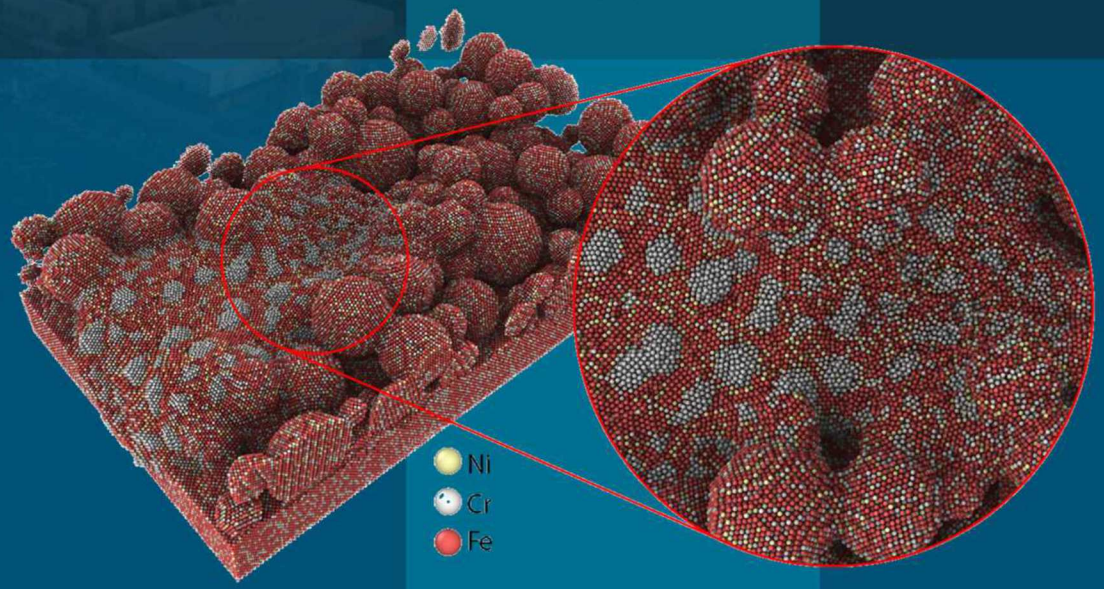
SAND2018-8843C

Effects of Elemental Segregation During Selective Laser Melting from Atomistic Simulations



PRESENTED BY

Mark Wilson, Andrew Kustas, and Michael Chandross

Computational Materials and Data Science

Sandia National Laboratories, Albuquerque, New Mexico

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.

Born Qualified Vision – additive manufacturing at Sandia

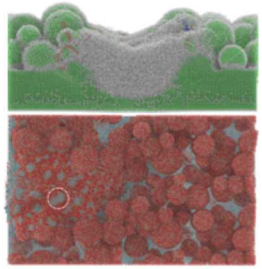
Part Scale Thermal & Solid Mechanics
Kyle Johnson, Kurtis Ford & Joe Bishop

Mesoscale Thermal Behavior
Mario Martinez & Brad Trembacki

Powder Spreading
Dan Bolintineanu

Part Scale Microstructure
Theron Rodgers

Powder Behavior
Materials modeling
Mark Wilson

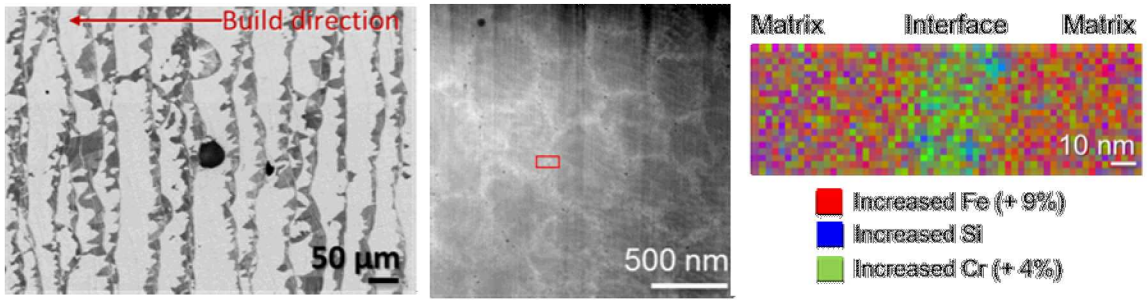


Mesoscale Texture/Solid Mechanics/CX
Judy Brown, Theron Rodgers and Kurtis Ford

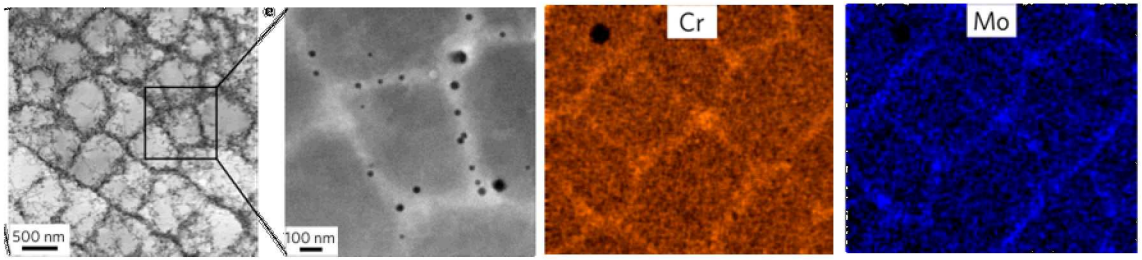
10^{-8} 10^{-6} 10^{-4} 10^{-2} 1

Length Scale (m)

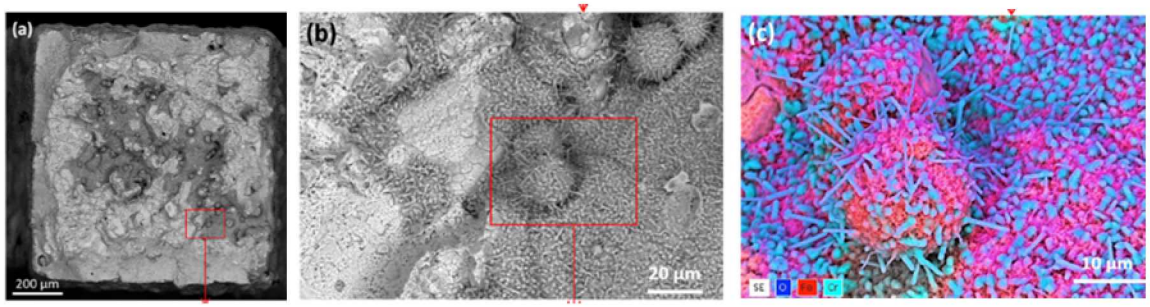
Chromium segregation is prevalent in AM of stainless steels



Schindelholz E., et al. J. of Electrochem. Soc., 2018

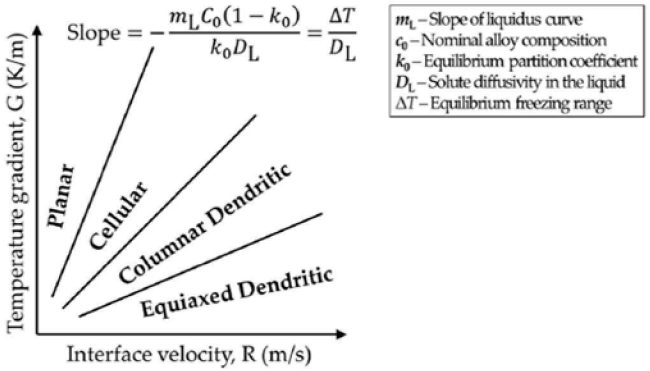


Wang, Y.M., et al. Nature Materials, 2017

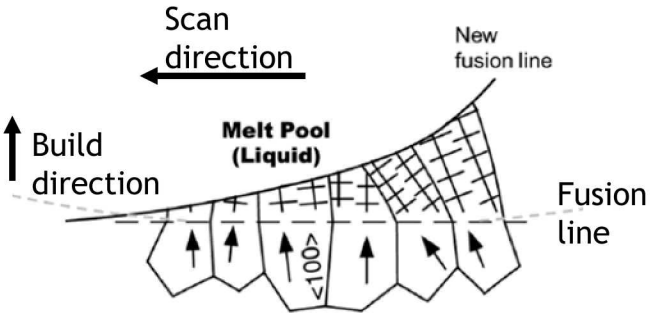


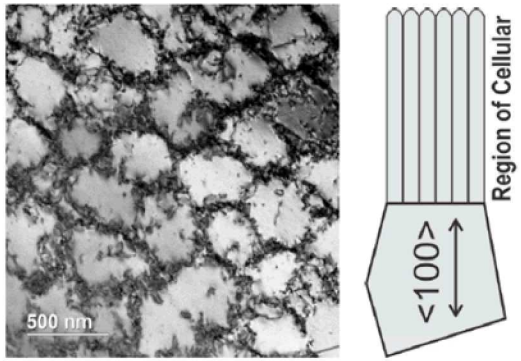
Boyce, B., Advanced Engineering Materials, 2017

Mechanism for solute segregation



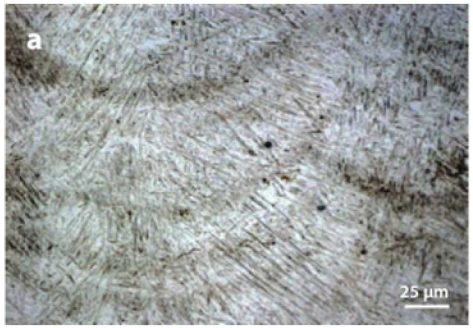
Fuyao Y. et al., Materials 2017

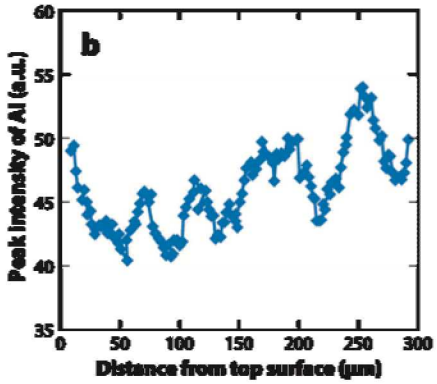




Wang, Y.M., et al. Nature Materials, 2017

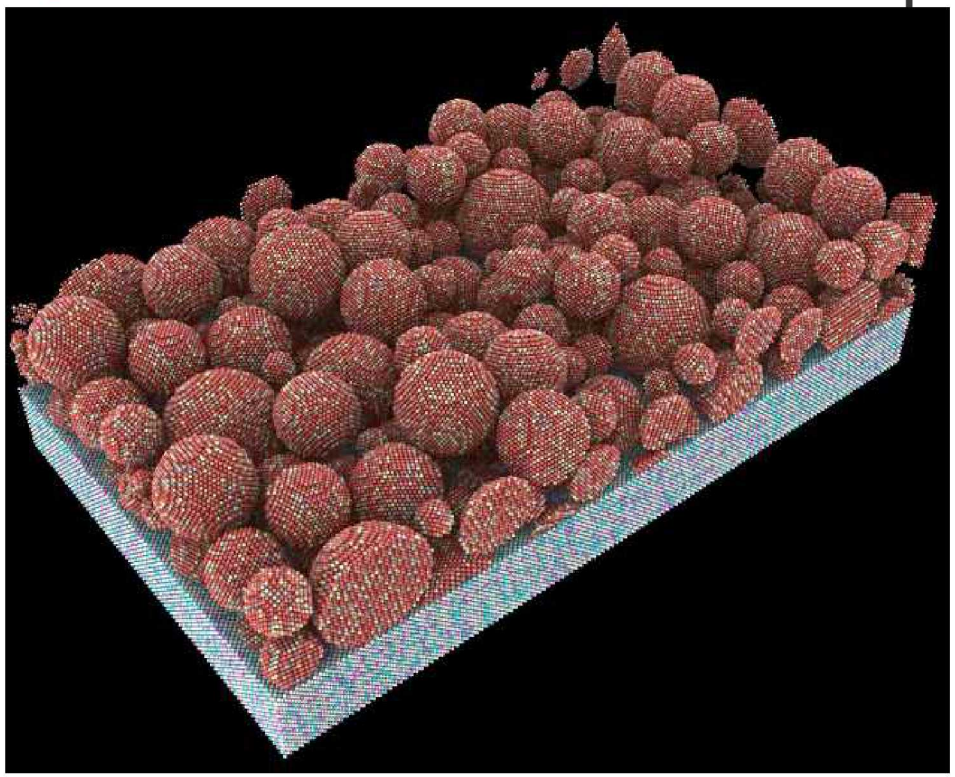
- Resultant microstructure is dependent upon the relationship between temperature gradient and solid-liquid interface velocity (G/R)
- Typically columnar-dendritic occur at the extents of the melt pool (largest temperature gradient) with equiaxed at surface
- Solute trapping – Diffusion limited process where cooling rates are sufficient to solidify into a non-equilibrium state

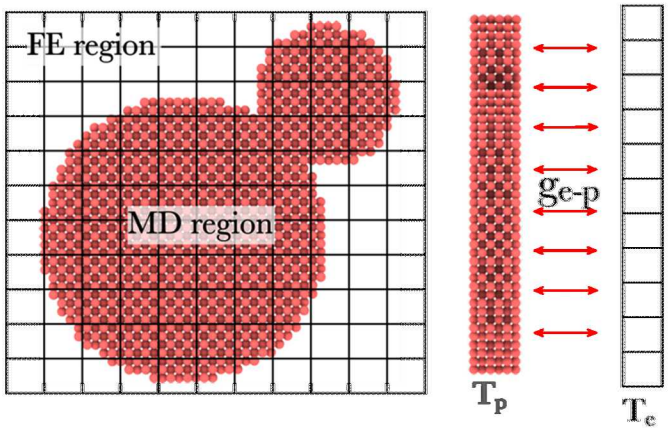




Berhaeghe, T., et al. Acta Mater. 2010

Multi-scale model of SLM process





Model parameterization

- Heat capacity: $C_e\,\rho_e$
- Conductivity: κ_e
- Electron-phonon coupling: g_{e-p}
- Damping coefficient: $\gamma_i = \gamma_p + \gamma_s$.
- Material approximation $Fe_{0.7}Cr_{0.18}Ni_{0.12}$

Material properties

$$C_e\,\rho_e\frac{\partial T_e}{\partial t} = \nabla(\kappa_e \nabla T_e) + g_{e-p}(T_e - T_a) + \alpha I_0 \beta \exp\left[-2\left(\frac{(x-x_l)^2}{\omega_x^2} + \frac{(y-y_l)^2}{\omega_y^2}\right) - \beta z\right]$$

Heat equation

electron-phonon coupling

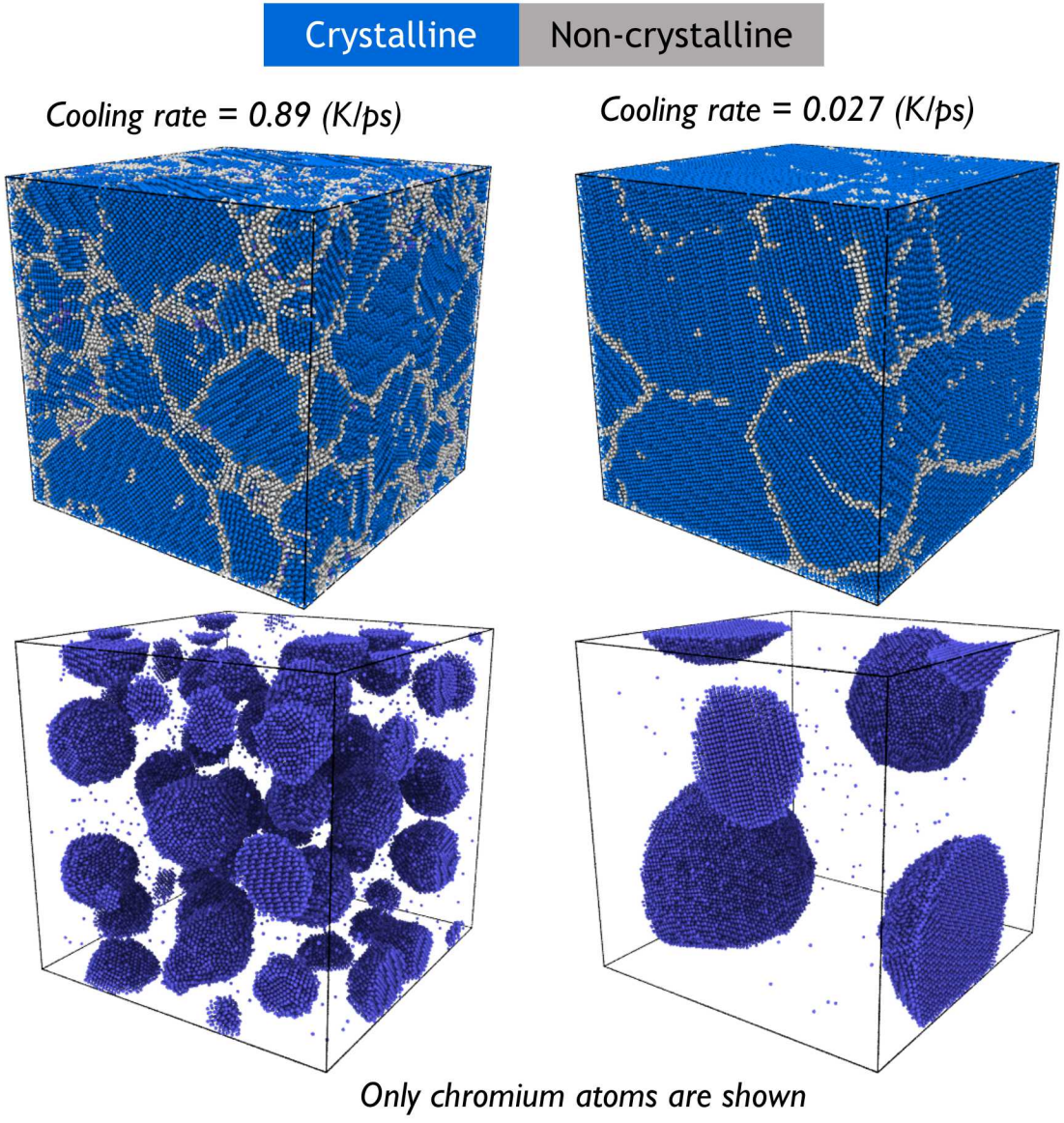
Gaussian energy source

- Source intensity I_0
- Spatial damping β
- Absorptivity α
- Source geometry ω_x , ω_y

Energy source properties

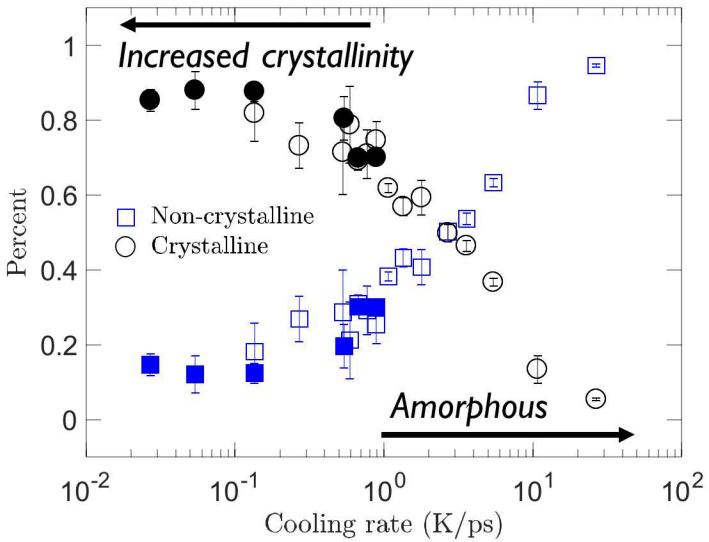
Similar to experiment, the SLM model also segregates chromium

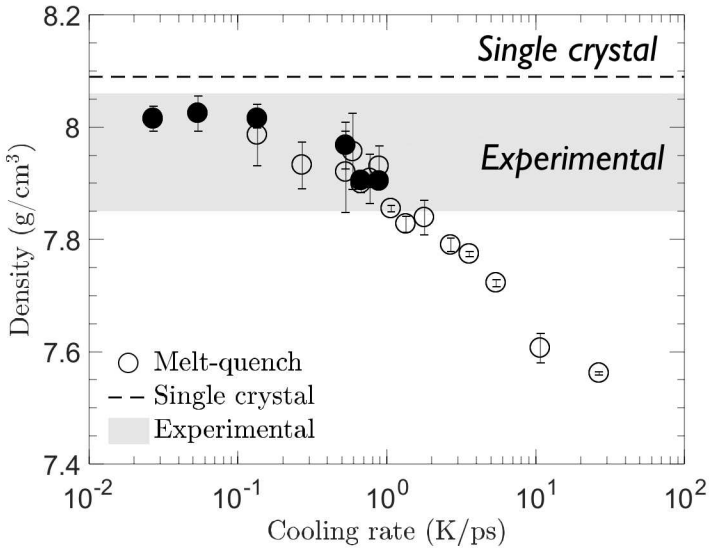
Structural properties

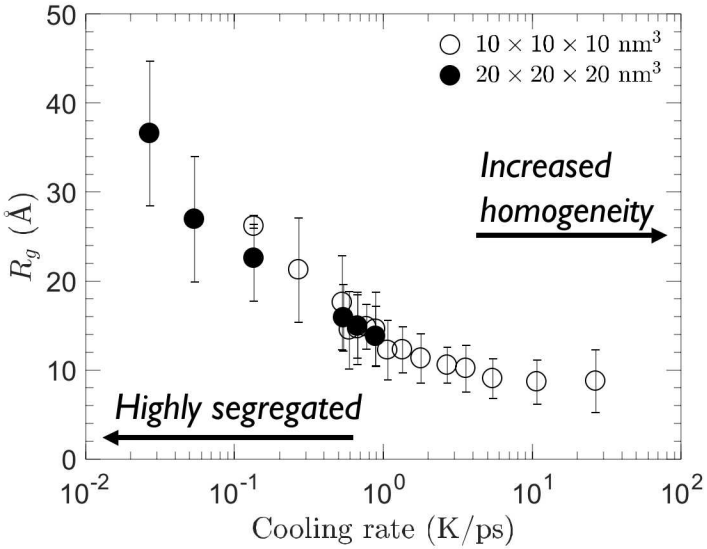


- Melt-quench procedure is performed with a linear temperature ramp to 300K
- Utilize a common neighbor analysis to identify crystalline structure
- Slower cooling rates develop increasing amounts of structure, with small percentages of interstitial structure (grain boundaries)
- Chromium is observed to localize oval regions that grow with lower cooling rates
- Diffusion limited process consistent with a solute trapping

Structural properties (cont.)

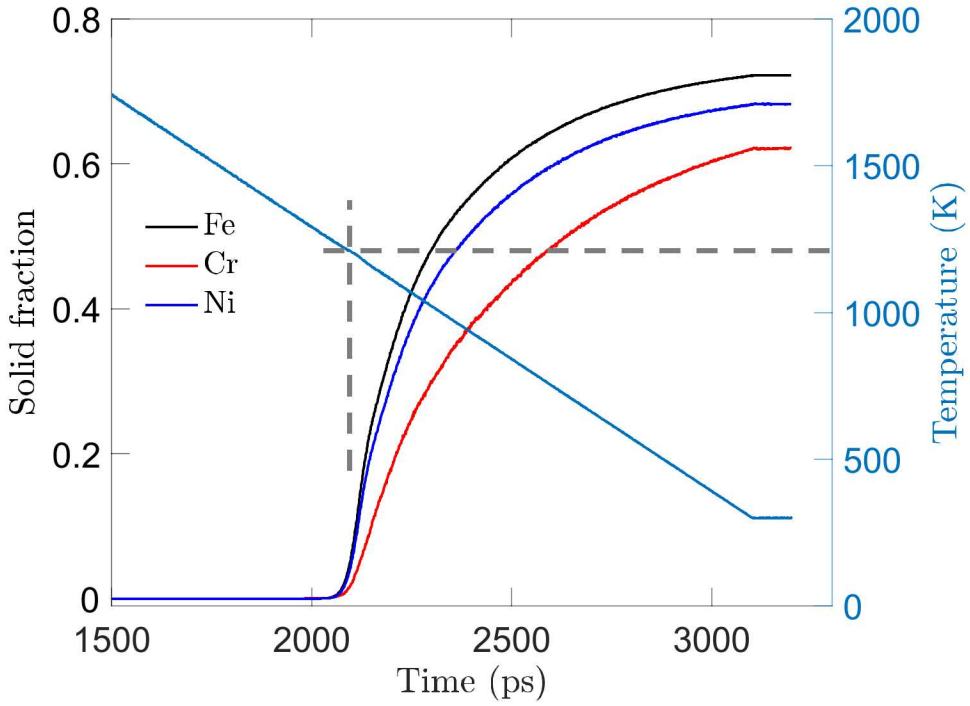






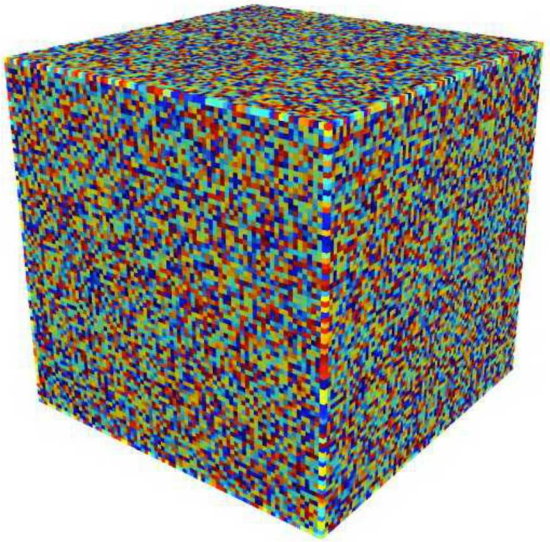
- Slower cooling rates develop increasing amounts of crystalline
- Decreasing rates show increases in density towards single crystal values (dashed lines). Experimental range is highlighted in grey.
- Use radius of gyration as a measure of chromium rich regions

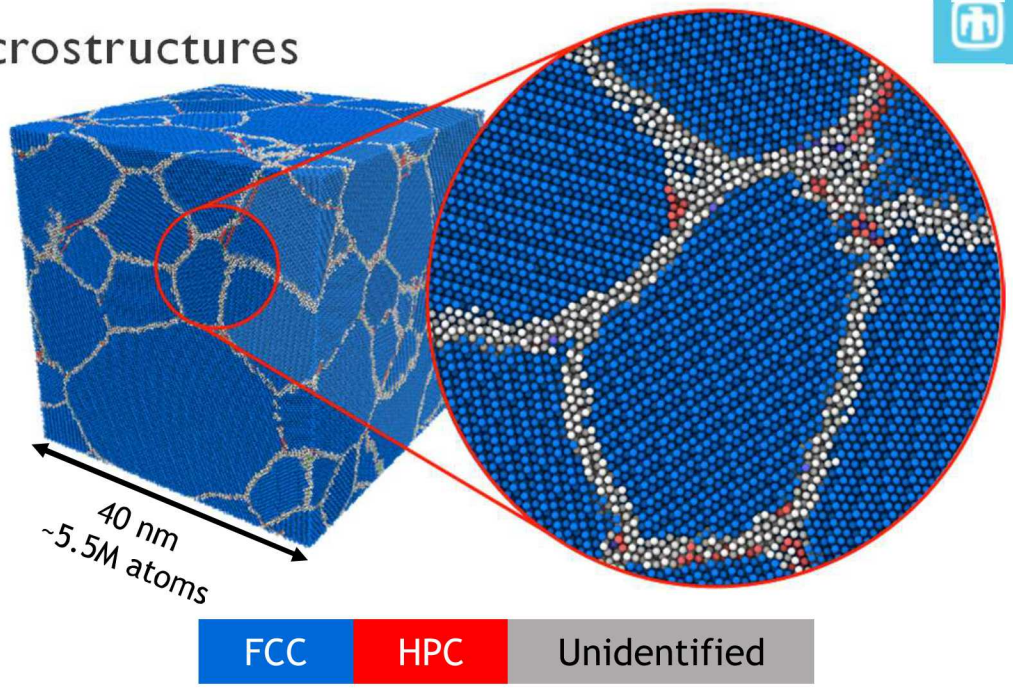
Elemental solidification

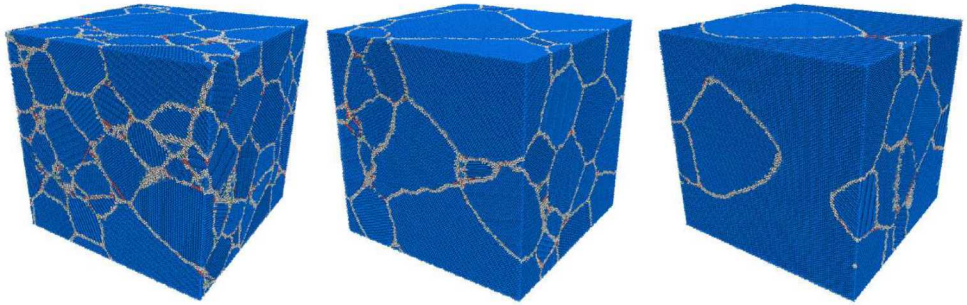


- Elemental, time dependent solid fraction indicates a chromium rich liquid phase
- Simulation is significantly undercooled with melt temperature of 304L SS ~1700K
- MD potential provides segregation properties as expected from rapid solidification process
- Simulation shows that changes in cooling rate can give rise to variations in structure and solute segregation
- Can we systematically study grain size and segregation effects on material properties?

Construction of atomistic microstructures



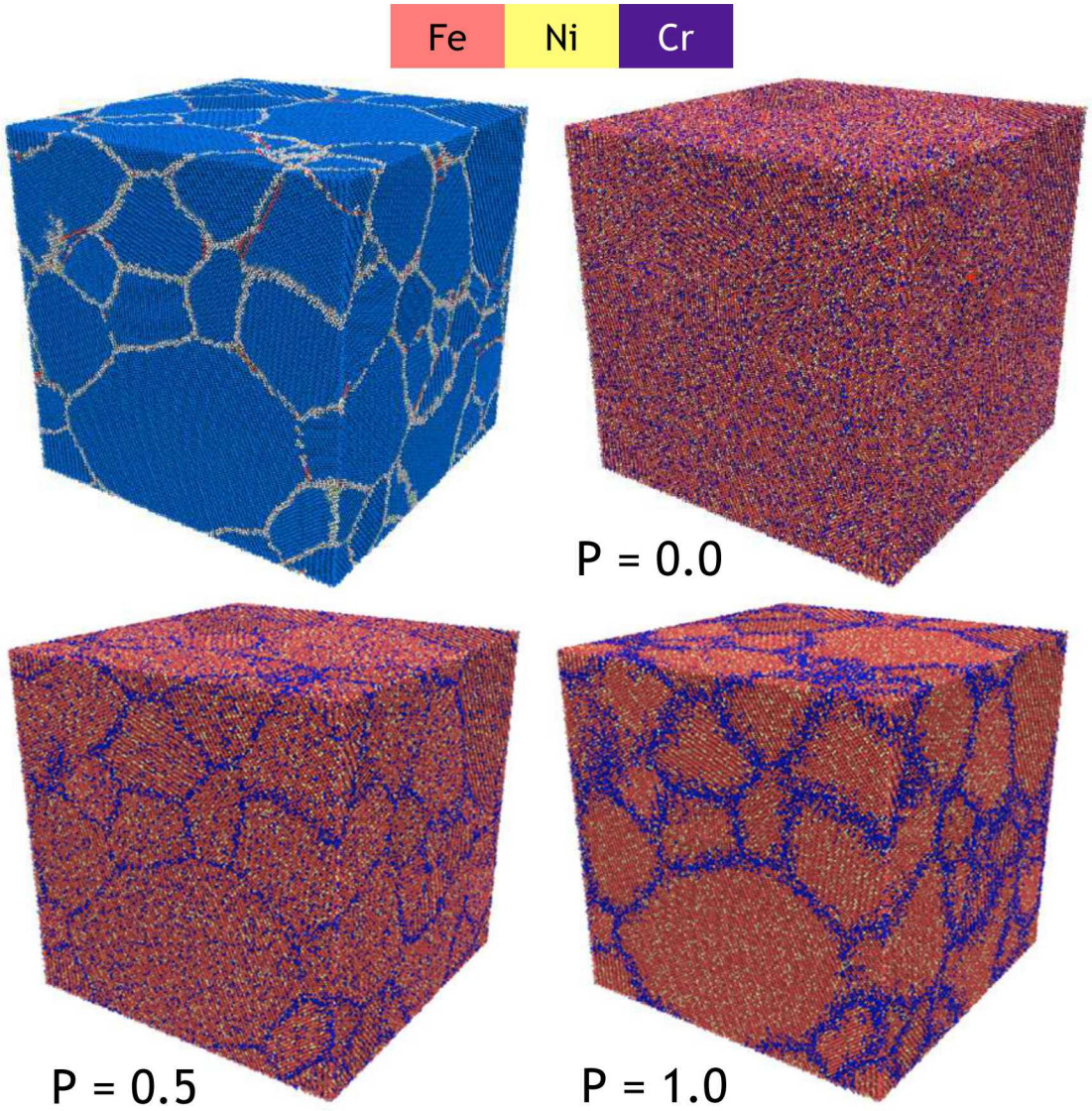




Average dia. = 8.0nm *Average dia. = 11.1nm* *Average dia. = 15.3nm*

- Evolution of probabilistic Pott's model provides volumetric microstructures
- Fill grain volumes with rotated atomic crystalline structures and anneal
- Build configurations with increasing average grain size

Elemental segregation of chromium

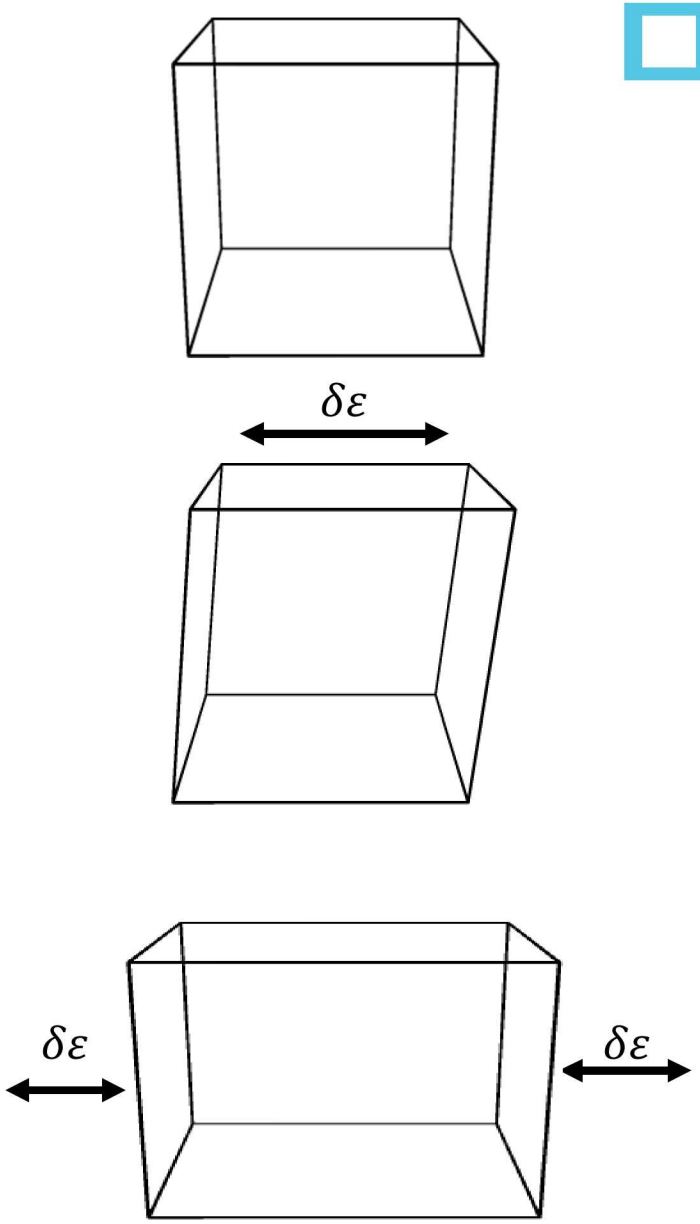


- Assign atom types probabilistically according to weight percentage $\mathrm{Fe_{0.7}Cr_{0.18}Ni_{0.12}}$
- The location of chromium atoms are preferentially placed on grain boundaries with a given probability (P)

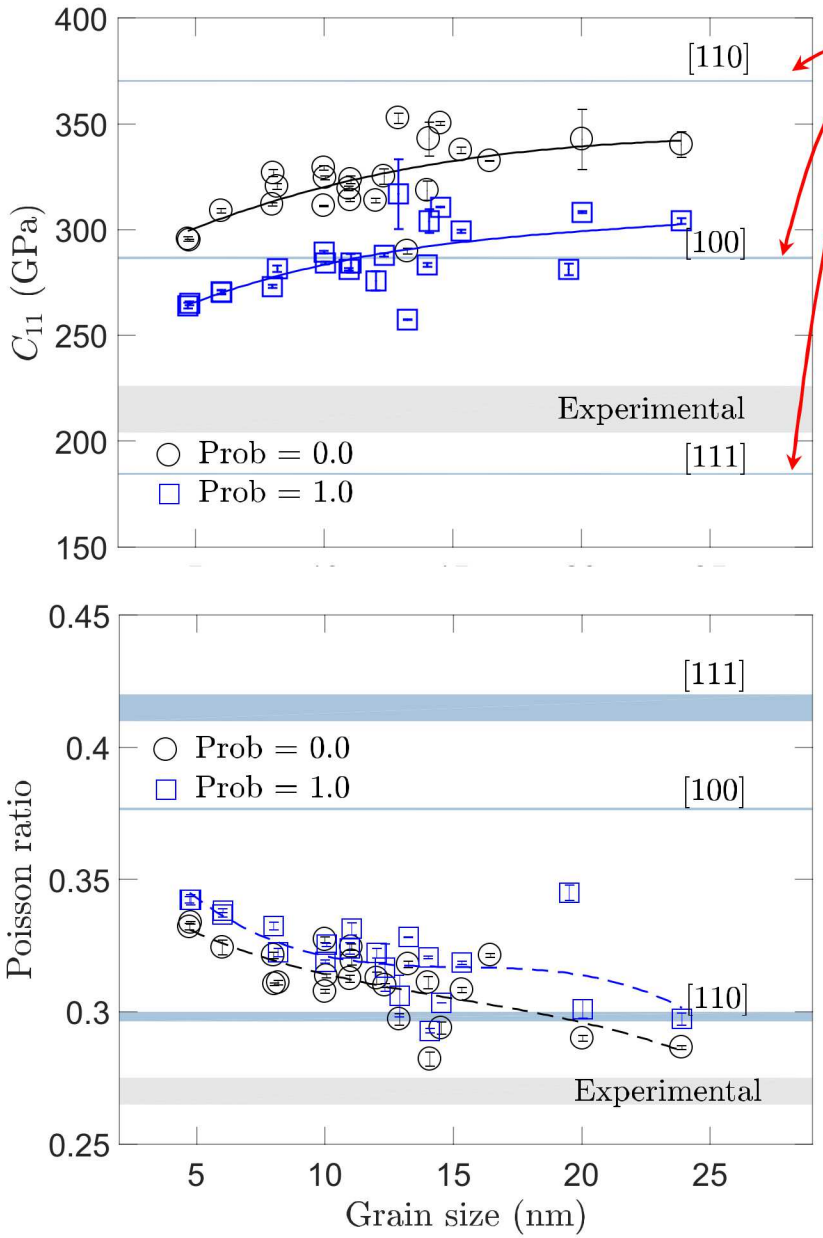
Elastic properties of single crystal

- Stress/pressure tensor is calculated, making small strain perturbations about equilibrium configurations
- Properties are a function of the MD potential, average results of tensor over a linear range of stress response
- Pure elemental moduli are in excellent agreement with experimental values, however the SS alloy is a different story

Property	Single crystal	Experimental
Density (g/cm3)	8.09 +/- 0.0006	7.85 - 8.06
C_{11} (GPa)	286.26 +/- 0.10	190 - 203
C_{12} (GPa)	172.84 +/- 0.05	132 - 135
C_{44} (GPa)	140.09 +/- 0.13	111 - 122
Bulk Modulus (GPa)	210.58 +/- 0.18	134 - 151
Poisson ratio	0.38+/-0.0001	0.265-0.275



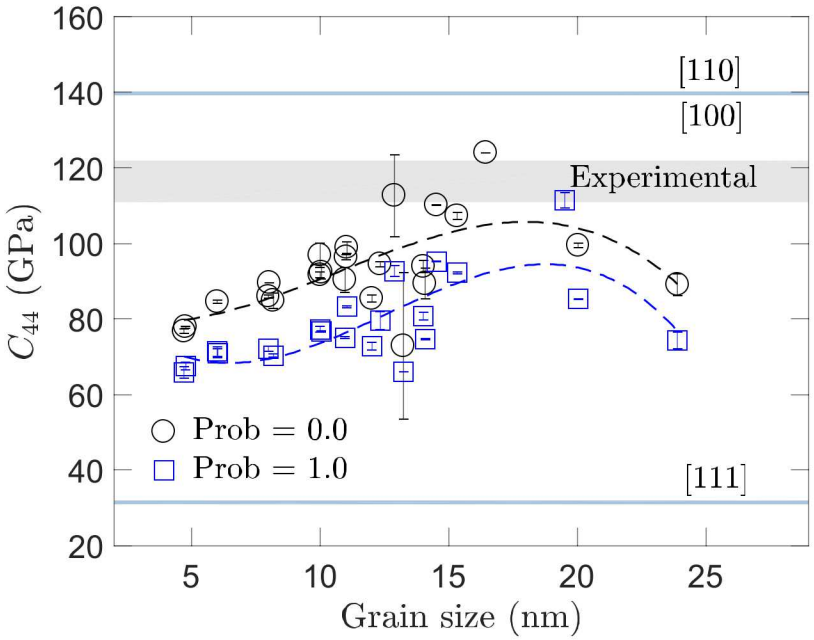
Elastic properties

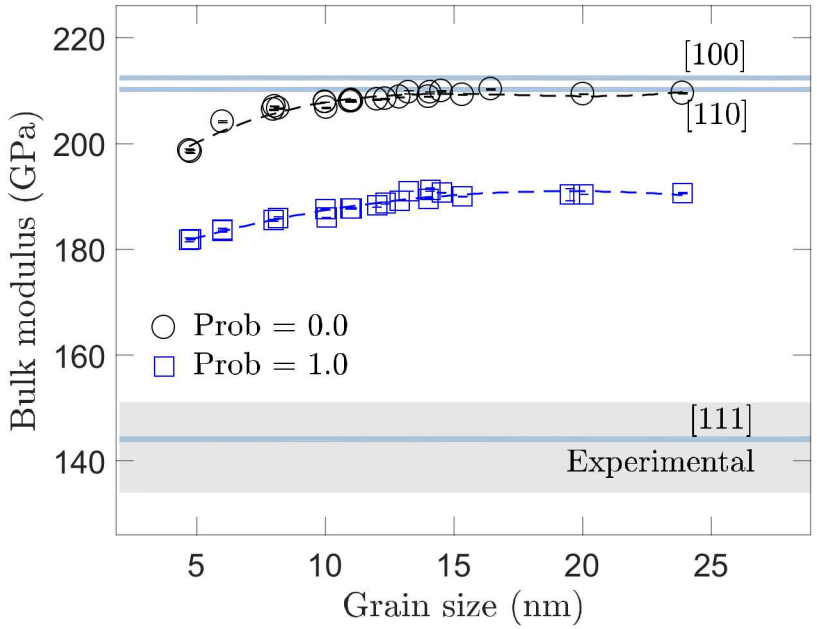


Single crystal orientation orthogonal to applied strain in [100]

- Averages and error bars are determined from the $\delta\varepsilon$ strain dependence of the MD potential
- Similar behavior for both probabilities of segregation is due to same crystalline structure
- Rule-of-mixtures should apply. Texture plays an important role here
- Segregated systems (squares) show lower C_{11} values relative to homogeneous polycrystalline alloy

Elastic properties (cont.)

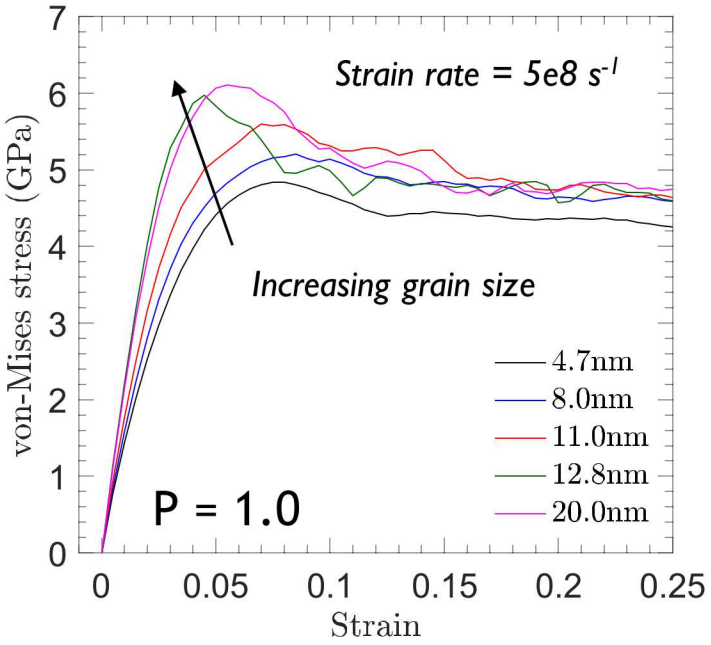


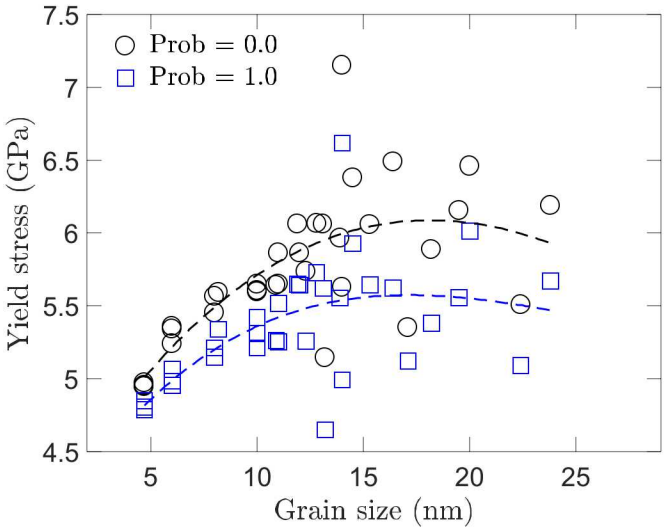


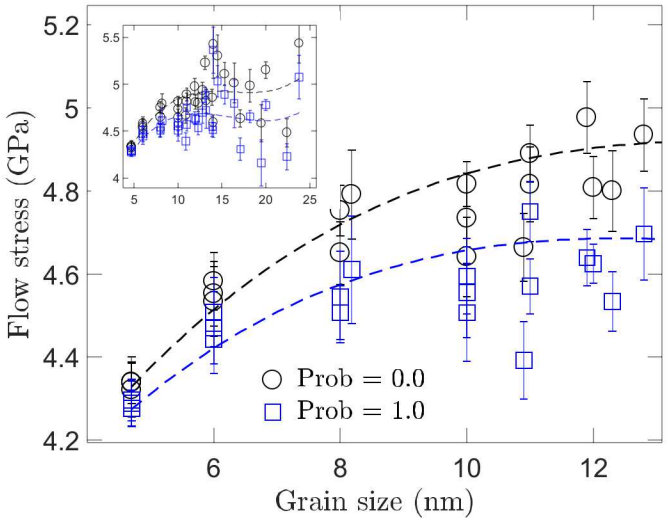
- Segregated systems show lower C_{44} and Bulk moduli values relative to homogeneous polycrystalline alloy
- Again, softening behavior is observed in both shear and compression

Mechanical properties

- Von Mises stress determined from dynamic uniaxial tension simulations
- Yield stress indicates trending behavior with increased grain size and chromium segregation
- Increase in yield stress and flow stress with grain size is suggestive of inverse Hall-Petch type behavior







Summary

- Atomistic molecular dynamics simulations are performed, modeling a single "laser" pass within a powder bed fusion process for a 304L SS. Chromium segregation is observed during solidification.
- Softening of the segregated alloy is observed with increased Poisson ratio and decreased moduli.
- Grain size dependence, along with yield and flow stress shows increasing trends providing evidence of inverse Hall-Petch behavior.
- Microstructure and solute segregation are coupled through cooling rate, but have independent effects on final material properties.
- Potentially tune part performance, modifying microstructure and segregation properties through their cooling rate dependence.