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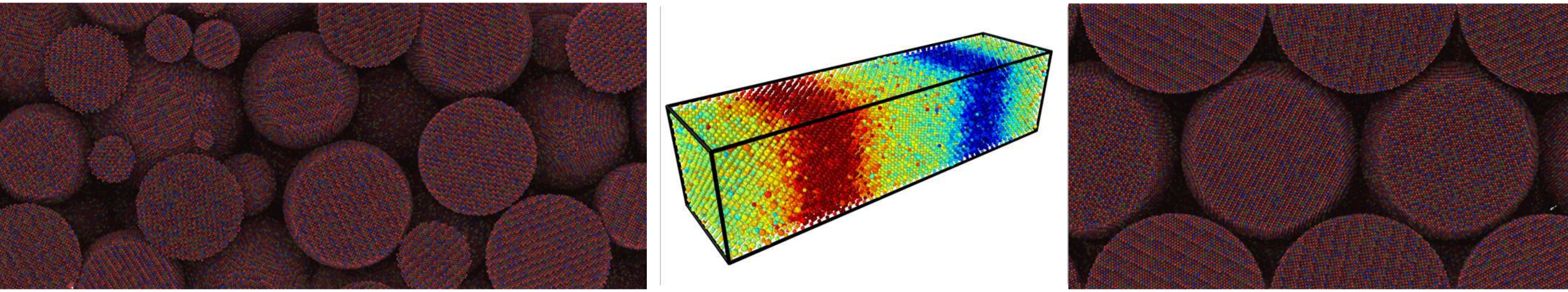


Thermal Conductivity within Nanoparticle Powder Beds

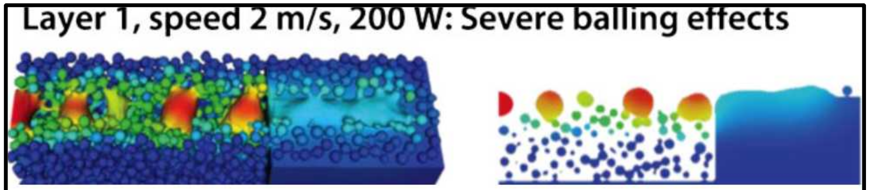
Solid Freeform Fabrication Symposium, August 10th 2016

Mark Wilson, Michael Chandross

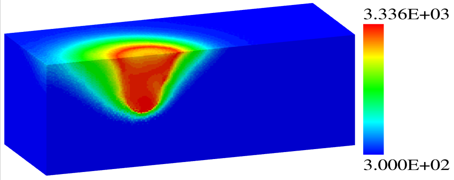
Computational Materials and Data Science

Motivation

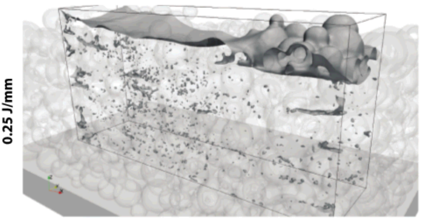
- Evolution of AM is challenged by process and quality issues, typically a function of control parameters, determined by a trial-and-error method.
- Modeling of the AM process powder beds are modeled at Thermo/mechanical continuum levels



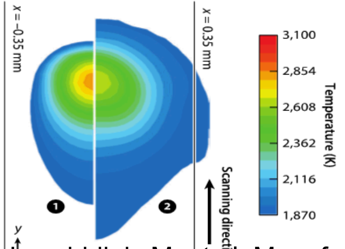
King, W. et al. Mat. Sci. & Tech. (2015)



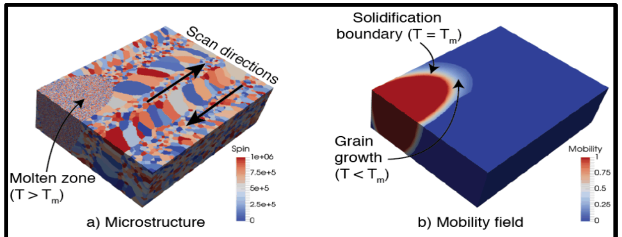
Martinez SNL,NM



Markl, M. et al.
Annu. Rev. Mater. Res (2016)



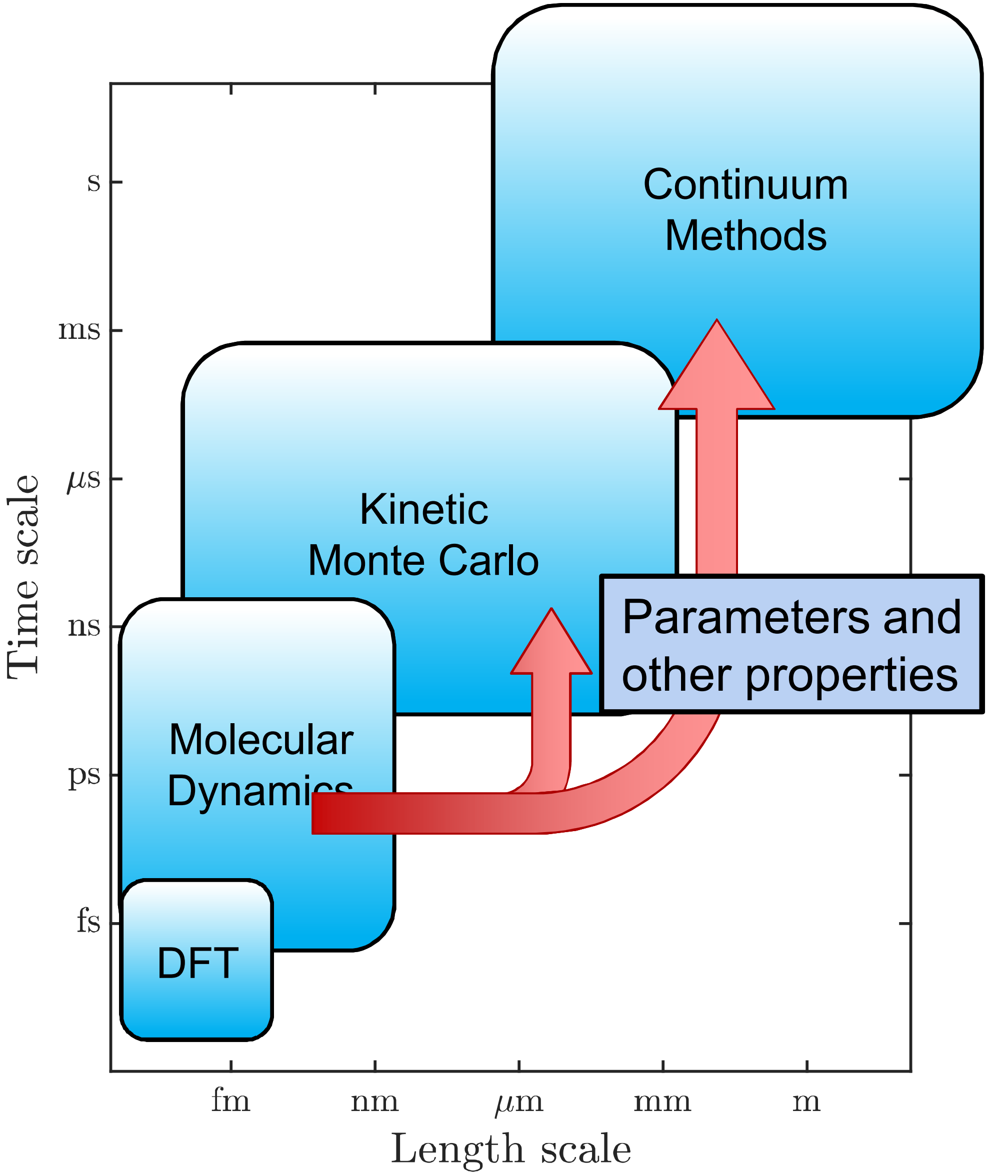
Jamshidinia M. et al. Manuf. Sci. Eng. Trans. (2013)



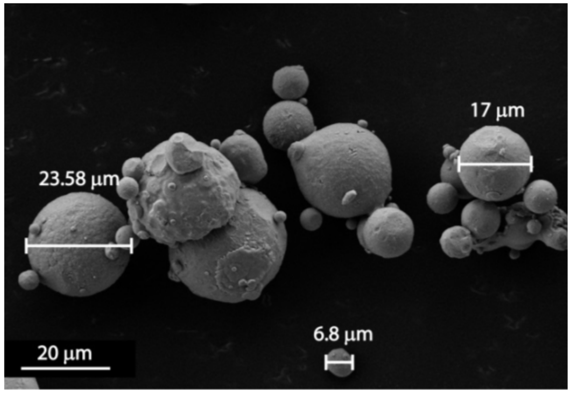
Rodgers T. et al., SNL,NM (2016)

- Gain a better understanding of thermal conduction within powder beds, beyond the continuum representation. Is this important? If so, to what degree?
- Molecular dynamics (MD) challenges to consider
  - Electron-mediated heat transfer is important in metals – Two Temperature Model (TTM)
  - Scale …

Modeling scale



- MD scale is substantially smaller than the ”part” scale



Manfredi, D. et al.

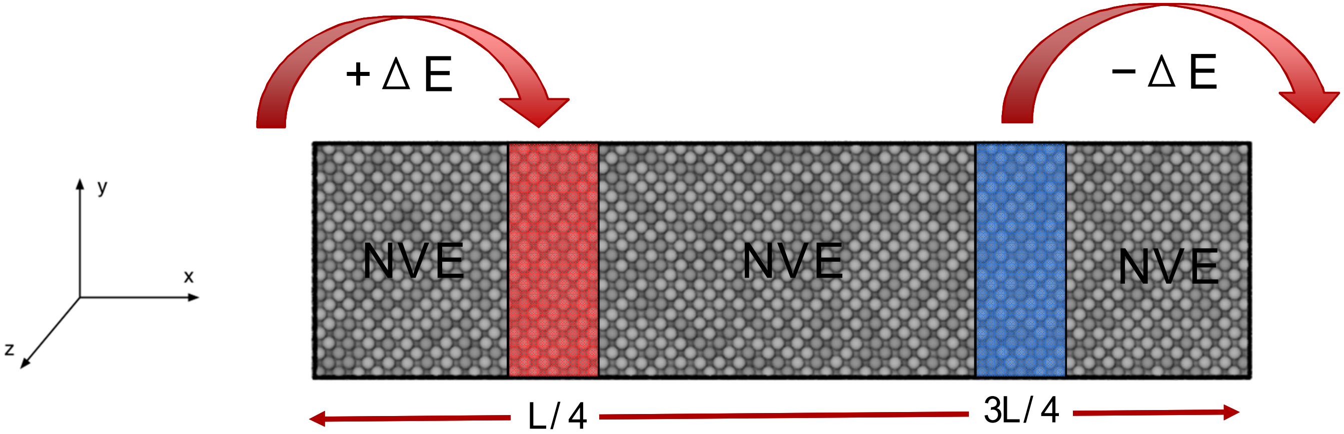
- Extrapolate to larger scales
- Goal: Inform other modeling approaches at various length and time scales
- Provide material specific parameters for upscale models

Methodology

- Fourier’s law of thermal conduction for small temperature gradients

$$\boxed{J = -\kappa \nabla T}$$

- Valid for all states of matter



- Heat flux is applied through a velocity renormalization method, conserving net linear momentum

$$J = \frac{\Delta E}{\Delta t\, 2A}\ [\mathrm{W/m^2}] \qquad \kappa = -\frac{J/A}{\partial T/\partial L}$$

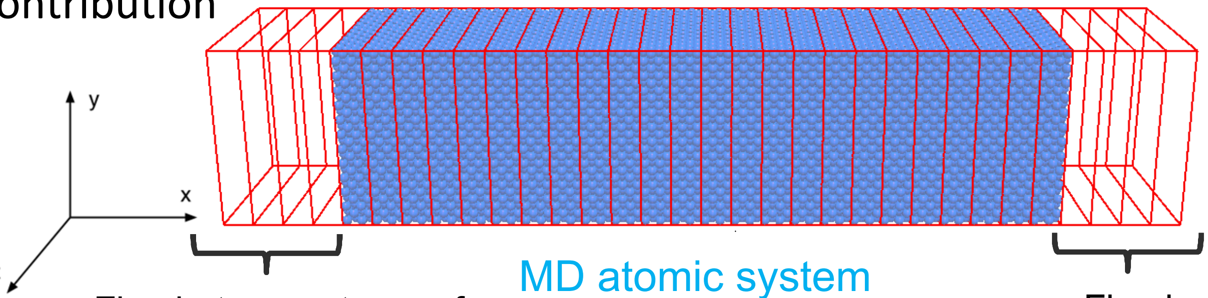
- System undergoes Newtonian dynamics through an NVE ensemble

Potential	lattice
Fe (Mendelev)	bcc
Al (Zhou)	fcc
304L SS (Bonny)	fcc

$Fe_{0.7}Cr_{0.18}Ni_{0.12}$

Two temperature model

- Spatial discretization of FE on top of MD system, implicitly model electronic contribution



Finite element mesh
Periodic in y,z, fixed in x

Fixed at mean temp of MD region

MD atomic system
Fully periodic BC's

Fixed at mean temp of MD region

- Electronic system and energy coupling between the two system is governed according

$$C_e \rho_e \frac{\partial T_e}{\partial t} = \nabla(\kappa_e \nabla T_e) - g_{e-p}(T_e - T_a) + \rho_e S_e$$

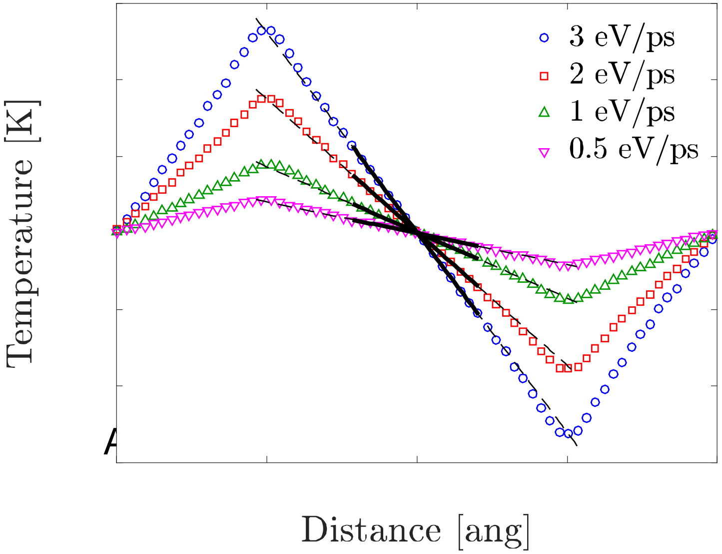
$$C_p \rho_p \frac{\partial T_p}{\partial t} = \nabla(\kappa_p \nabla T_p) + g_{e-p}(T_e - T_a)$$

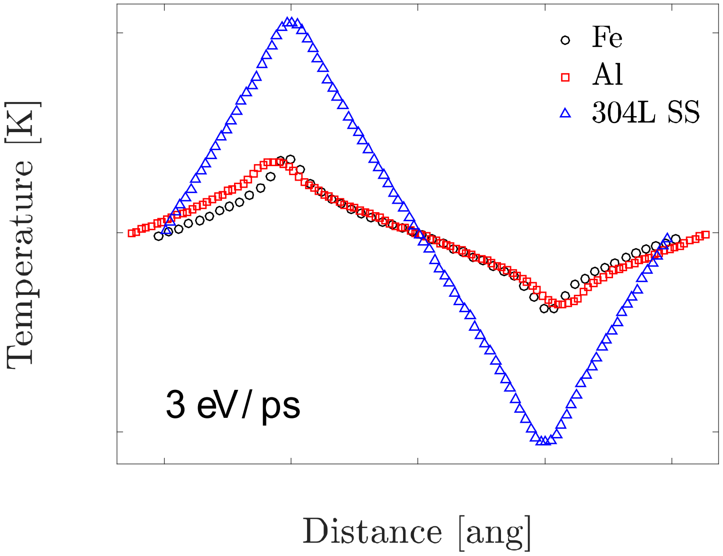
- Parameterization

$C_e \rho_e$ $C_p \rho_p$	▪ **Heat capacity:** estimated from free electron density (electronic), Dulong-Petit law (phonon)
κ_e κ_p	▪ **Thermal conductivity:** Franz-Wiedemann law (electronic), direct method MD (phonon)
g_{e-p}	▪ **Electron-phonon coupling:** DFT calculations of electronic DOS, pump-probe experiments

Wagner. et al, Comput. Methods appl. Mech. Engrg. (2008)

Phonon heat conduction results



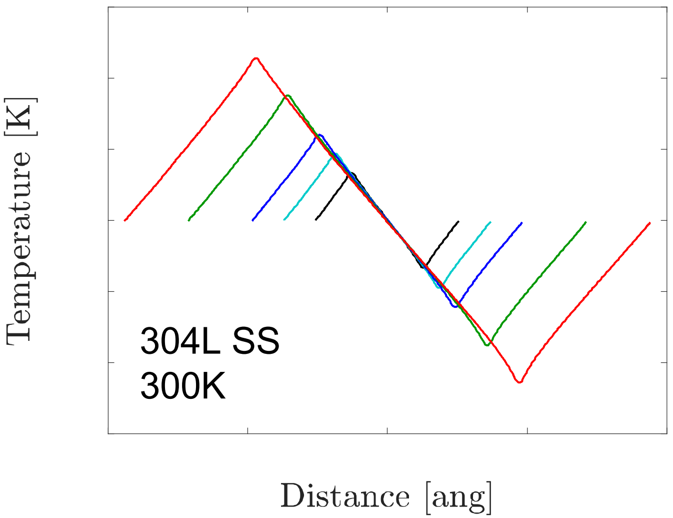


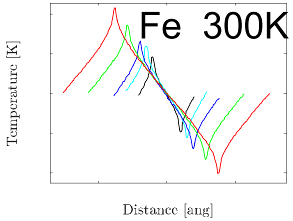
- Determination of temperature profile discretizes the MD simulation spatially along the x axis
- The error in calculated conductivity resides in determination of slope of thermal profile

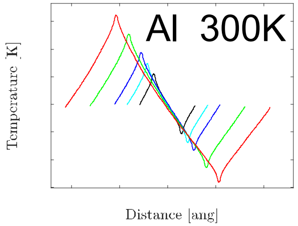
Zhou. X., et al, Phys Rev B. (2009)

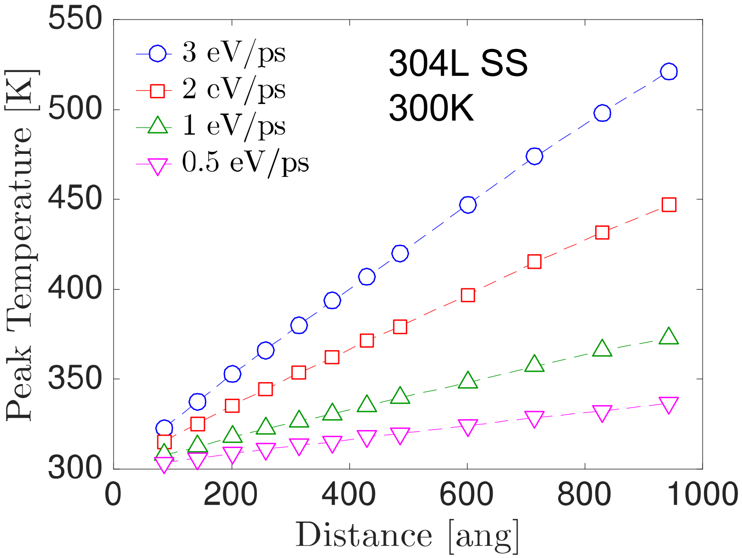
- Profile shape gives indications of general thermal behavior of system
  - Greater temp at extrema - slower energy transfer
  - Linear profile – slower energy transfer

Phonon system size effects



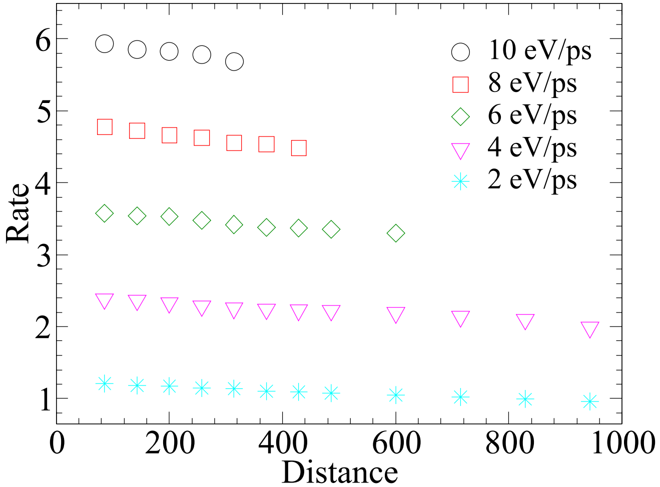




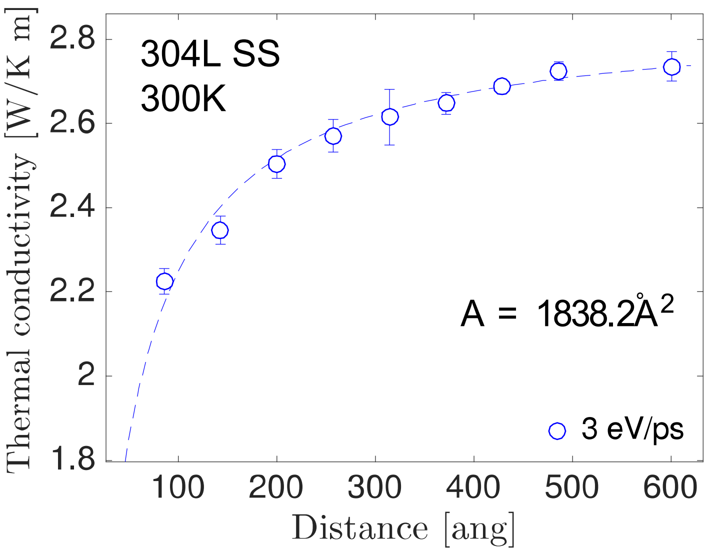


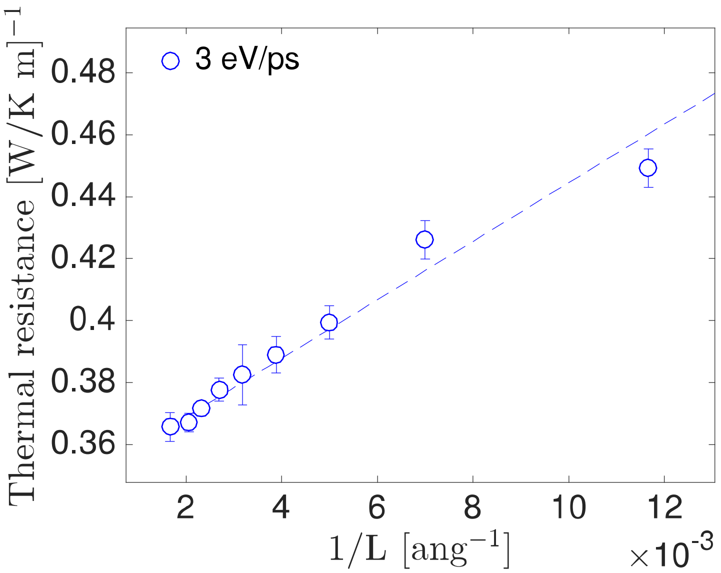
- Employ direct method over multiple system sizes
- Peak temperature indicates strong dependent on system size
- Rate of energy transfer through material

$$\boxed{R_t = \frac{Q}{t} = \kappa A \frac{(T_{source} - T_{sink})}{D}}$$



Phonon system size effects





- Extrapolate to bulk properties – Matthiessen rule

$$\boxed{\frac{1}{\kappa} = \frac{1}{\kappa_\infty} + \frac{\alpha}{L}}$$

- Mean free path, group velocity of acoustic phonon can be determined under a simple model

Heino, P., Microelectronics J., (2003)

$$\boxed{\frac{1}{\kappa} = \frac{2}{nk_B v}\left(\frac{1}{\ell_{MFP}} + \frac{4}{L}\right)}$$

Potential	lattice	v [m/s]	v_{exp} [m/s]	ℓ_{MFP} [nm]
Fe (Mendelev)	bcc	5766	5130	9.32
Al (Zhou)	fcc	5100	5939	4.48
304L SS (Bonny)	fcc	6225	5790	7.6

Temperature / flux dependence

Potential	lattice	Temp [K]	κ_p [W/m K]	κ_p [W/m K]	κ_{exp} [W/m K]	T_D [K]
Fe (Mendelev)	bcc	300	32.5	-	80	420
Al (Zhou)	fcc	300	10.8	≈ 6	205-240	394
304L SS (Bonny)	fcc	300	2.92	-	14.0-16.3	468

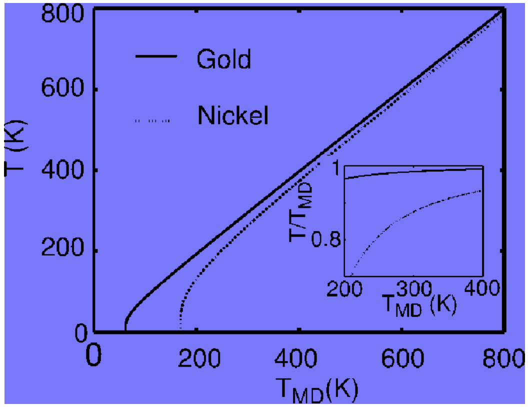
This work

Jain A. et al, Phys Rev B. (2016) – k_p

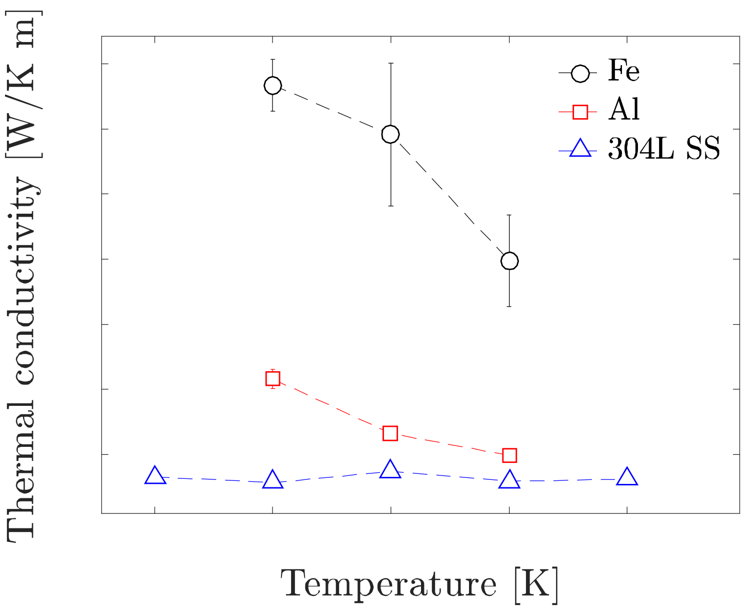
Ashcroft and Mermin – T_D

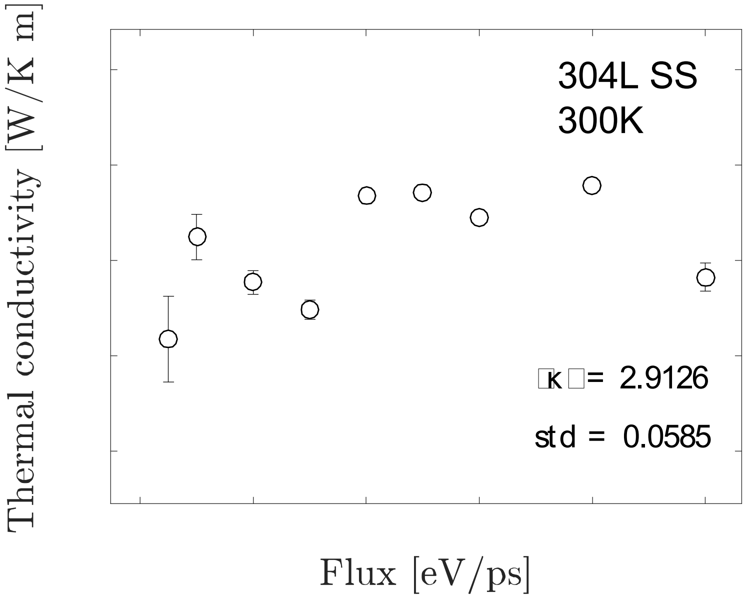
Graves R.S. et al, Int J Thermo. (1991) – 304L k_exp

Winter J., et al, Phys Rev B (2016) – 304L T_D



Heino, P., et al, Microelectronics J., (2003)

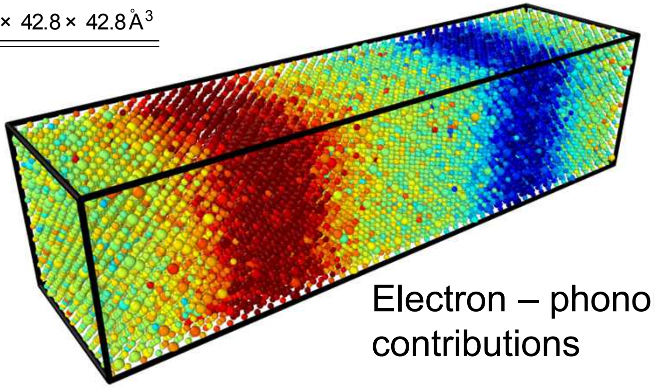




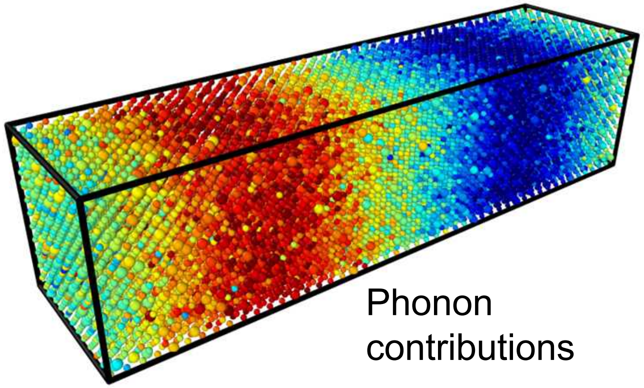
Comparison with TTM

$\approx 30,000$ atoms

$171.5 \times 42.8 \times 42.8 \text{Å}^3$



Electron – phonon contributions



Phonon contributions

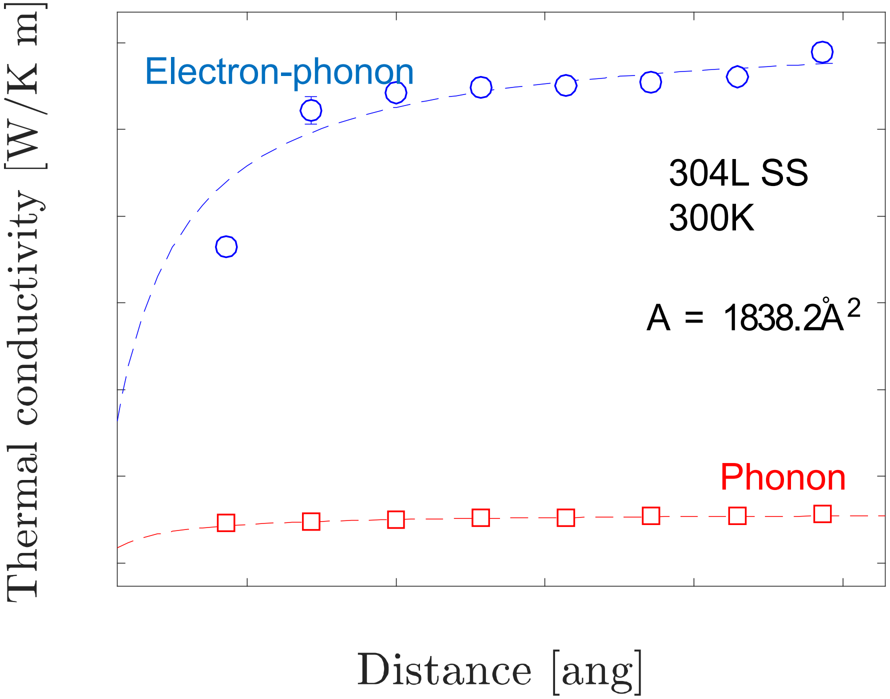
Temperature [K]

304L SS
300K

- Shape of the thermal profile indicates improved conductance with the addition of the TTM
- Increased heat flux is necessary to achieve similar resultant slope

$$\kappa = -\frac{J/A}{\partial T/\partial L}$$

Comparison with TTM



- Observe a plateau region for 304L SS, suggesting that distance dependence maybe less important when including TTM
- Elevated conductivity results from TTM. Considerations:
  - Correct parameterization of TTM?
  - Free electron density - $C_e \rho_e$
  - Temperature relative to Debye temperature

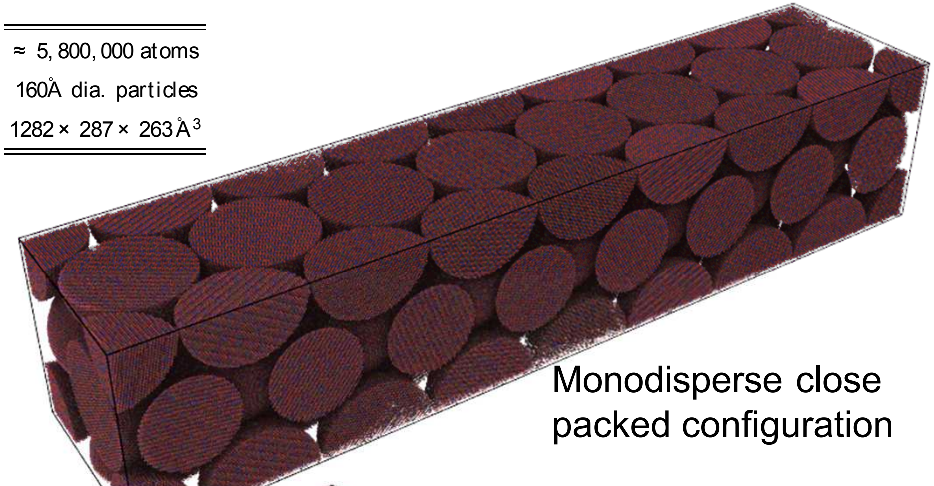
Potential	lattice	temp [K]	κ_p [W/m K]	κ_{TTM} [W/m K]	κ_{exp} [W/m K]
Fe (Mendelev)	bcc	300	32.5		80
Al (Zhou)	fcc	300	10.8	321.98 ± 12.01(800Å)	205-240
304L SS (Bonny)	fcc	300	2.92	31.02 ± 0.96	14.0-16.3

Nanoparticle powder beds

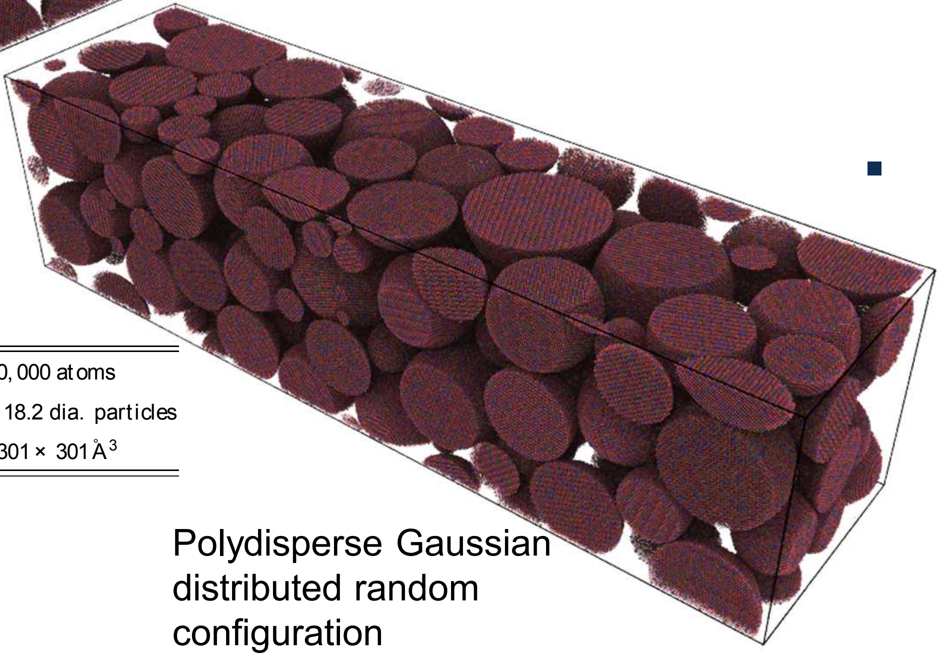
≈ 5, 800, 000 atoms

160Å dia. particles

1282 × 287 × 263 $Å^3$



Monodisperse close packed configuration



≈ 5, 730, 000 atoms

< 41.8 > Å ± 18.2 dia. particles

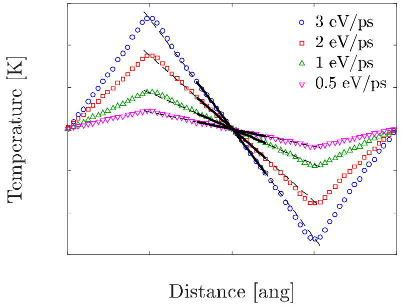
1152 × 301 × 301 $Å^3$

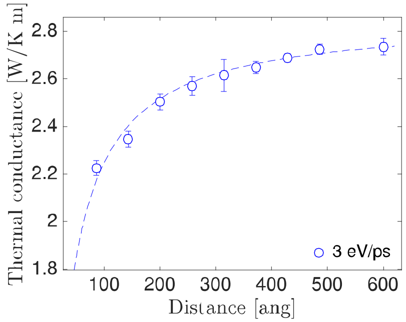
Polydisperse Gaussian distributed random configuration

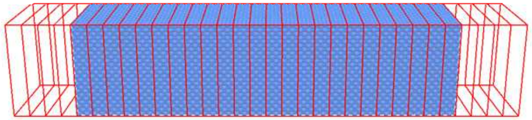
- Approach for creation of atomistic powder bed, initial configuration
- Mono/poly disperse configurations
- GOAL: Extrapolation of results to micrometer scales, using a similar approach to the determination of bulk conductivity properties
- Observations / considerations:
    - Small dia. particles leads to cohesive polycrystalline material at temperature.
    - Parameterization of TTM model, decrease in the number of free electrons
    - Discontinuous nature of configuration leads to decreased phonon contribution to conductivity

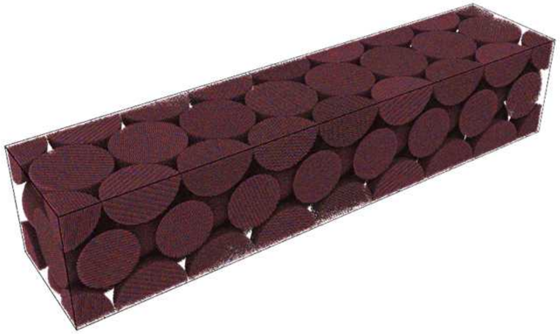
Summary

- Utilize MD and the “direct method” to study thermal conduction within crystalline metallic systems
- Showed that resulting conductance values can be extrapolated to bulk system properties utilizing a simple model of thermal resistivity
- Introduced a two-temperature model, so as to incorporate electronic contributions to thermal conductance
- Initial results indicate that the model overshoots experimental conductance values
- Approach to studying thermal conductivity within powder beds was discussed



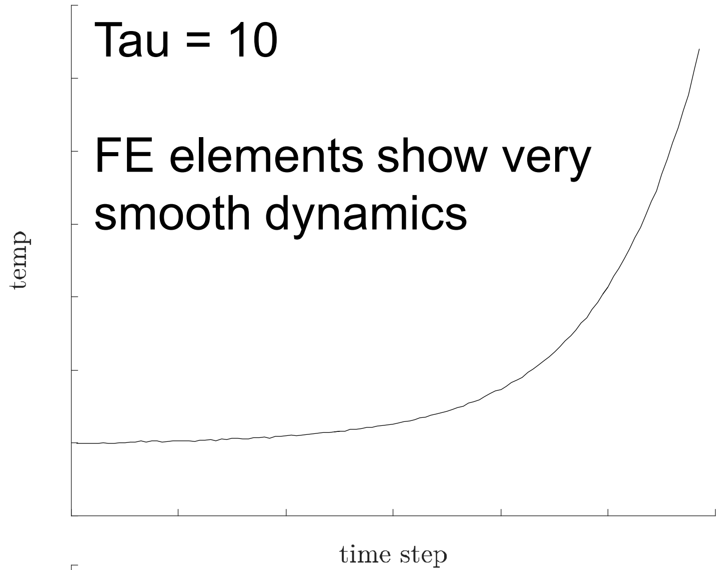






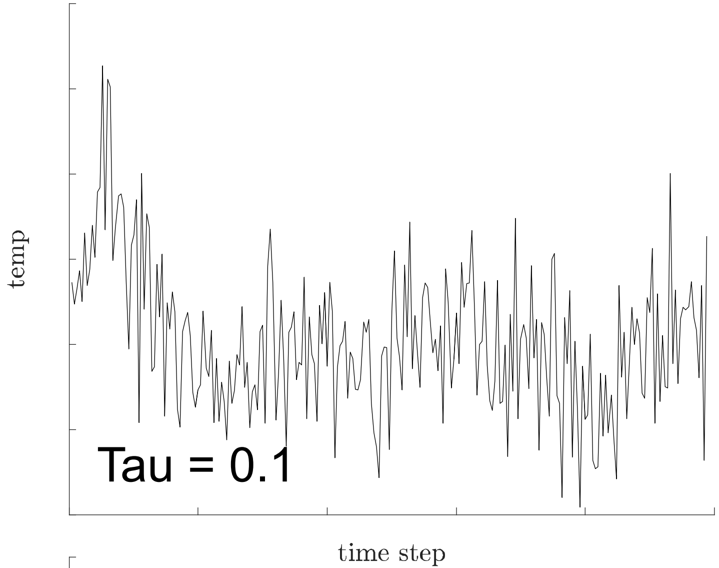
Time filtering

Aluminum: G_e-p times a factor of 10;
Equilibrium conditions -- No heat source

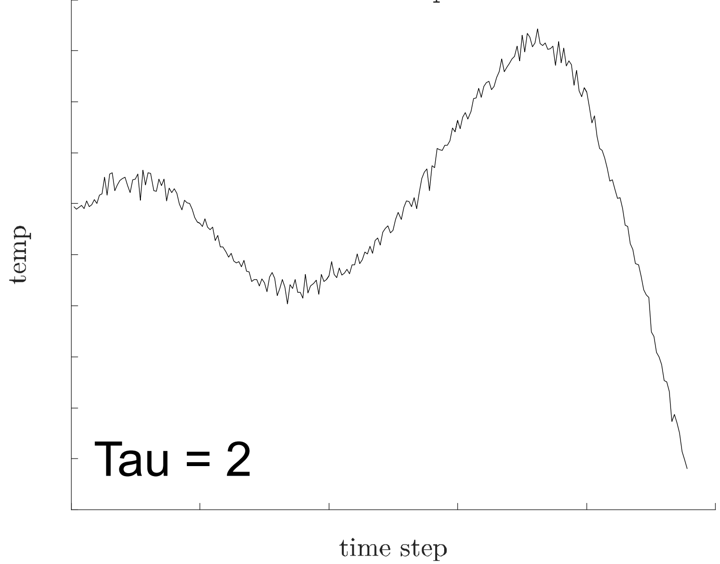


Tau = 10

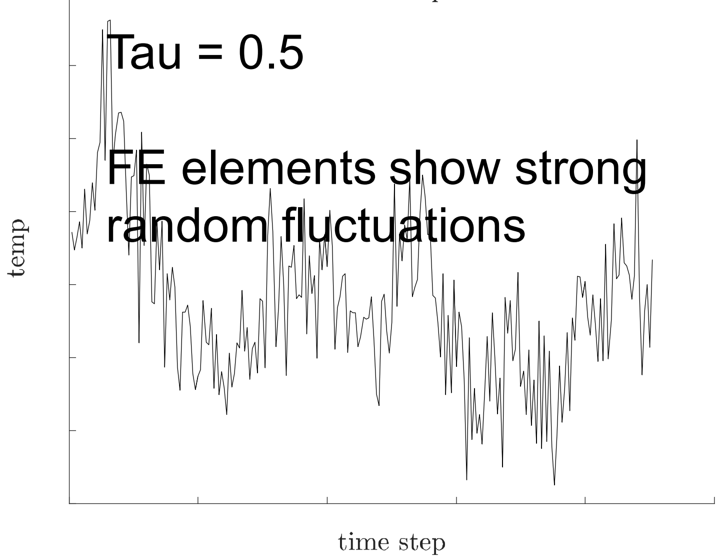
FE elements show very smooth dynamics



Tau = 0.1



Tau = 2



Tau = 0.5

FE elements show strong random fluctuations

Time filtering

Aluminum: G_e-p known value;
Equilibrium conditions -- No heat source