Mesoscale Priority Research Direction

Predicting Mesoscale Material Kinetics with Atomistically-based Computation

Opportunity

Materials design often plays kinetics against the equilibrium phase diagram to create materials with novel functionality due to structure at the mesoscale. Today, as the materials community turns to self-assembly and additive manufacturing, control of the mesoscale kinetics is becoming important in an ever broader range of materials. With time and length scales too large for MD and too small for conventional continuum techniques, new approaches are needed to understand and control kinetics at the mesoscale. These approaches must have the predictive power of atomistic methods but be able to handle the mesoscale.

Approach

As supercomputers approach the exascale, several techniques are emerging to predict mesoscale kinetics:

- Phase field modeling informed by ab initio and MD results for free energies and transport models, linked by:
  - Information passing with pre-computation,
  - Top-down multiscale via in-situ tabulation.
- Nucleation rates from transition state theory, metadynamics, non-equilibrium MD and off-lattice KMC.
- Leveraging the push to exascale computation to do explicit verification of mesoscale kinetics models through judicious use of extremely large-scale simulation.

Meso Challenge

- Can rates of non-equilibrium mesoscale processes be predicted: microstructural evolution in Li-ion battery electrodes, failure processes in advanced turbine composites, swelling in irradiated materials?
- How can successful nanoscopic computational methodologies (DFT, classical MD, etc.) be extended to predict mesoscale rates when the time and length scales are beyond their conventional capabilities?

Impact

Mesoscale material systems important for our energy future depend on kinetics that are inherently mesoscopic:

- Energy storage systems: fabrication and operation of next-generation electrodes for batteries, supercapacitors.
- Nuclear energy materials: design and synthesis of microstructures and their evolution during aging.

References: A. Arsenlis et al., Comp. Meth. Appl. Mech. Engng 196, 1-13 (2006).
D. R. Mason et al., J. Phys.: Condens. Matter 16, S2679-S2697 (2004).

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