrix}\right)$$

$$D_{ph}\left(\begin{smallmatrix}\boldsymbol{\kappa}\\ \nu\end{smallmatrix}\right) \approx 0$$



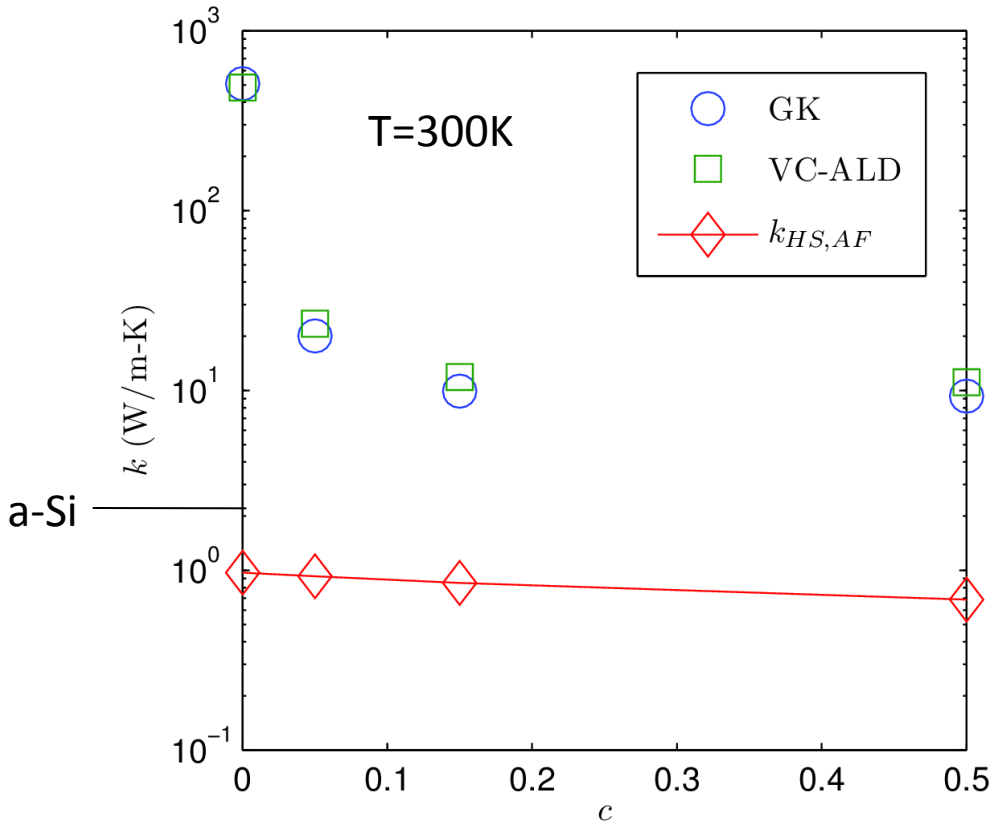
In a disordered material, it is not possible (in general) to specify v_g and τ independently

$$k_{AF} = \sum_{modes} \frac{k_B}{V} D_{AF}\left(\omega\left(\begin{smallmatrix}\boldsymbol{\kappa}=\mathbf{0}\\ \nu\end{smallmatrix}\right)\right)$$

PRB 59, 3551–3559 (1999)

high-scatter limit: SW Si

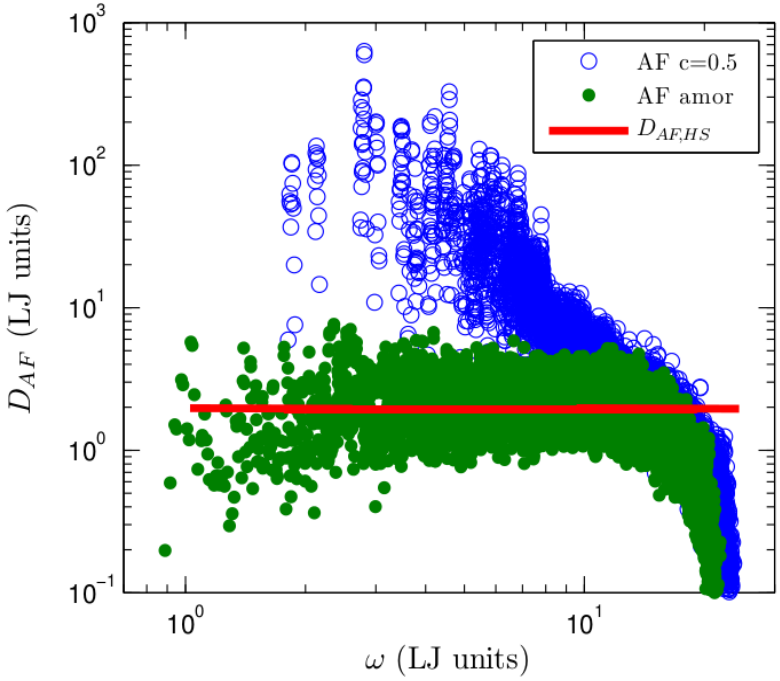
$$k_{AF,HS} = \frac{k_B}{V_b} b v_s a$$



high-scatter limit: LJ Ar

$$k_{AF} = \sum_{modes} \frac{k_B}{V} D_{AF}(\omega(\kappa=0_{\nu}))$$

$$k_{AF,HS} = \frac{k_B}{V_b} b v_s a$$



a-Ar