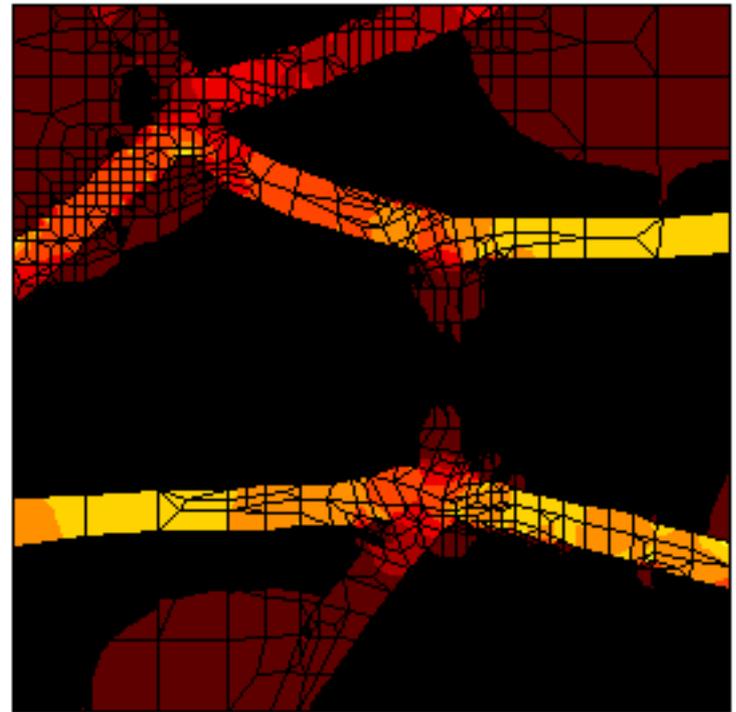


ITR: Computational Tools for Multicomponent Materials Design

Zi-Kui Liu, Long-Qing Chen, Padma Raghavan, Qiang Du (Penn State)
Stephen Langer (NIST), Christopher Wolverton (Ford). ITR-0205232

Property Simulations

OOF software computes macroscopic properties from images of material microstructure. OOF2, developed in conjunction with the ITR project, adds new physics, new computational techniques, and parallelism to OOF. It will form the basis of a future 3D version of the code.



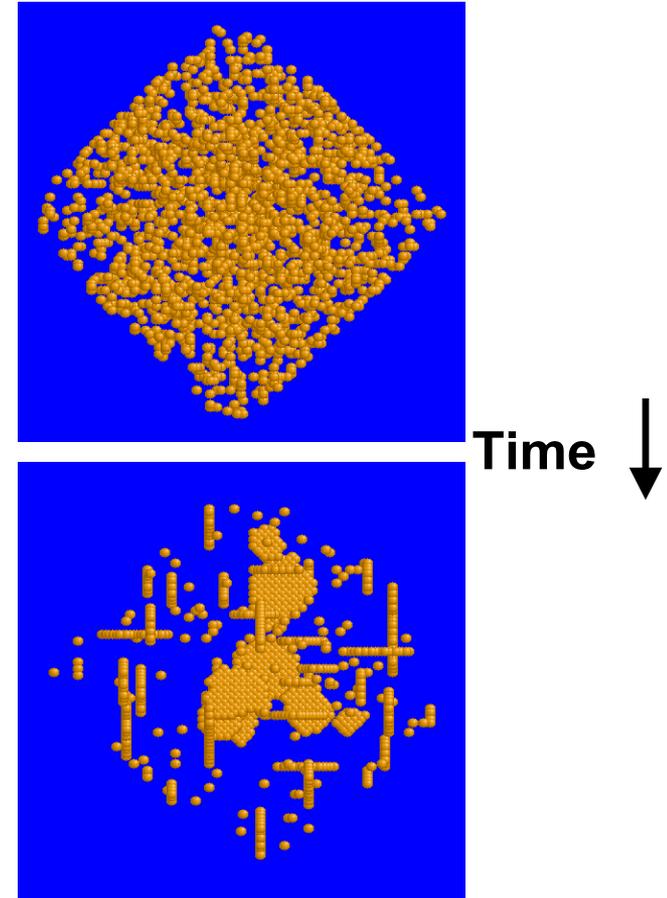
Ion diffusion along grain boundaries in a simulated electrode.

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First-principles Morphological Evolution of Nanoscale Particles

In what could be called a century-old form of nanotechnology, industrial alloys are often strengthened significantly via precipitation hardening. In this process, solute is added to a metal, and precipitated out of the metal host matrix via heat treatment below the solubility limit. However, despite the importance of this process, and its study for a century, the details of many precipitation processes are often elusive to experiments, as the precipitates are often nanometer scale, and sometimes as small as one atomic plane thick! We have applied a quantum-mechanical predictive modeling approach combined with Kinetic Monte Carlo simulations to the formation of precipitates in the Al-Cu system. This allows us, for the first time, to “see” how atoms come together to form precipitates, and how they grow and strengthen materials as they do.



Cu atoms in an Al-Cu alloy. The simulation starts (upper panel) with Cu atoms randomly distributed, and over time, they form single atomic layer thick plate-like precipitates (bottom panel).

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Algorithmic Development

- Improved optimization algorithms for phase diagram calculation
- Faster marching algorithms for phase field simulations
- Adaptive meshing near interfaces
- Accelerated elasticity solvers

