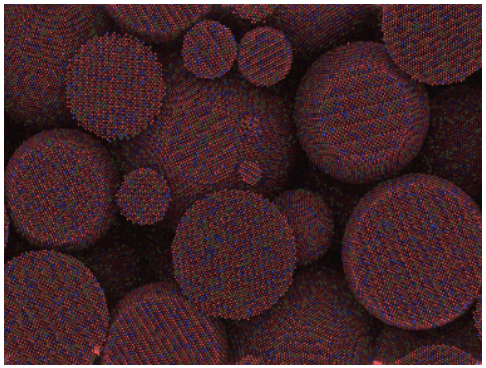
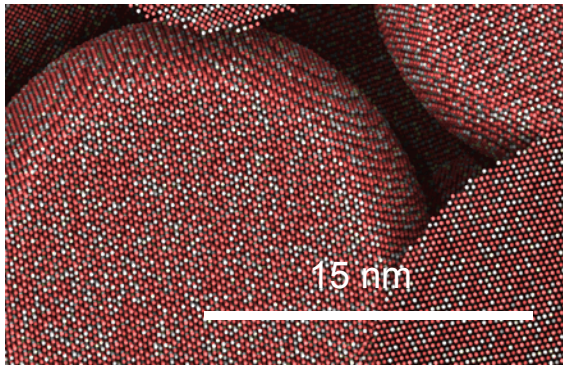
SAND2017-11144C





Atomistic details of metal additive manufacturing in powder beds

Mark Wilson and Michael Chandross

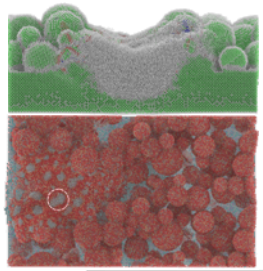
Computational Materials and Data Science

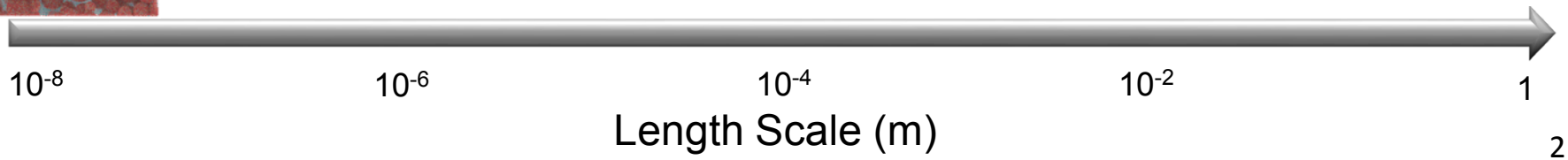
Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

AM Modeling at SNL

Codes
LAMMPS, SPPARKS,
Sierra/Aria,
Sierra/Adagio

Powder Behavior
Mark Wilson





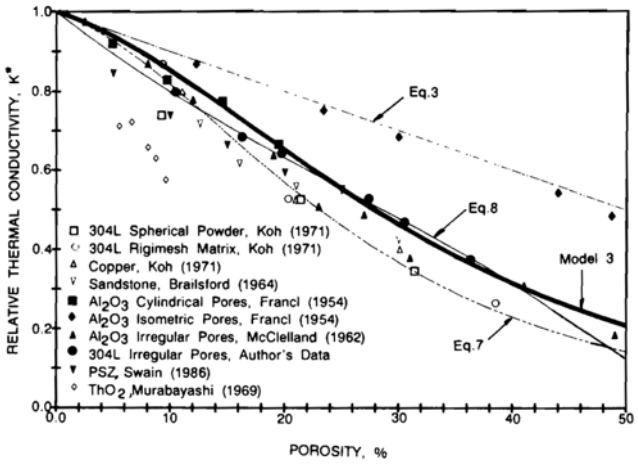
Motivation

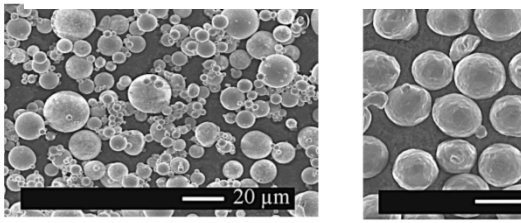
Characterization of powder properties is critical in developing process-structure relationships

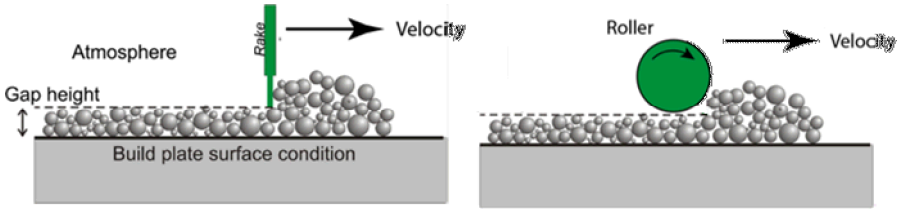
Multiple contributions to thermal conductivity within powder bed environments

- Packing fraction – porosity/topology
- Chemical composition
- Particle morphology – contact area
- Environment: convection and radiative
- Radial size
- Poly-disperse size distribution

GOAL: explore relative contributions to thermal conductivity at the atomistic scale

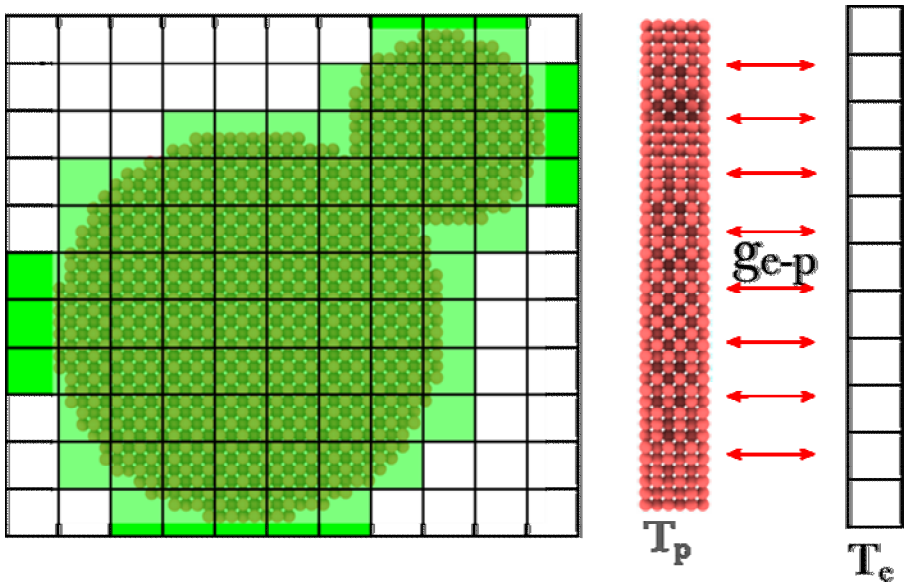






Agapiou et al. J Heat Trans (1989)
Rombouts et al. J. Appl. Phys (2005)

Computational model



$$C_e(T_e)\,\rho_e\frac{\partial T_e}{\partial t} = \nabla(\kappa_e(T_e)\nabla T_e) - g_{e-p}(T_e - T_p) + g_s T_a'$$

Heat equation

electron-phonon coupling

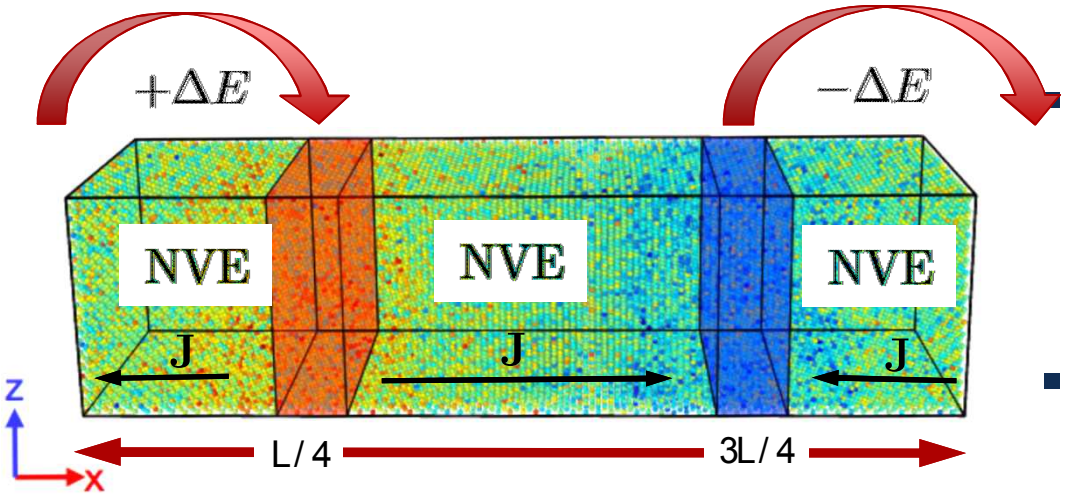
electron stopping energy

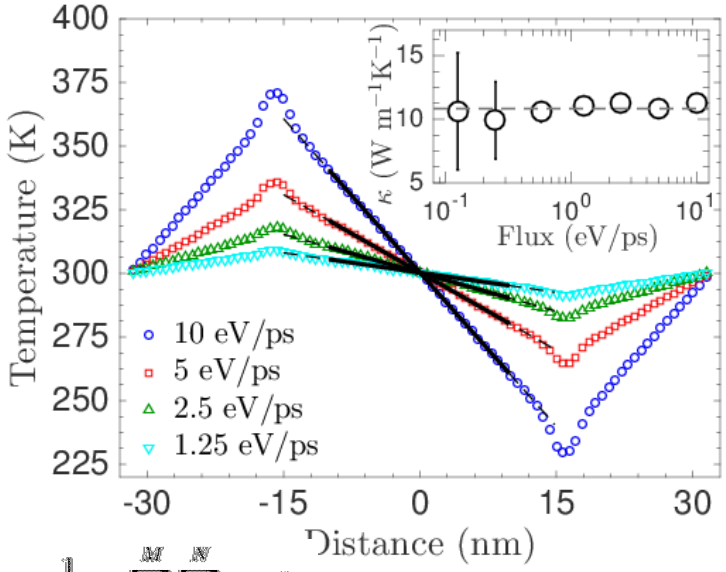
Parameterization

- **Heat capacity:** $C_e\,\rho_e$
  estimated from free electron density, electronic DOS
  Lin et al., Phys. Rev. B. (2008)
- **Conductivity:** κ_e
  Franz-Wiedemann law (electronic), direct method MD (phonon)
- **Electron-phonon coupling:** g_{e-p}
  DFT calculations of electronic DOS, pump-probe experiments
- **Damping coefficient:** $\gamma_i = \gamma_p + \gamma_s$.
  frictional contributions, electron-ion interaction, electron stopping
- **Material approximations:**
  304L SS $Fe_{0.7}Cr_{0.18}Ni_{0.12}$
  Inconel 718 $Fe_{0.3}Cr_{0.2}Ni_{0.50}$

Rutherford and Duffy, J. Phys. Condens. Matter (2007)
Jones R., Int. J. Num. Meth. Engin (2010)

Thermal conductivity via the "direct" method





$$\langle T_{slab} \rangle = \frac{1}{3NMk_B} \sum_{i=1}^{M} \sum_{i=1}^{N} m_i \mathbf{v}_i^2$$

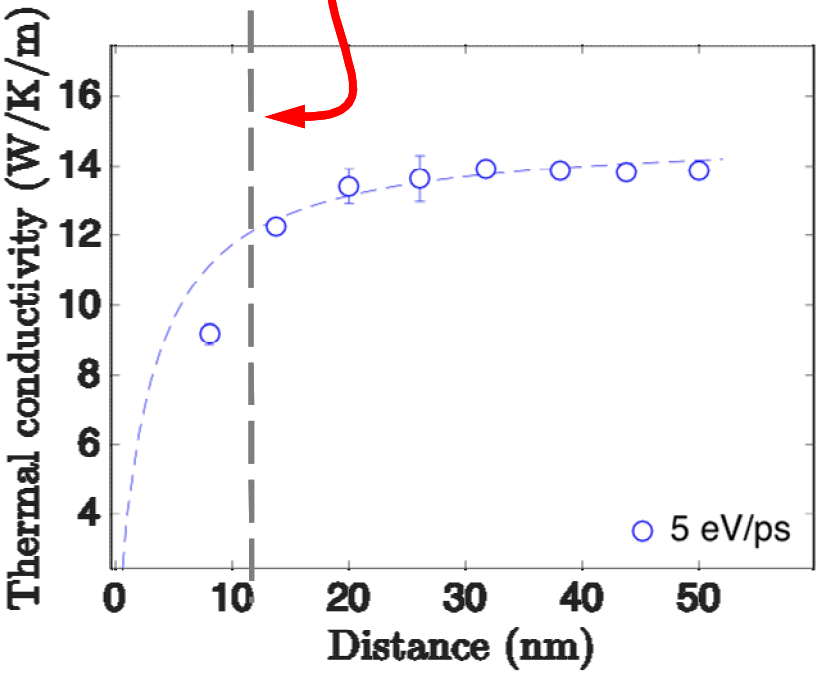
- Fourier's law of thermal conduction for small temperature gradients $\mathbf{J} = -\kappa \nabla T$
- Heat flux is applied through a velocity renormalization method, conserving net linear momentum

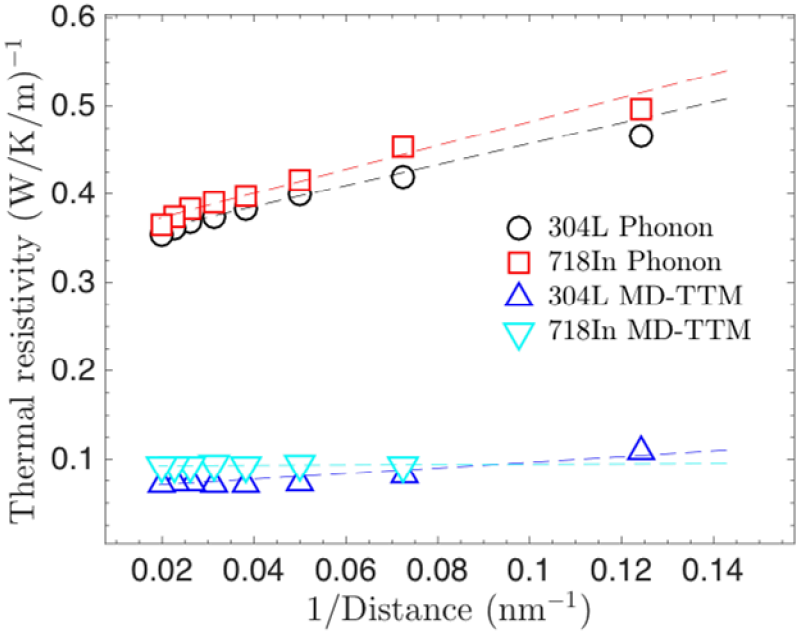
$$\kappa = -\frac{J/A}{\partial T/\partial L} \qquad J = \frac{\Delta E}{\Delta t\, 2\, A} \; [\mathrm{W/m^2}]$$

- System undergoes Newtonian dynamics through an NVE ensemble, embedded atom methods

Finite system size effects

Phonon mean free path: ~10 nm



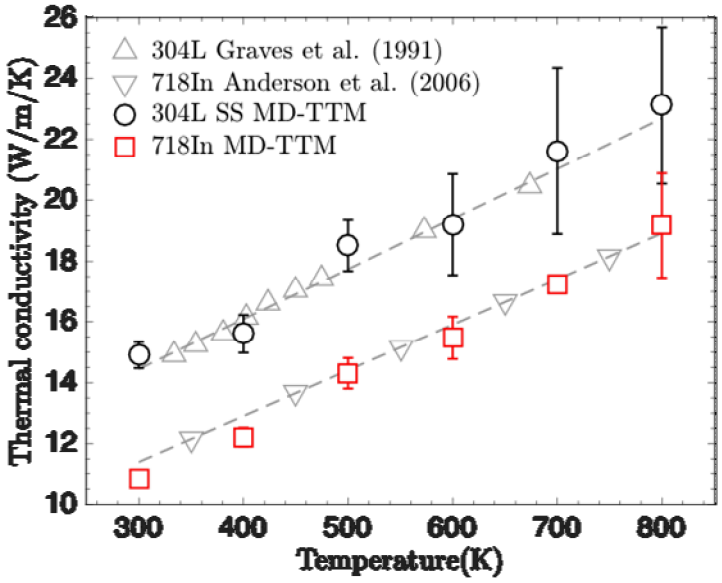


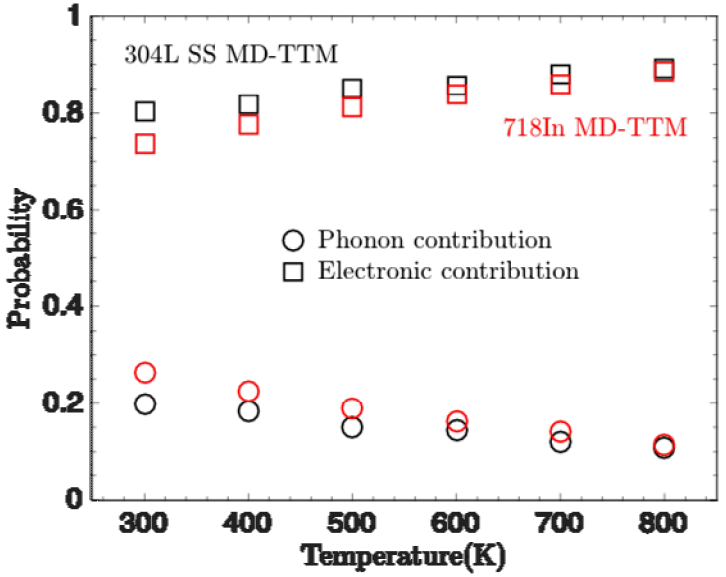
- Extrapolate to bulk properties – Matthiessen rule
- Mean free path, group velocity of acoustic phonon can be determined under a simple model

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

Heino. et al, Microelectronics J. (2003)

Single crystal - temperature dependence



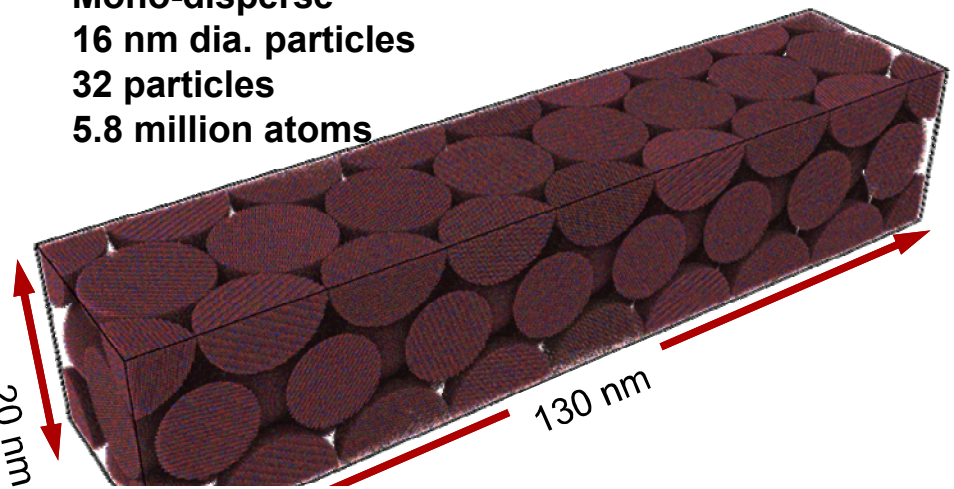


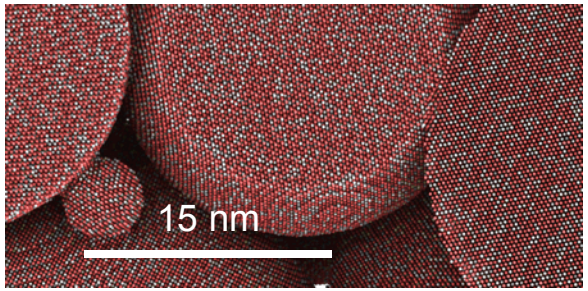
- Verification of parameterization for both 304L SS and 718 Inconel show agreement with experimentally determined bulk values
- Both materials, energy transport is dominated by electronic contributions, behavior increases with higher temperatures

Graves, et al. Int. J. Thermophysics (1991)
Anderson, Int. J. Machine Tools and Manuf. (2006)

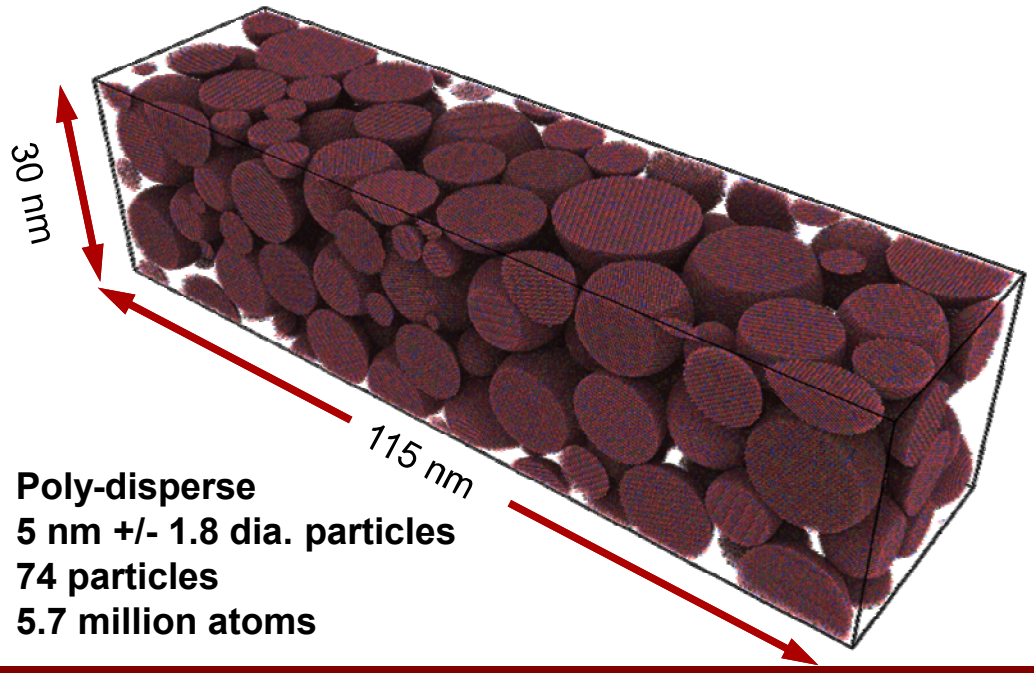
Nanoparticle powder beds

Mono-disperse
16 nm dia. particles
32 particles
5.8 million atoms





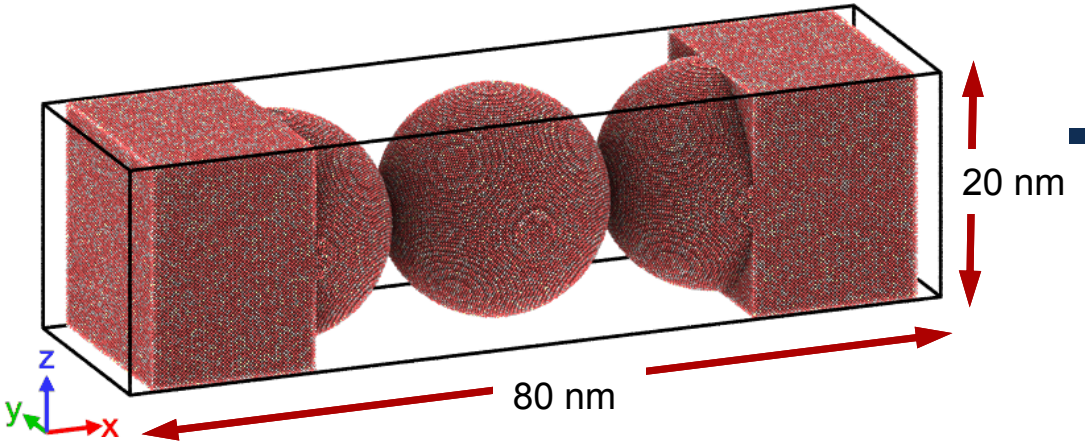
- Packed particle configurations are generated from DEM simulations
- Interstitial regions between particles are modeled as vacuum
- Particles are mobile, results in variations in contact area

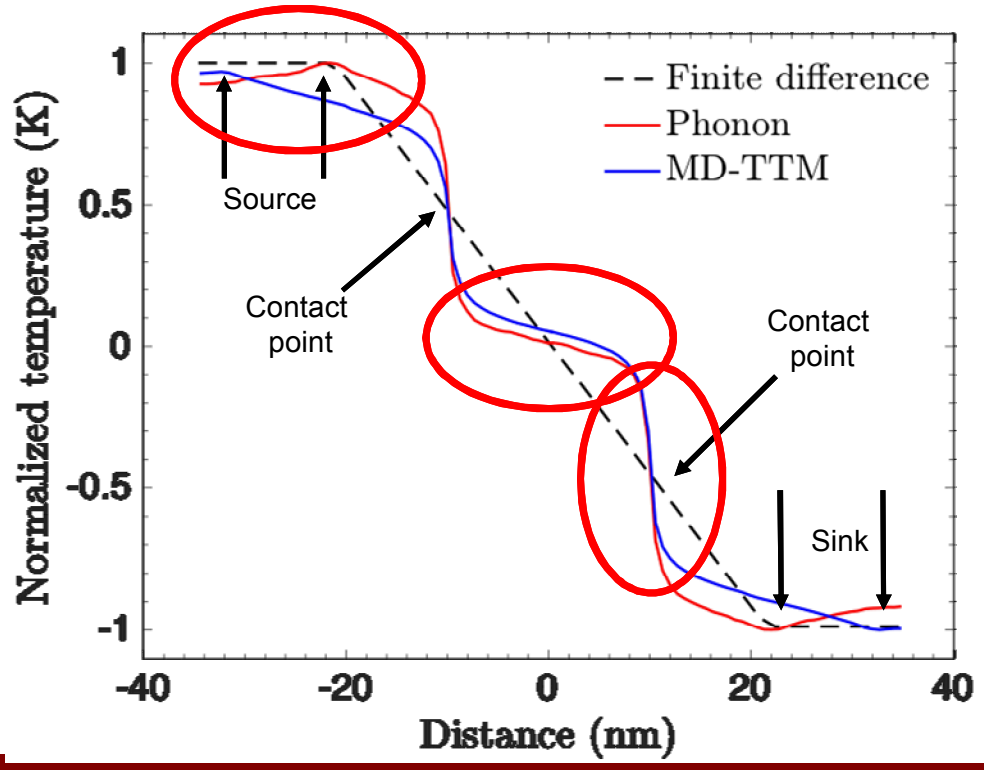


Poly-disperse
5 nm +/- 1.8 dia. particles
74 particles
5.7 million atoms

Using a similar approach to the determination of bulk conductivity properties, investigate size and distribution dependence on thermal conductivity

“Ideal” example of particle contact

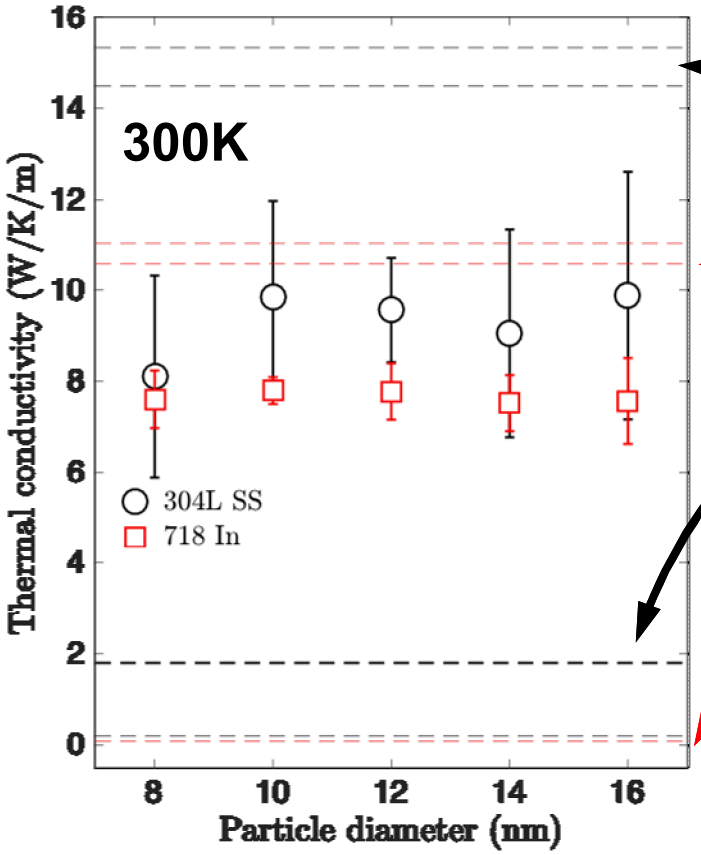




- Diffuse energy transmission within finite difference approach leads to linear profile within steady state
- Reflective phonon, phonon-phonon, and phonon-source/sink interactions give rise to topological information contained in profile

MD-TTM exhibits thermal profile consistent with present topology

Mono-disperse size dependence



304L SS: single crystal MD-TTM value with error Exp. 14.5 (W/K/m)

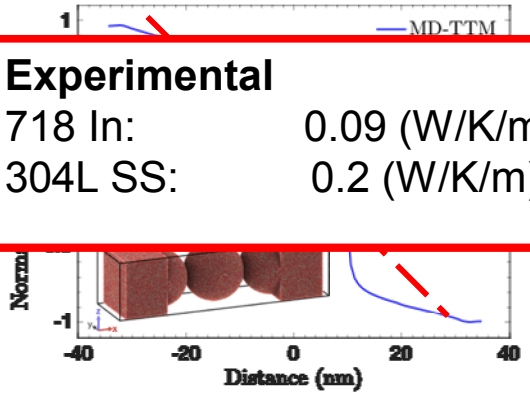
718 In: single crystal MD-TTM value with error Exp. 11.4 (W/K/m)

Estimate of lower bound 1.8 (W/K/m)

Experimental

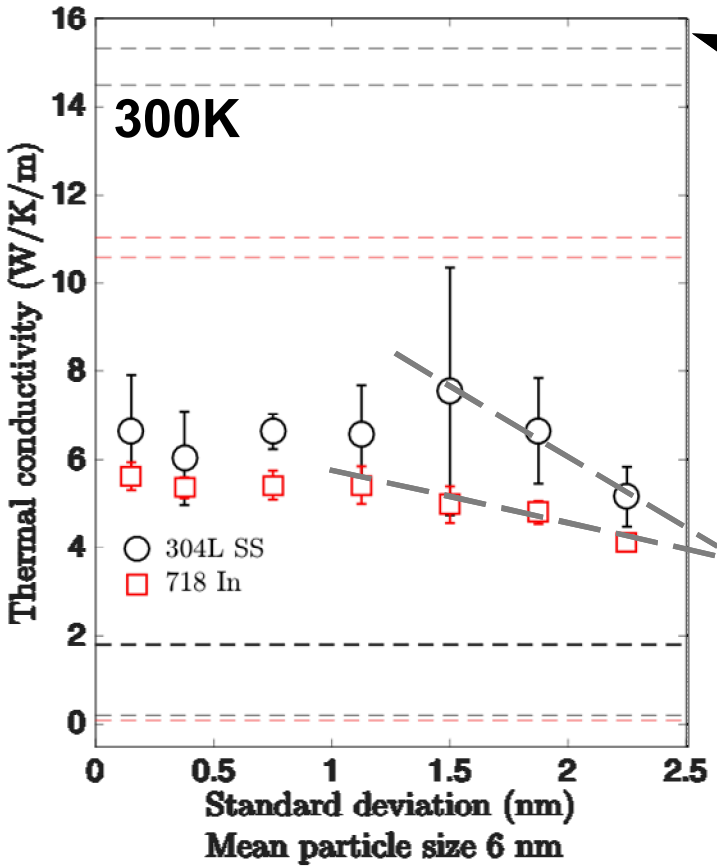
718 In: 0.09 (W/K/m)

304L SS: 0.2 (W/K/m)



- Mono-disperse beds exhibit a conductivity nearly a factor of 1.5 less than single crystal

Distribution dependence

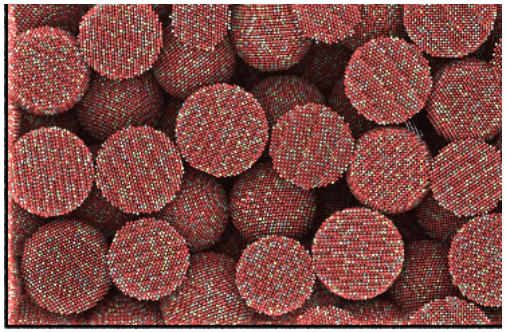


304L SS: single crystal MD-TTM value with error Exp. 14.5 (W/K/m)

718 In: single crystal MD-TTM value with error Exp. 11.4 (W/K/m)

- Poly-disperse beds exhibit a conductivity nearly a factor of 2 less than single crystal

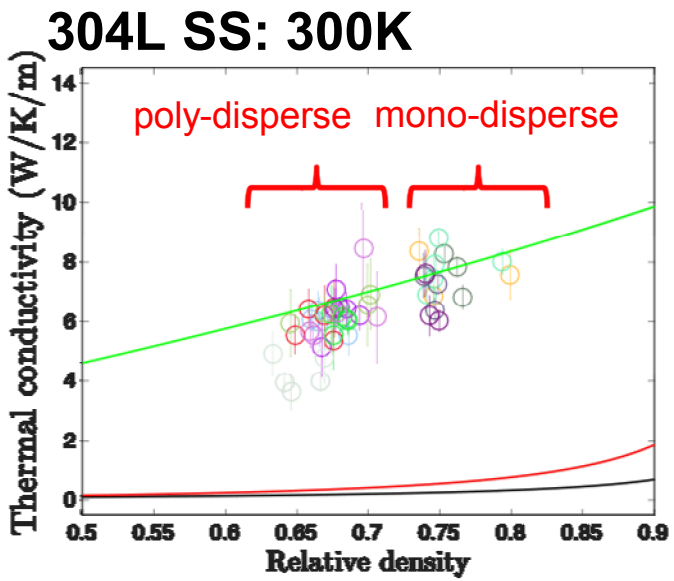
Trending behavior?

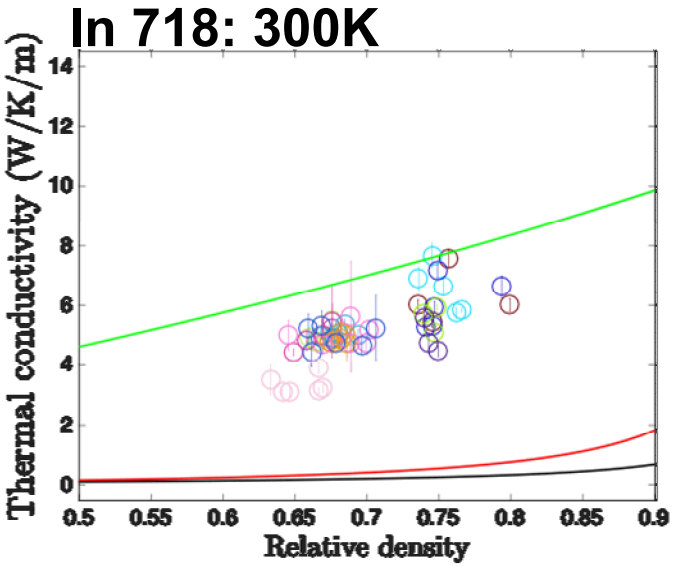


Lots of pathways

Fewer pathways

Relative density and analytical results





- Geometry based analytical models
  - contact area relative to particle size, effective conductivities (solidus/gas), effective porosity

Gonzo (2002)

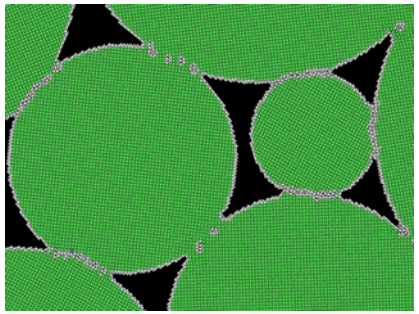
$$\frac{k_{\text{eff}}}{k_1} = \alpha \frac{[1 + 2\beta'(1-\phi)]}{[1 - \beta'(1-\phi)]}$$

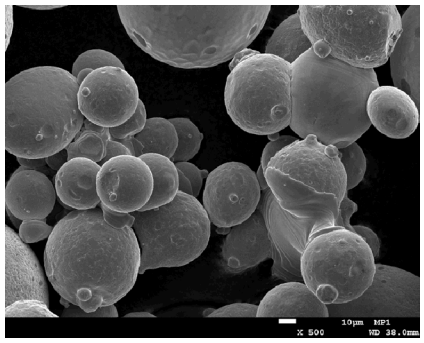
Chiew (1980)

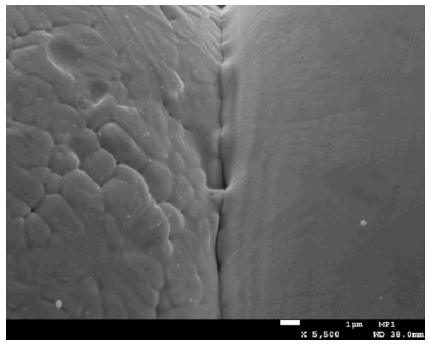
$$\frac{k_{\text{eff}}}{k_1} = \frac{1 + 2\beta\phi + (K_2 - 3\beta^2)\phi^2}{1 - \beta\phi}$$

Maxwell (1874)

$$\frac{k_{\text{eff}}}{k_1} = \frac{1 + 2\beta\phi}{1 - \beta\phi}$$

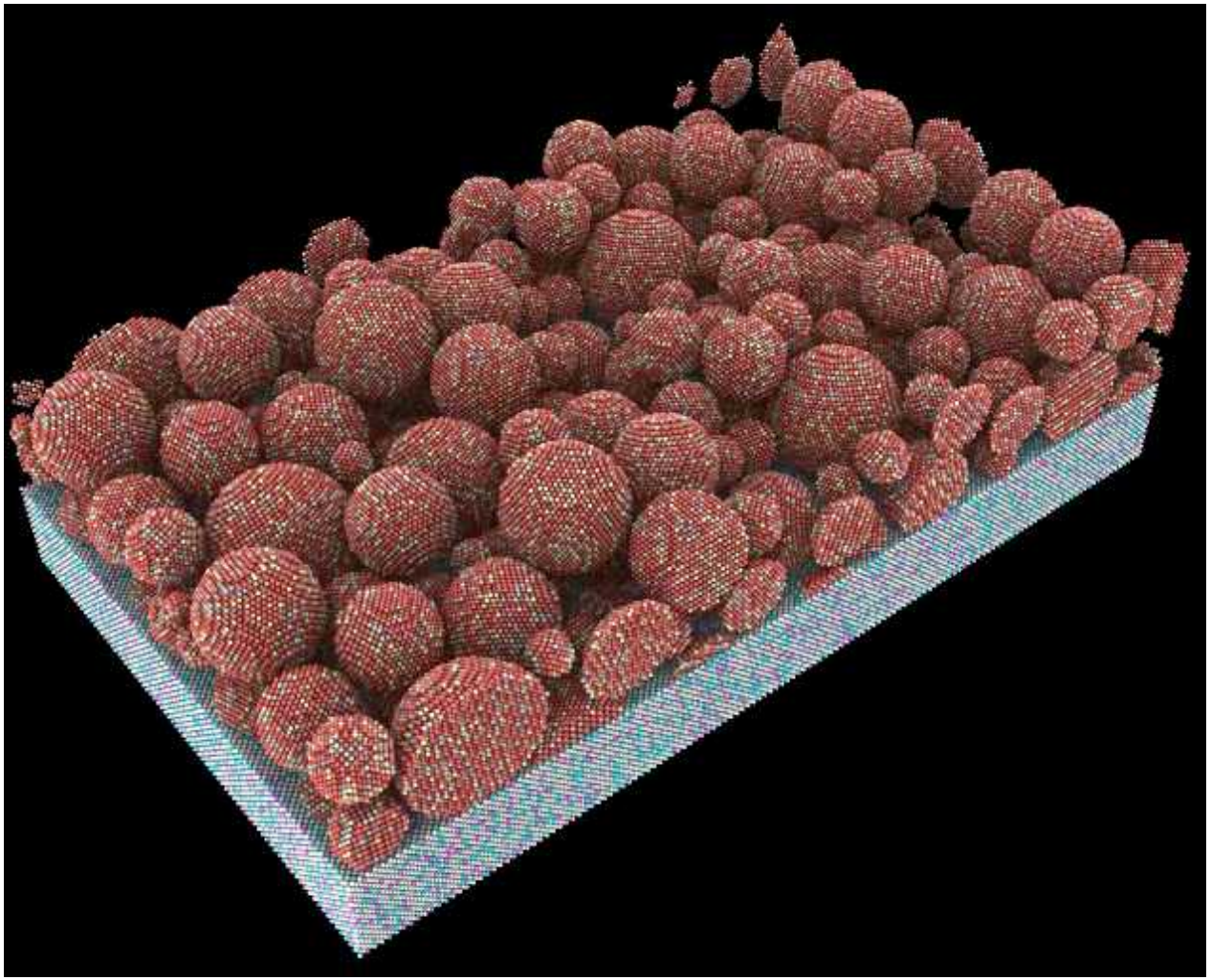






Slotwinski, J. of Research of the NIST (2014)

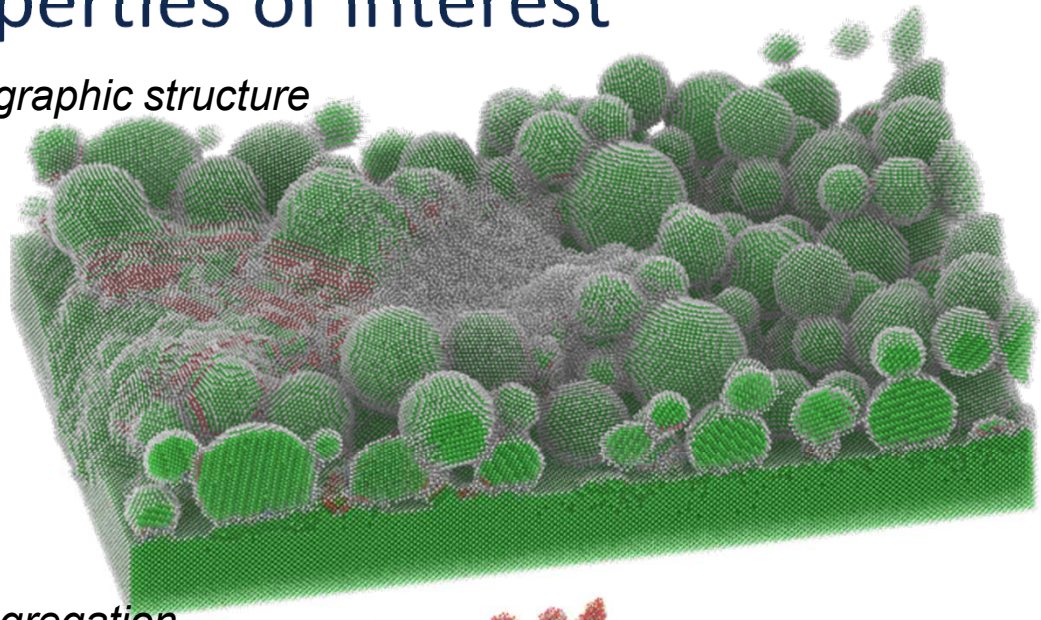
SLM in nanoparticle powder beds



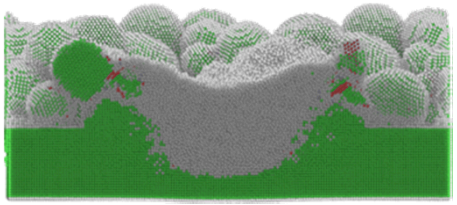
- ~200 W laser source
- Scan velocity: 10m/s
- Longest dimension ~100 nm

Properties of interest

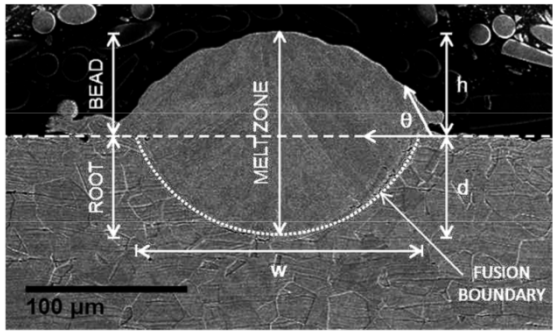
Crystallographic structure



Scan direction: Into page

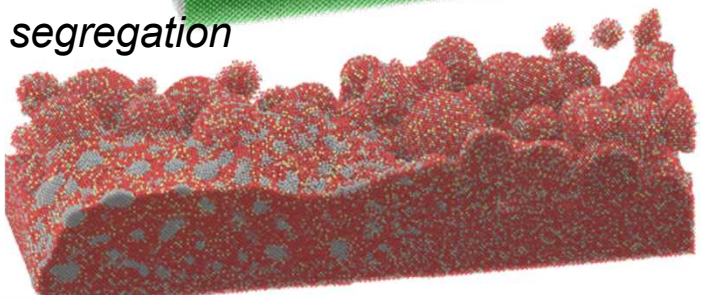


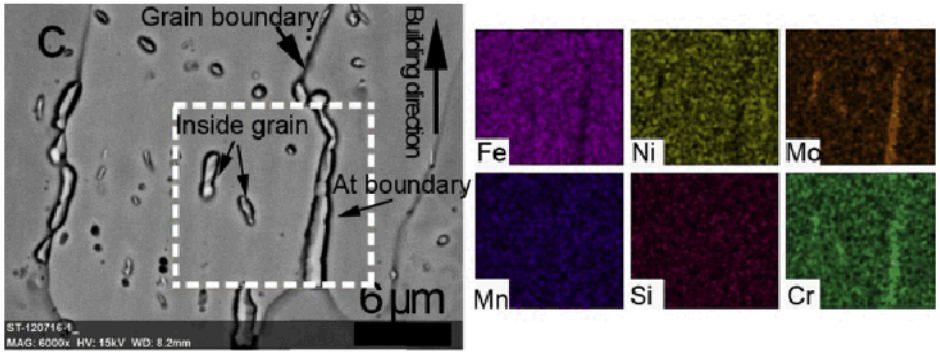
Defect nucleation and incomplete melting of powder



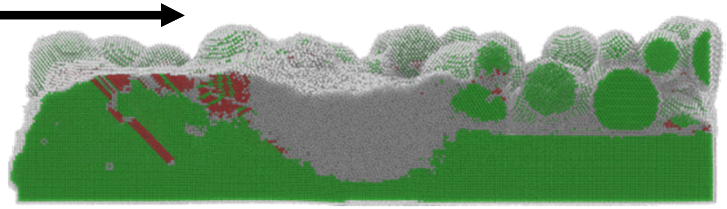
Roehling et al. Acta Materialia (2017)

Solute segregation





Scan direction

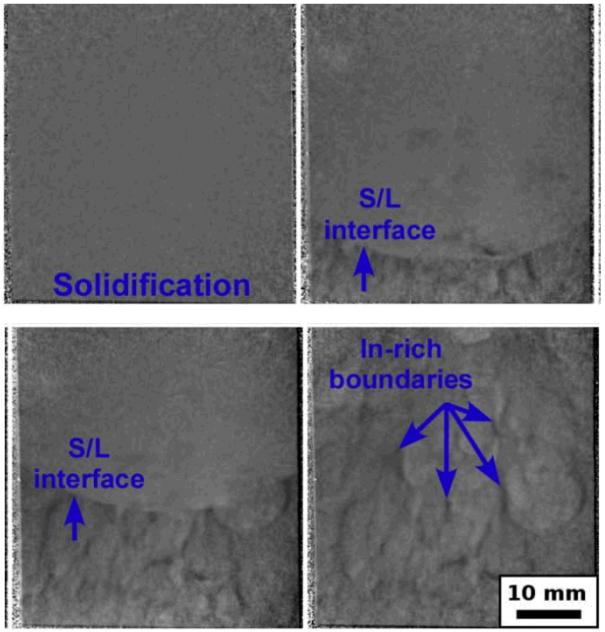


Powder size and distribution dependent melt pool geometries

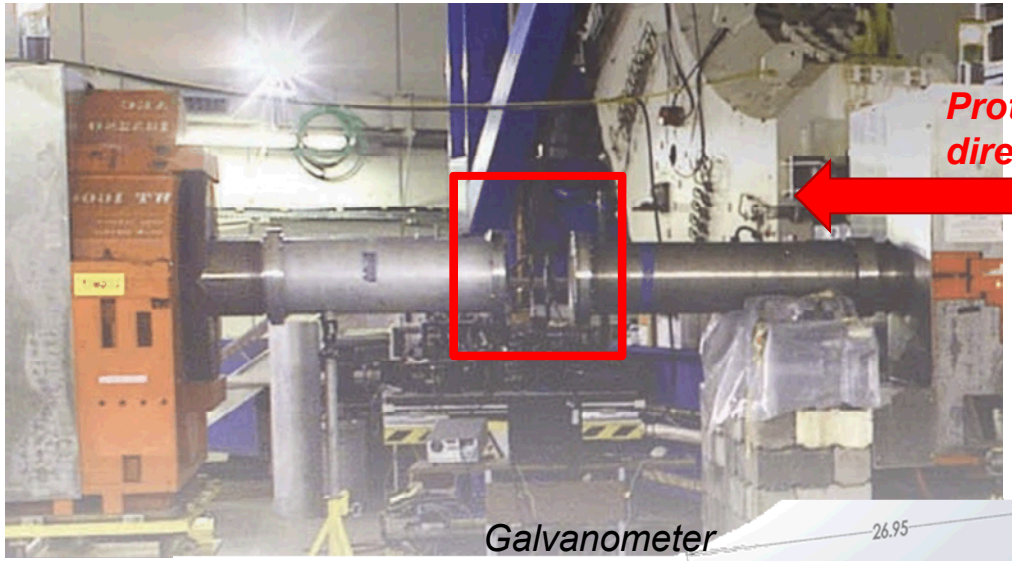
Zhong Y, J. Nuclear Mat. of (2017)

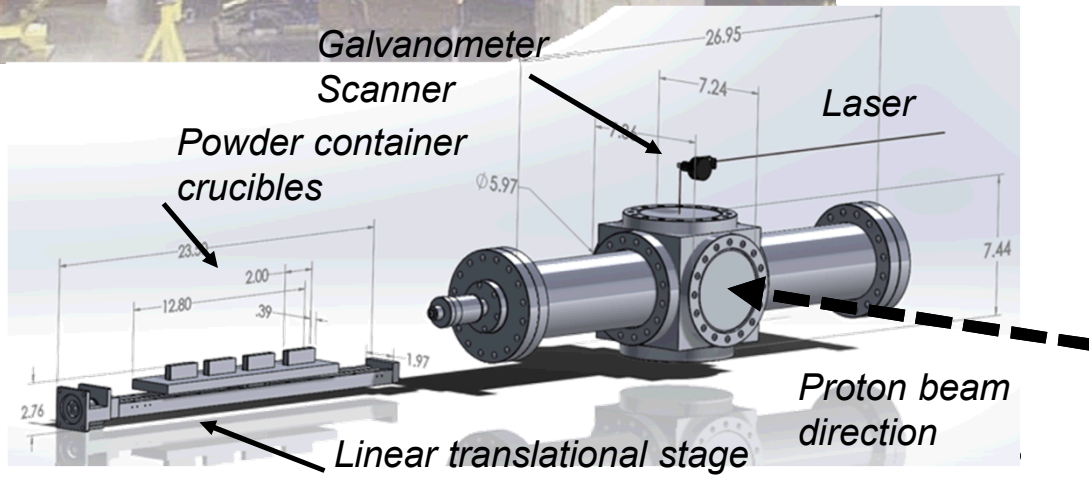
Model Validation

- Proposal to utilize LANSCE proton radiography facility at LANL
- Establish an *in situ* **through material** observation of melting and solidification
- Rapid 160 ns imaging frame rate



Clarke A., et al. Sci. Rep. (2013)





Summary

- Multiscale MD and continuum level model is utilized to study metal alloy particle systems. Determination of thermal conductivity and a single SLM laser pass is modeled in nano-scale powder beds.

- Model predicts conductivity values which extrapolate to bulk system properties accurately. Poly/mono-disperse results showed conductivity values near a factor of 2 lower than single crystal values, lacking size dependence, with decreasing trends with increasing width of distribution.

- “Direct method” indicates the importance of structural topology when features of interest are on the order of the MFP (particle contacts).

- Atomistic SLM process provides opportunity to investigate defect nucleation, solute segregation and melt pool geometry.