Computational Micro(μ)-structure Physics Group

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XSEDE
Extreme Science and Engineering Discovery Environment

DISCOVER INNOVATE ARL TRANSITION

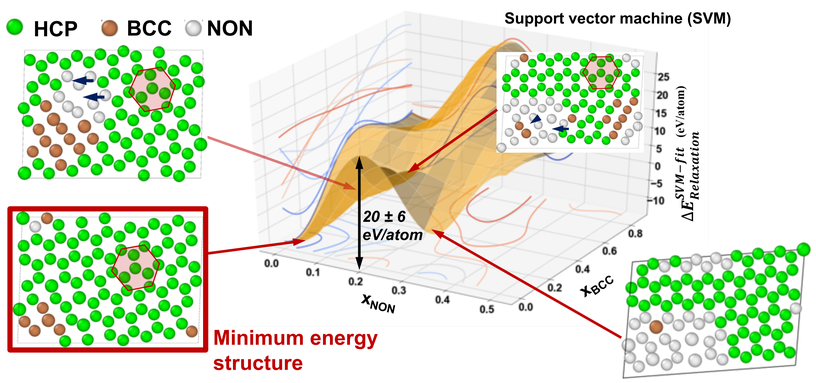
Phase transformations, dislocation plasticity & microstructure evolution

Time

10^{-1} - 10^{4} s

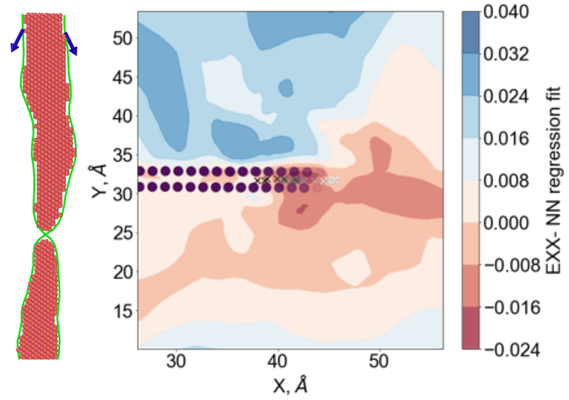
Atomistics-ML coupling for accessing higher temporal & spatial scales

Map equilibrium energy-structure surface for precipitation in alloys



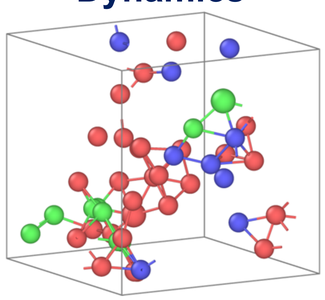
Energy landscape as input for meso-scale simulations

Extract continuum fields around defect substructures

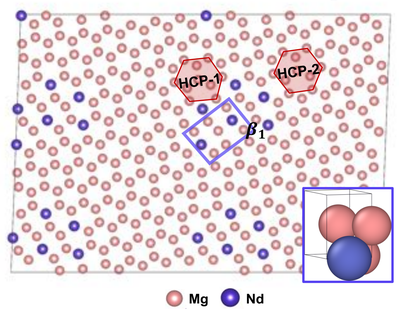


Nucleation in liquid and solid states

Liquid structure from *ab inito* Molecular Dynamics

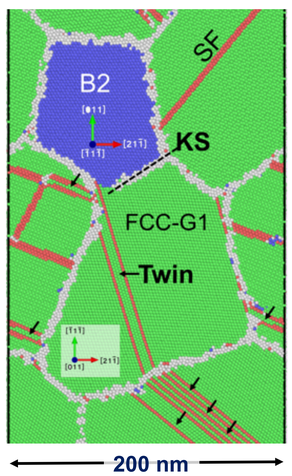


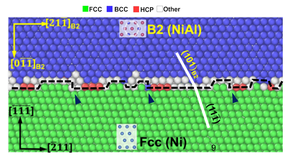
Precipitate structure from Kohn-Sham density functional theory



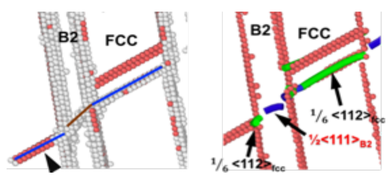
Microstructurally informed simulations

Molecular dynamics of microstructures with orientation relationships





Kurdjumov-Sachs (KS) interface



Slip transfer across a Kurdjumov-Sachs interface

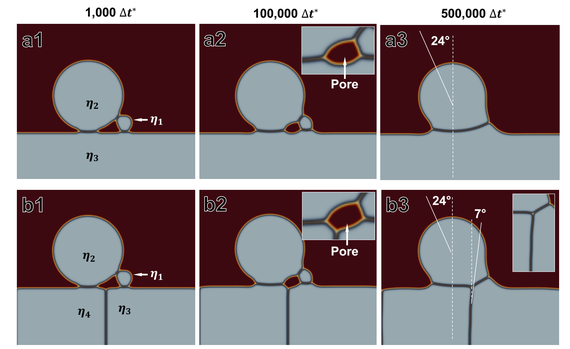
Mesoscale simulations of processes

Phase-field modelling of multi-particle solid-state sintering process

$$F = \int_V \left[f(\rho, \eta_i) + \frac{1}{2}\kappa_\rho |\nabla\rho|^2 + \frac{1}{2}\sum_{i=1}^{i=N} \kappa_{\eta_i} |\nabla\eta_i|^2 \right] dV$$

$$\frac{\partial\rho}{\partial t} = \nabla . D \nabla \frac{\delta F}{\delta \rho}$$

$$\frac{\partial\eta_i}{\partial t} = -L\frac{\delta F}{\delta \eta_i}$$



Selected publications

1. Choudhuri, D., **Matteson, S***. and **Knox, R.***, Nucleation of coupled body-centered-cubic and closed-packed structures in liquid Ni-Cr alloys. *Scripta Materialia*, *199*, p.113857. (2021)
2. Local structure and bonding environment of intermetallic β1 precipitate phase nucleus in binary Mg-Nd. *Computational Materials Science*, *187*, p.110111. (2021)
3. Choudhuri, D. and **Blake, L.***, Particle curvature effects on microstructural evolution during solid-state sintering: phenomenological insights from phase-field simulations. *Journal of Materials Science,* 56(12), pp.7474-7493. (2021)
4. Structural changes during crystallization and vitrification of dilute FCC-based binary alloys. *Materialia*, 12, p.100816. (2020)
5. Choudhuri, D. and **CampBell, A.***, Interface dominated deformation mechanisms in two-phase fcc/B2 nanostructures: Nishiyama-Wasserman vs. Kurdjumov-Sachs interfaces. *Computational Materials Science*, 177, p.109577. (2020)
6. **Paranjape, P.***, Srinivasan, S.G. and Choudhuri, D., Correlation between bonding, vacancy migration mechanisms, and creep in model binary and ternary hcp-Mg solid solutions. *Journal of Applied Physics*, 128(14), p.145103. (2020)
7. Deformation of lamellar FCC-B2 nanostructures containing Kurdjumov-Sachs interfaces: Relation between interfacial structure and plasticity. *International Journal of Plasticity*, 125, pp.191-209. (2020)
8. Enhancing strength and strain hardenability via deformation twinning in fcc-based high entropy alloys reinforced with intermetallic compounds. *Acta Materialia*, 165, pp.420-430. (2019)

* Student co-authors

10^{-9} s

10^{-12} s

10^{-10} m

10^{-9} m

10^{-6} m

Length