

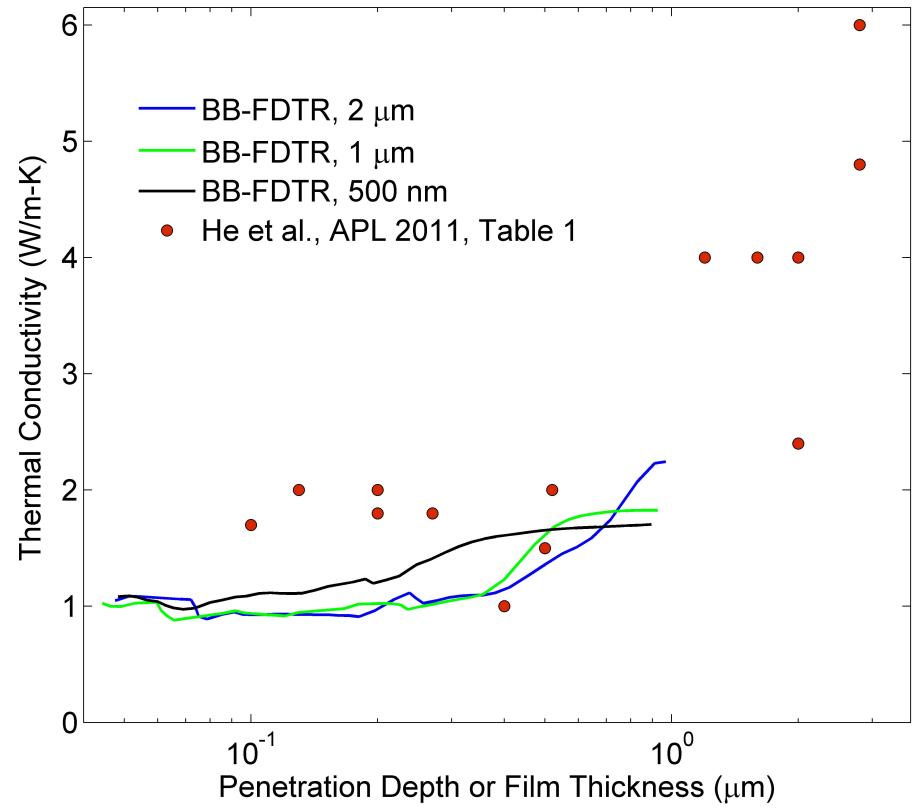
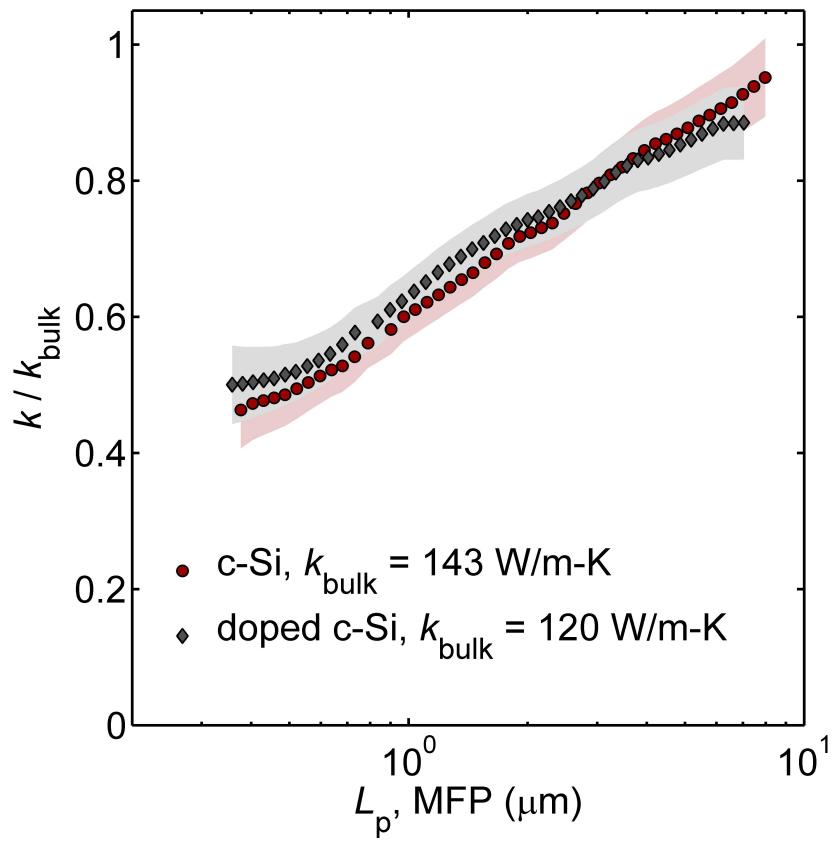
# Predicting Mean Free Paths in Disordered Systems

**Lin Hu, Scott N. Schiffres,  
Jonathan A. Malen, and Alan J. H. McGaughey**

Department of Mechanical Engineering  
Carnegie Mellon University

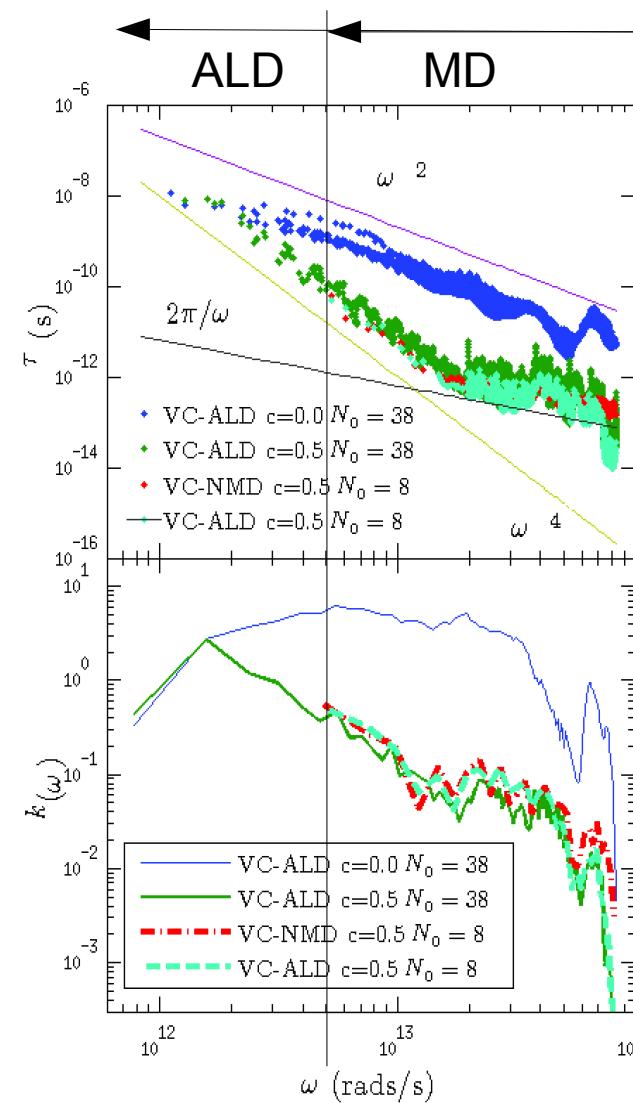
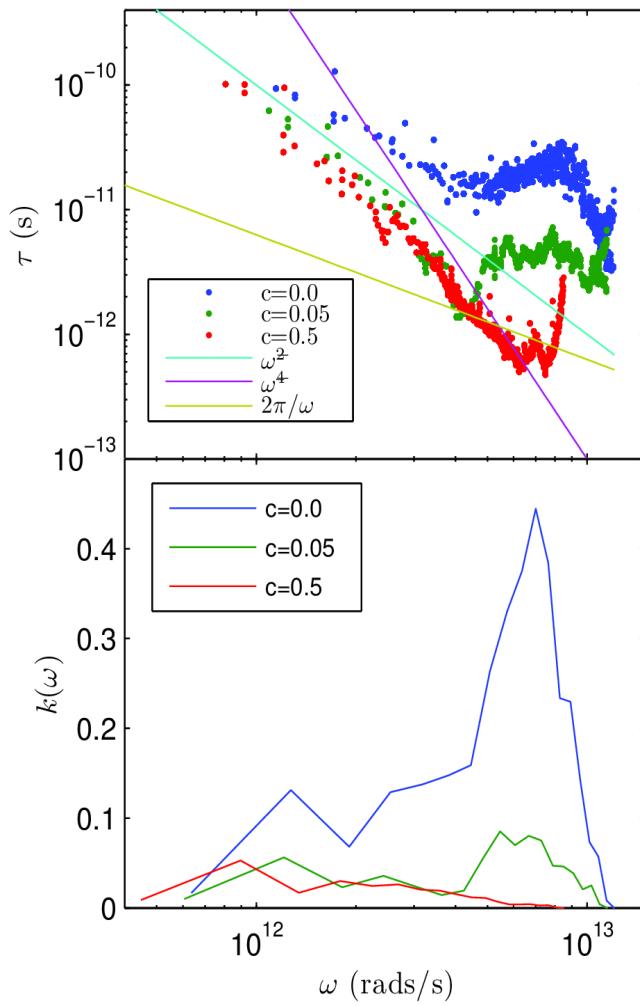
February, 20<sup>th</sup> 2012

# Background & Motivation



# Phonon Spectrum: LJ Ar vs SW Si

MD



MD-based:

1E4 modes

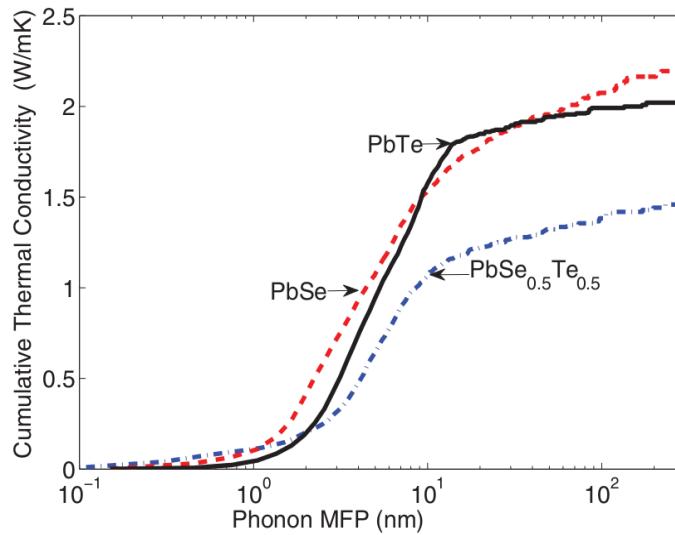
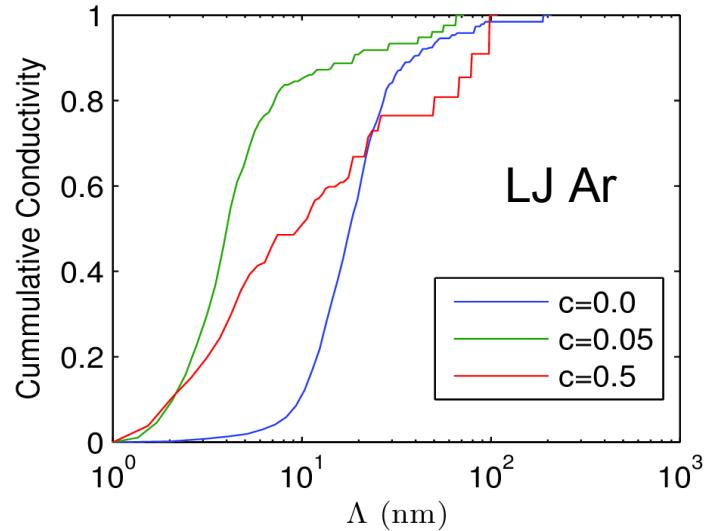
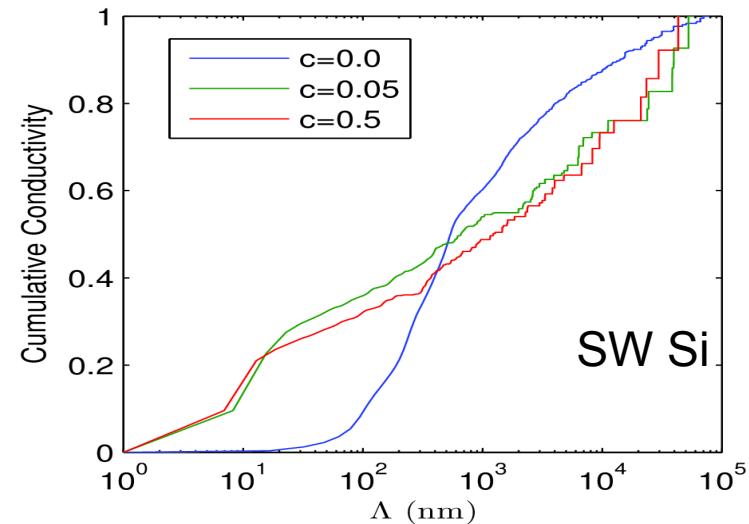
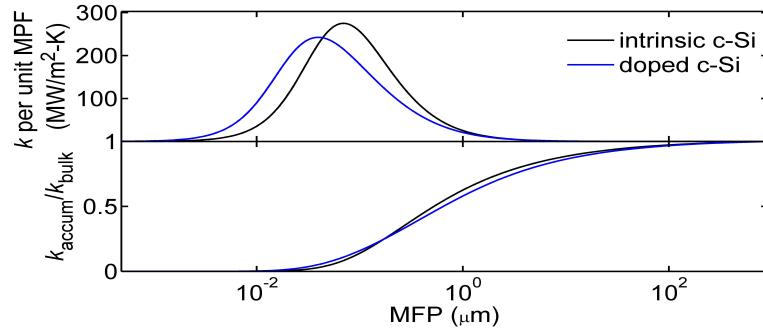
(7 days)\*(100 cpu)

ALD:

1E6 modes

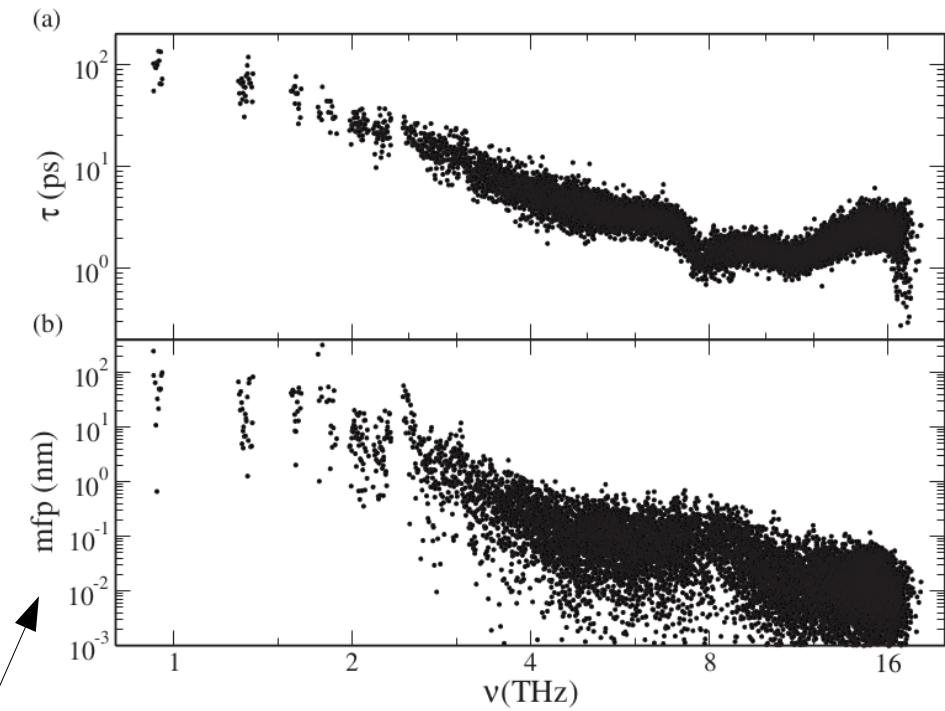
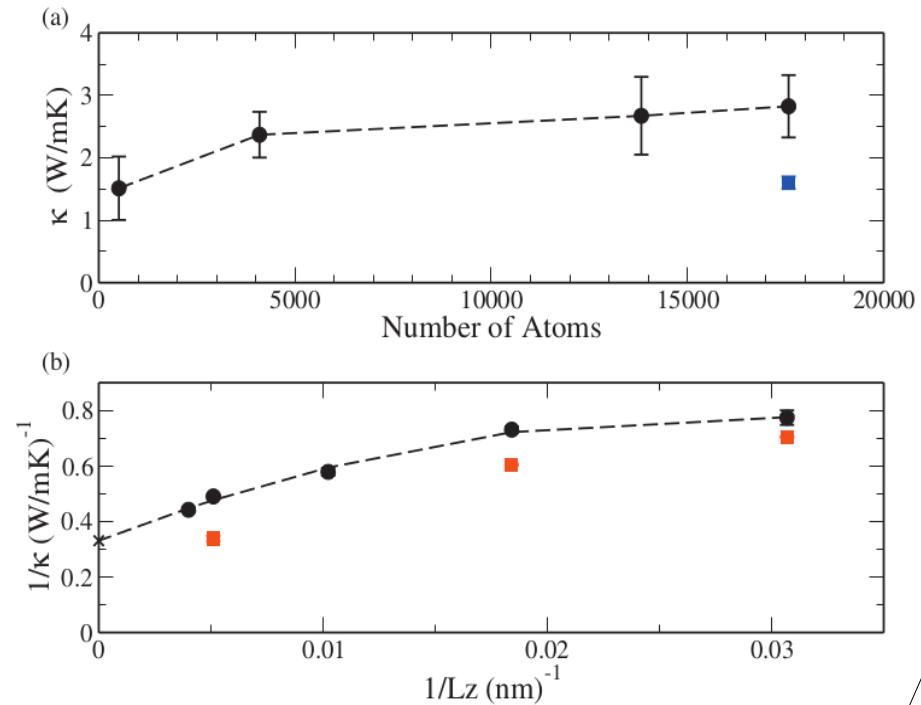
(7 days)\*(12 cpu)

# Conductivity Accumulation

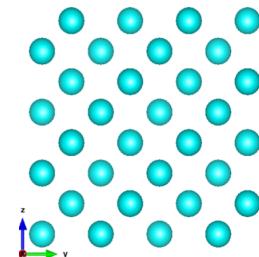
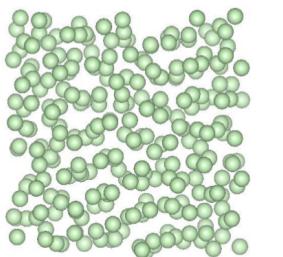


PHYSICAL REVIEW B 85, 184303 (2012)

# MFP in a-Si: from Tersoff and MD



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

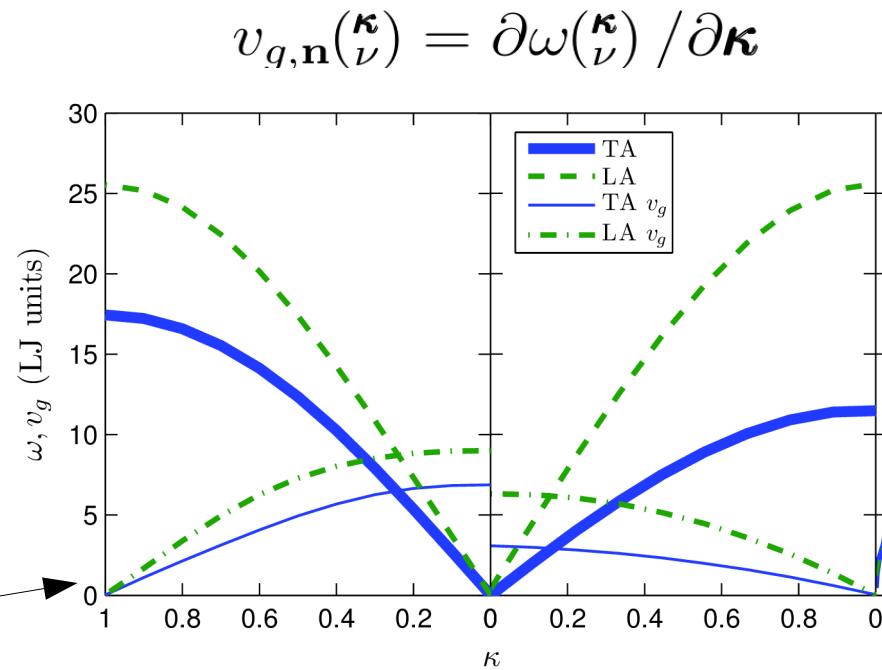
# Thermal Transport: Ordered and Disordered

$$k_{ph,\mathbf{n}} = \sum_{\boldsymbol{\kappa}} \sum_{\nu} \frac{k_B}{V} \mathbf{v}_{g,\mathbf{n}}^2(\boldsymbol{\kappa}) \tau(\boldsymbol{\kappa})$$

$$D_{ph}(\boldsymbol{\kappa}) = \mathbf{v}_g^2(\boldsymbol{\kappa}) \tau(\boldsymbol{\kappa})$$

$$\Lambda(\boldsymbol{\kappa}) = |\mathbf{v}_g| \tau(\boldsymbol{\kappa})$$

$$D_{ph}(\boldsymbol{\kappa}) \approx 0$$



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

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

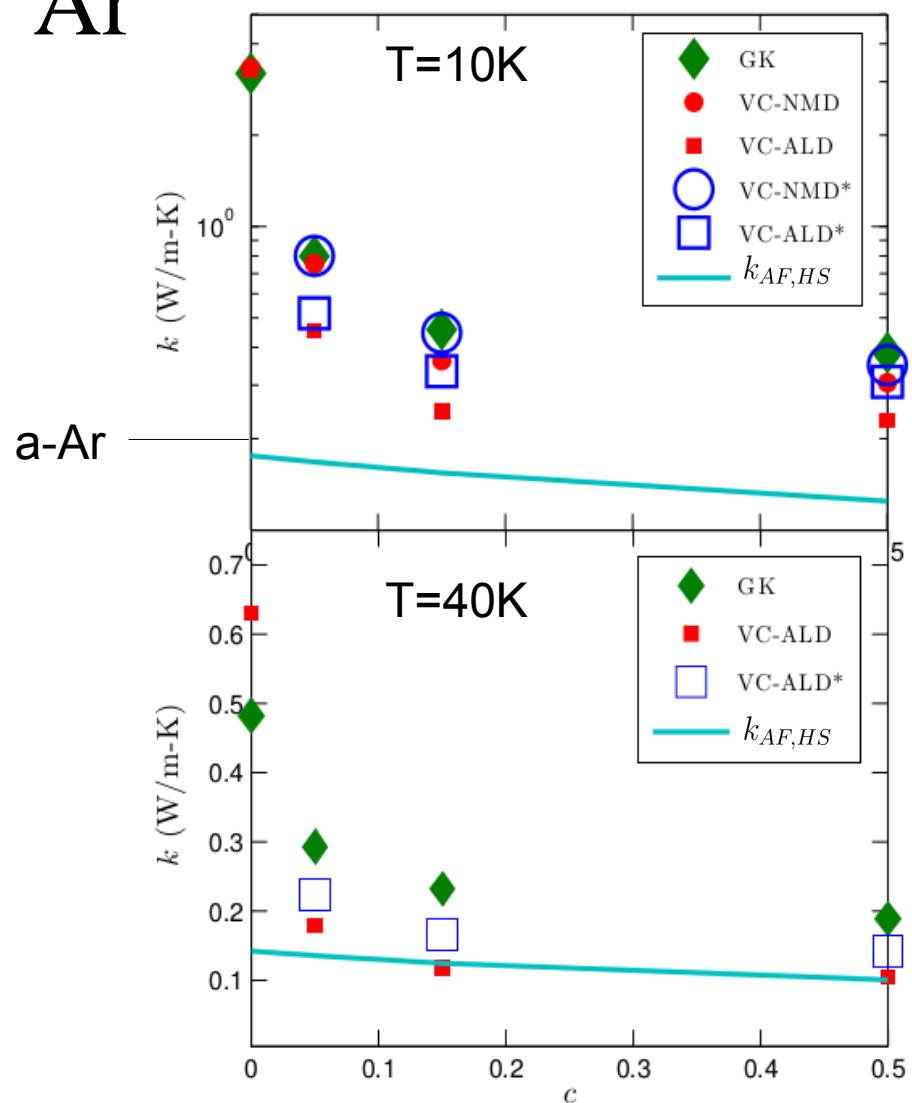
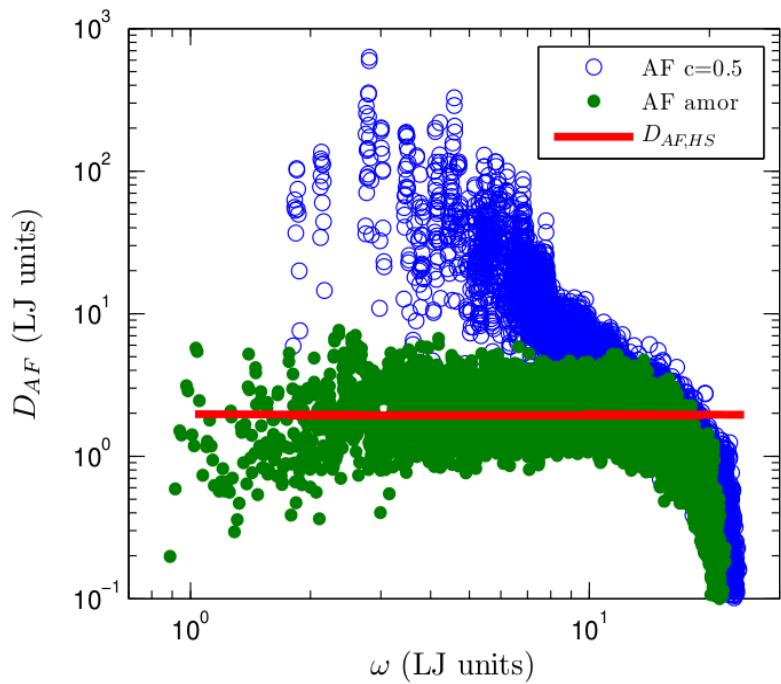
Phys. Rev. B 59, 3551–3559 (1999)

[http://prb.aps.org/abstract/PRB/v59/i5/p3551\\_1](http://prb.aps.org/abstract/PRB/v59/i5/p3551_1)

# High-Scatter Limit: LJ Ar

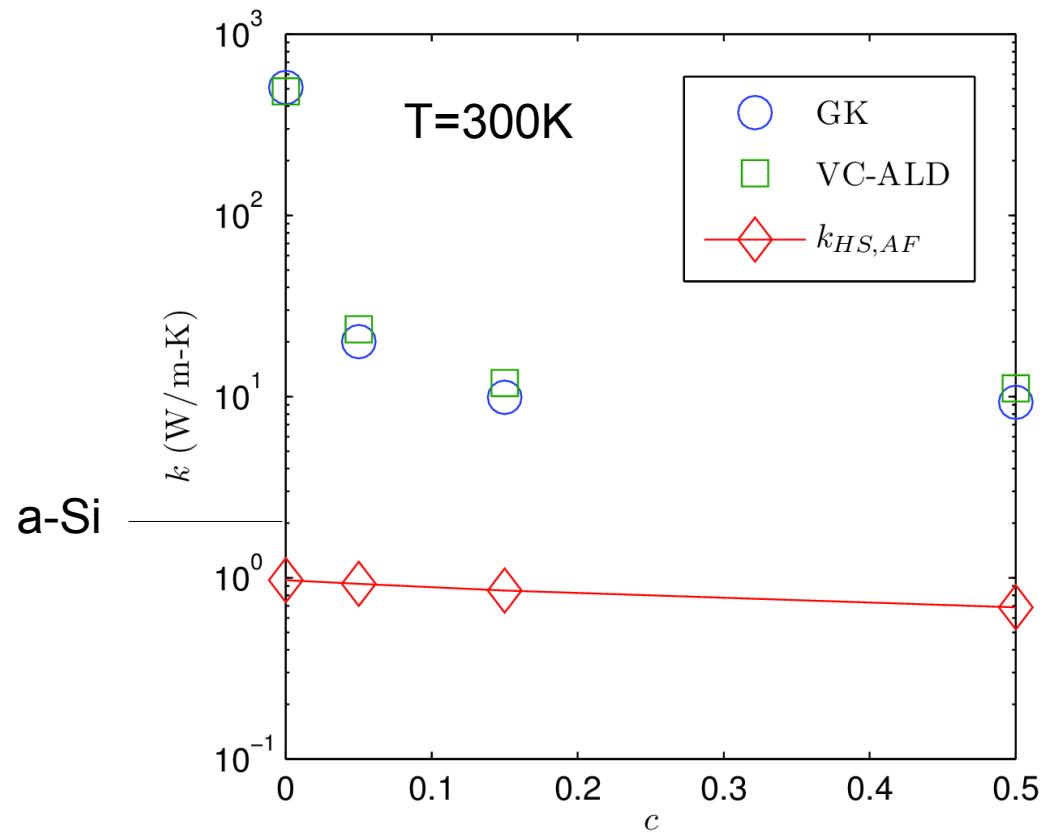
$$k_{AF} = \sum_{modes} \frac{k_B}{V} D_{AF}(\omega(\kappa=0))$$

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



# High-Scatter Limit: SW Si

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

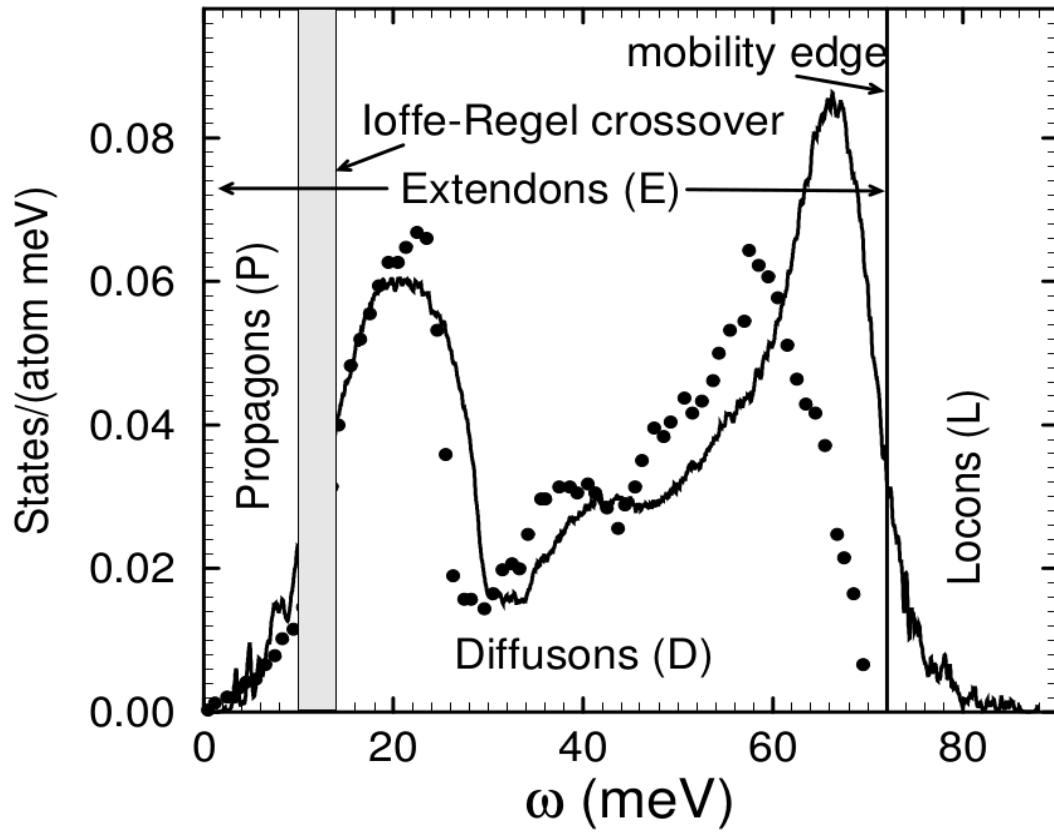


# Propagons, Diffusons, Locons

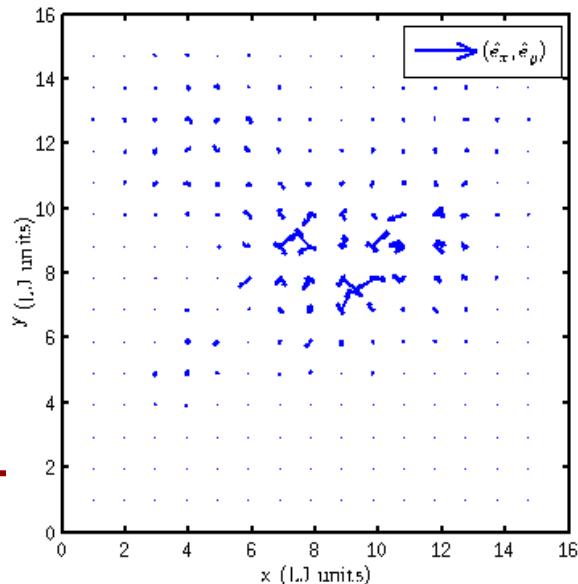
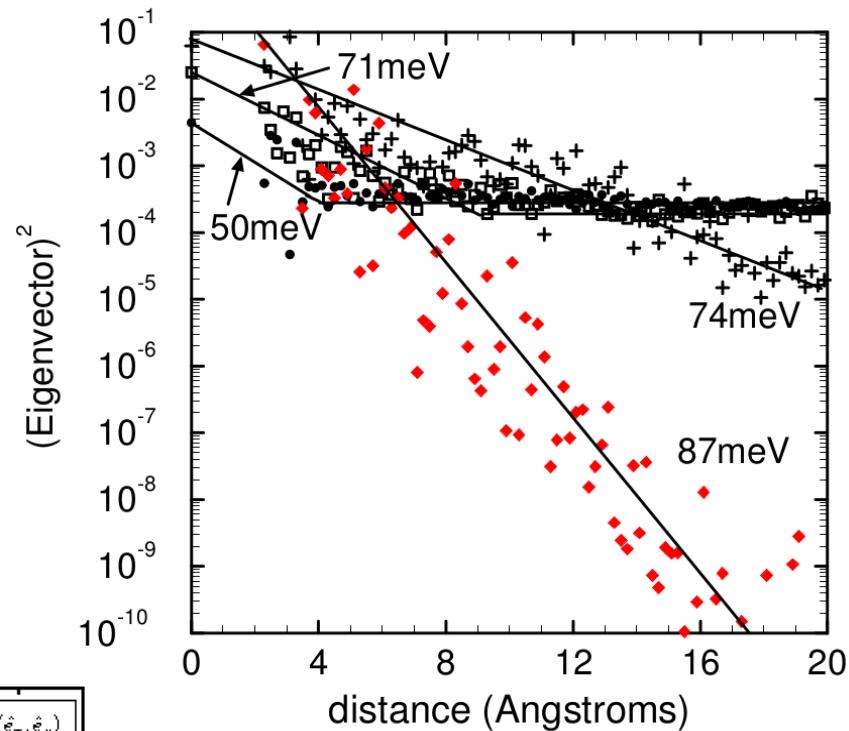
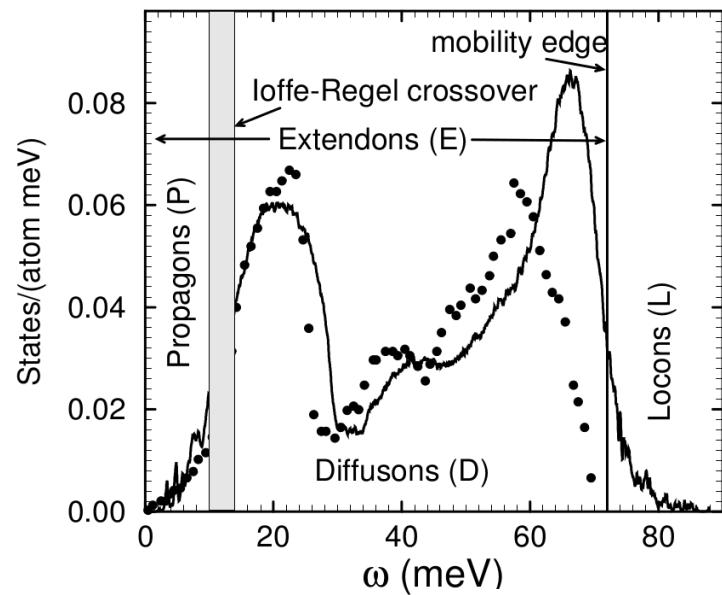
Numerical studies of amorphous silicon show that the lowest 4% of vibrational modes are plane-wave like (“propagons”) and the highest 3% of modes are localized (“locons”). The rest are neither plane-wave like nor localized. We call them “diffusons.”

\cite{diffusons\_allen\_1999}

vibrons { extendons { propagons  
                                  diffusons  
                                  } }  
                                  locons



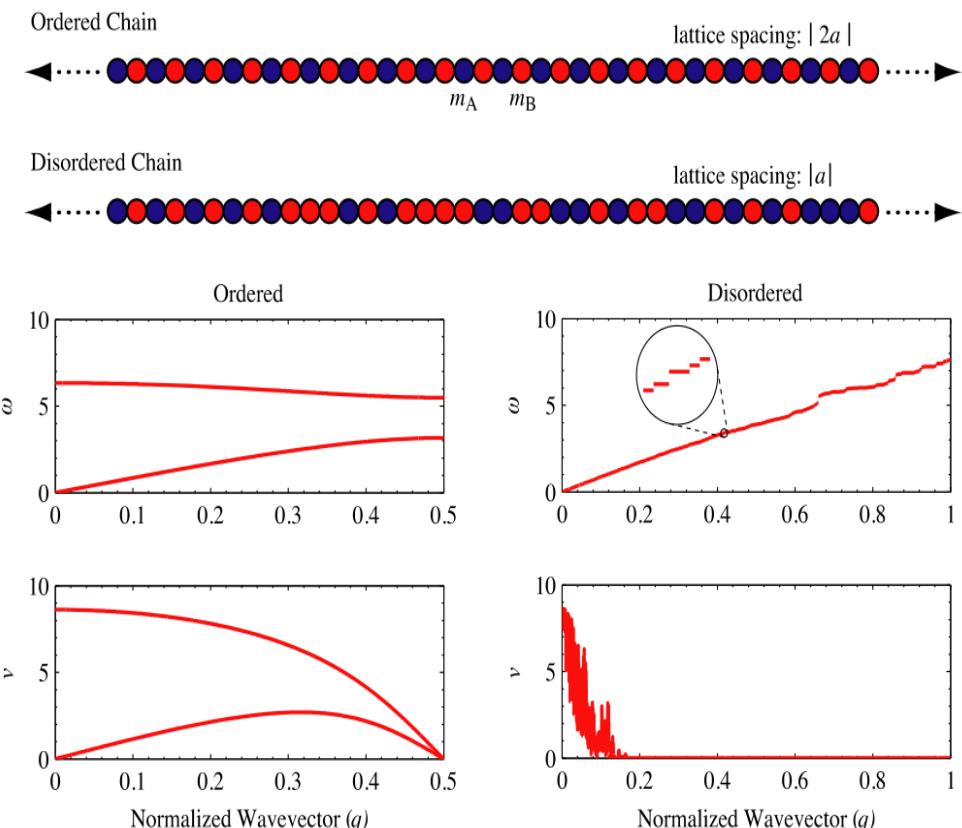
# Propagons, Diffusons, Locons



# Disordered Mode Group Velocity

$v_g$  from “zone-folding”:

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

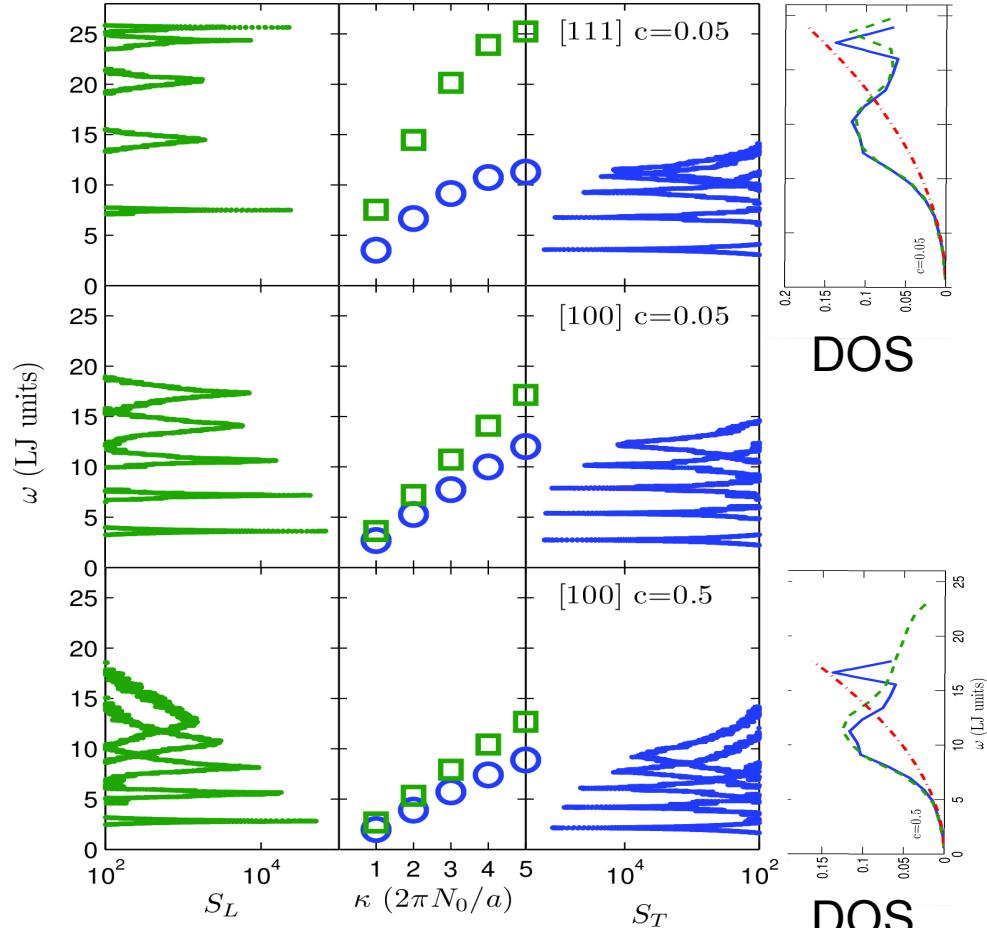
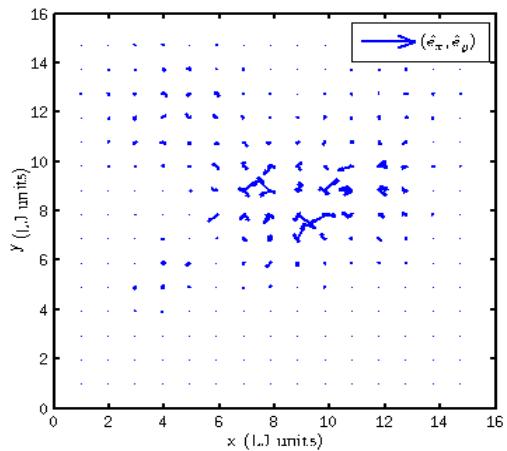
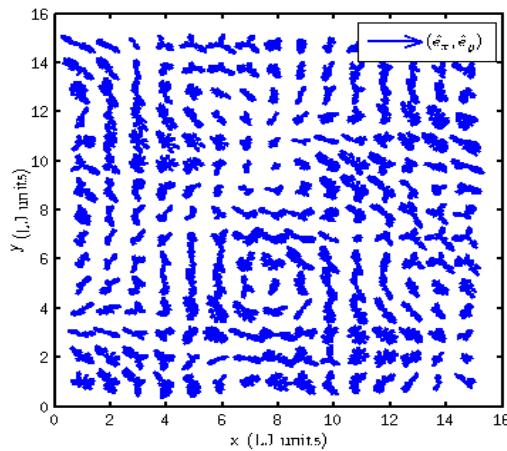
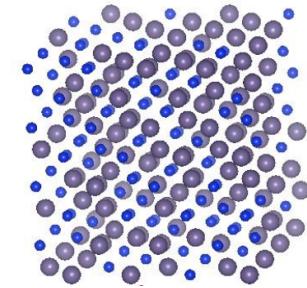


$v_g$  from near [000]:

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

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

# Disordered Mode Group Velocity



[https://github.com/jasonlarkin/disorder/blob/master/paper/vc/prb\\_vc\\_jl\\_011813.pdf](https://github.com/jasonlarkin/disorder/blob/master/paper/vc/prb_vc_jl_011813.pdf)

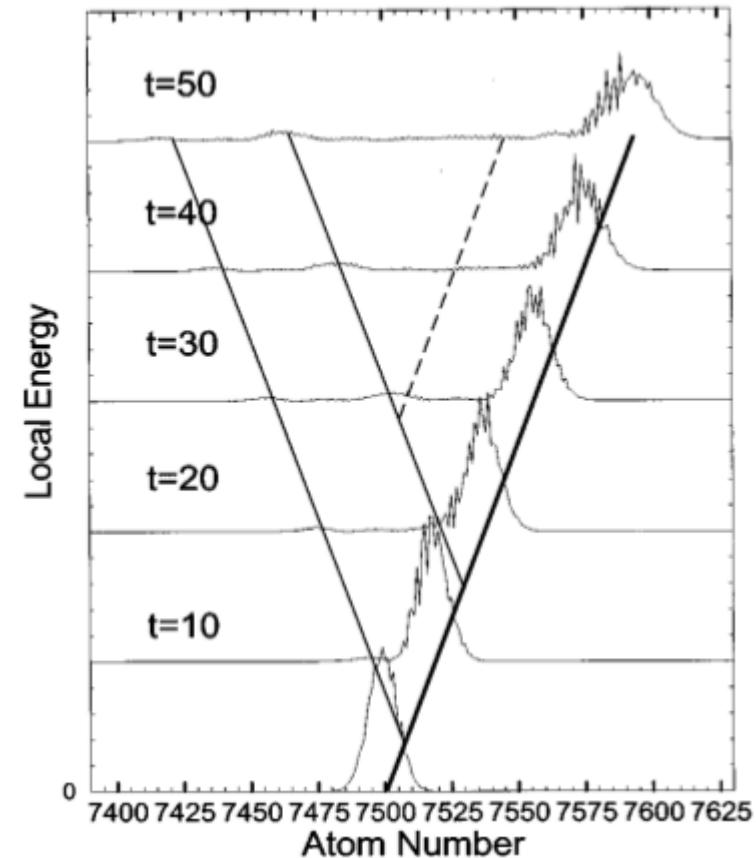
# Extra

# Ballistic vs. Diffusive Transport

Table I. Modes of time evolution of a packet.

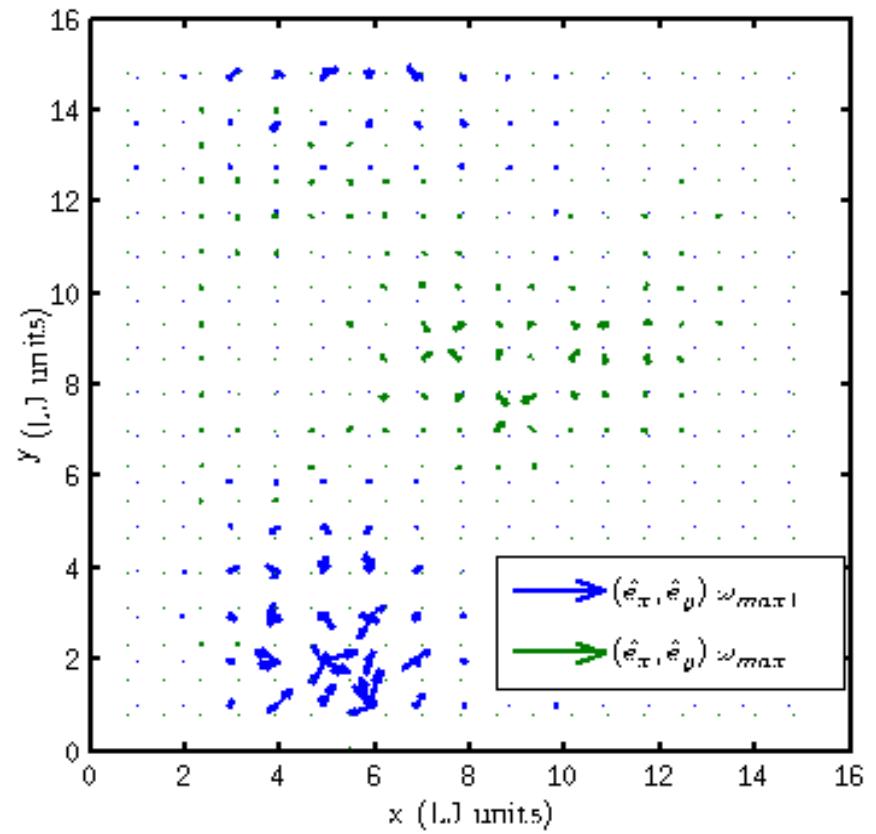
	Center of pulse	Squared width of pulse
propagating	$\mathbf{R}_0 + \mathbf{v}t$	$b^2 + a_0^2 t^2 / b^2$
diffusing	$\mathbf{R}_0$	$b^2 + 2Dt$
localized	$\mathbf{R}_0$	$\xi^2$

$R(t)$

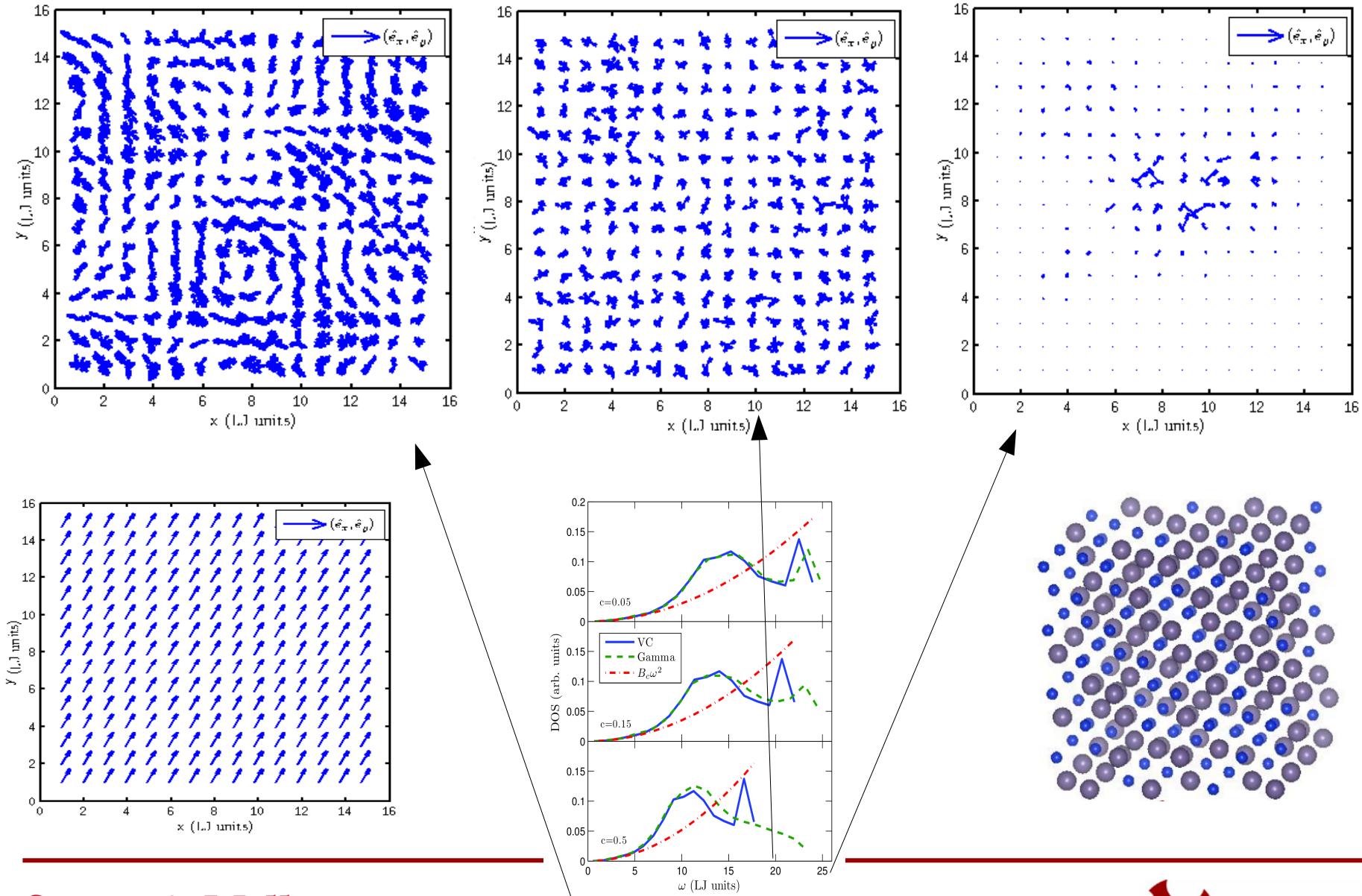


Am. J. Phys., Vol. 66, No. 6, June 1998

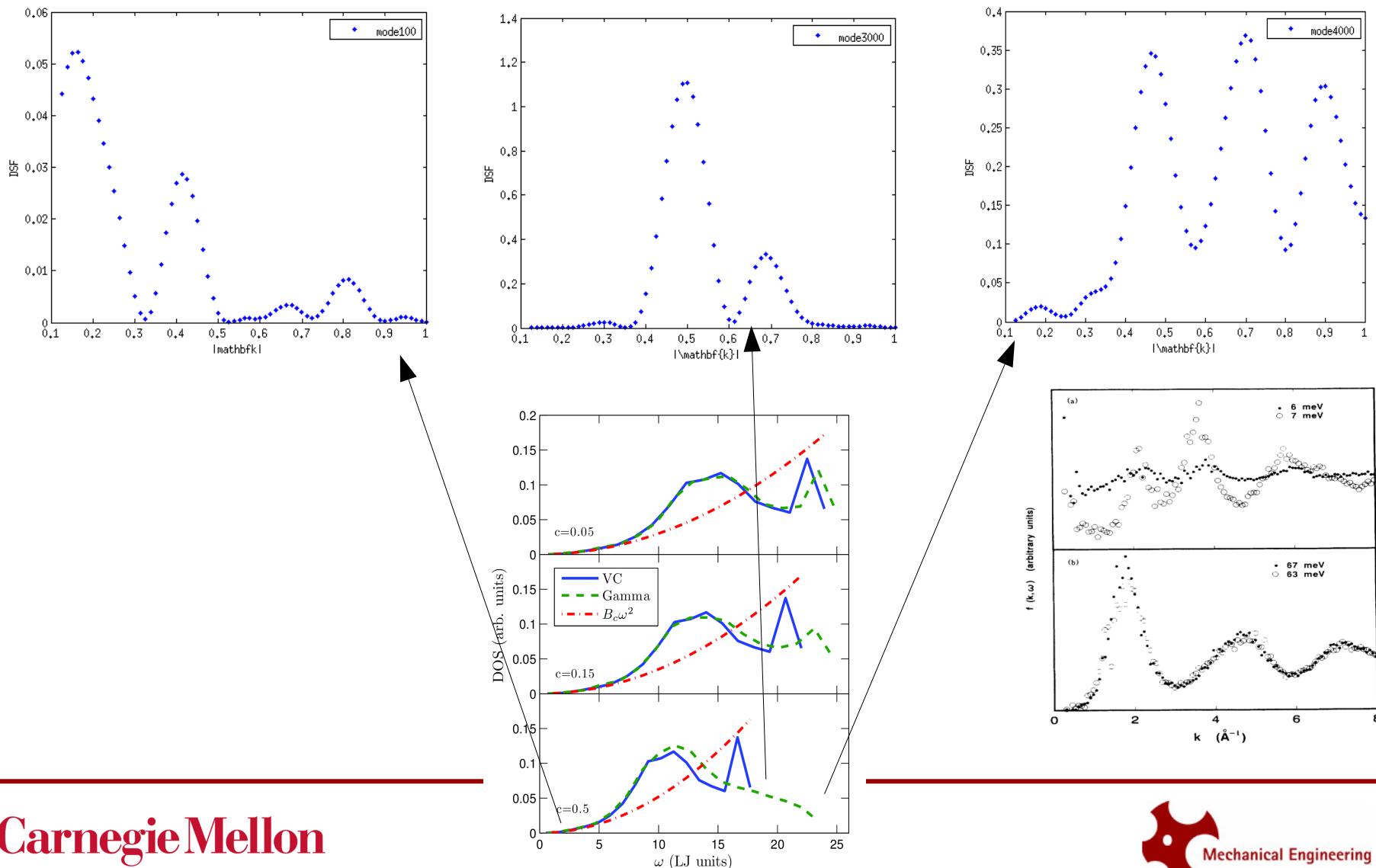
# Localized Modes



# Mode Localization



# Disordered Mode Plane-Wave Character



# Disordered Modes Group Velocity: Zone-Folding

