

MULTISCALE SIMULATION OF POLYCRYSTALLINE MATERIALS

SCIENTIFIC ACHIEVEMENT

We have developed the conceptual and computational framework for a novel, hierarchical multiscale simulation approach for predicting the thermo-mechanical behavior of polycrystalline materials. The approach incorporates linkages between the three most relevant length and time-scale regimes controlling the evolution of polycrystalline microstructures, including the atomic-level, the microstructural length and time scales (the ‘mesoscale’), and the continuum level, the ultimate goal being the development of a dynamical mesoscopic computational platform which realistically incorporates atomic-level and interfacial materials processes and parameters. Using grain growth as a first case study, we have demonstrated how these three levels can be linked. First, we have performed molecular-dynamics simulations of grain growth in a nanocrystalline-Pd microstructure. These simulations revealed the presence of two growth mechanisms, (a) curvature-driven grain-boundary migration and (b) grain rotations with subsequent grain coalescence. These insights were captured quantitatively in the form of a theory of diffusion-accommodated grain rotation, which then enables mesoscale simulations in which the objects evolving in space and time are the grain boundaries and grain junctions rather than the atoms. This allowed us to determine the growth topology and long-time growth kinetics for a system containing a very large number of grains of arbitrary average size, and on a time scale governed by the grain-boundary mobility, energy and diffusivity rather than atomistic time scales. We are presently incorporating the anisotropic elastic effects of applied stress, by meshing the grain interiors such that the grain-interior nodes link up with the already discretized grain boundaries and grain junctions delimiting each grain. This will then allow us to elucidate the coupling between grain growth and high-temperature, grain-boundary diffusion controlled plastic deformation.

SIGNIFICANCE

Understanding the precise manner in which materials microstructure and its evolution controls the performance and lifetime of engineering materials has represented one of the greatest forefronts in materials research throughout the last century. Based on empirically developed principles, this understanding has now evolved to a point where microstructurally-designed materials are playing an increasingly important role in many technologies. However, in spite of these remarkable achievements, there is still no comprehensive fundamental understanding of the processes and underlying mechanisms that control microstructural evolution under the usual driving forces of temperature and stress. It is well known that ultimately one needs to understand the dynamical behavior of, and interaction among, microstructural elements (such as dislocations, grain and phase boundaries, voids, cracks and precipitates) in response to external and internal stresses. Successful implementation of this multiscale approach offers a roadmap for the achievement of this ambitious goal. This type of approach now represents the centerpiece of a recently formed, DOE/BES funded multi-laboratory computational thrust within the Computational Materials Science Network (CMSN), titled *Microstructural Effects on the Mechanics of Materials*.

REFERENCES

Combined Atomistic and Mesoscale Simulation of Grain Growth in Nanocrystalline Thin Films, A. J. Haslam, D. Moldovan, S. R. Phillpot, D. Wolf and H. Gleiter, *Comput. Mat. Sci.* 23, 15-32 (2001).
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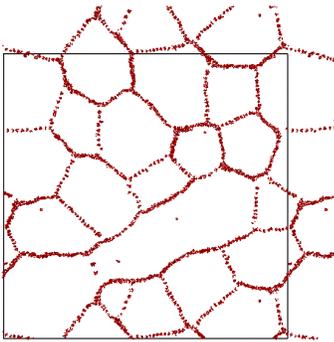
PERFORMERS

A. Haslam, D. Moldovan, V. Yamakov, D. Wolf and S. Phillpot, Materials Science Division, Argonne National Laboratory, and H. Gleiter, Inst. for Nanotechnology, Forschungszentrum Karlsruhe, Germany

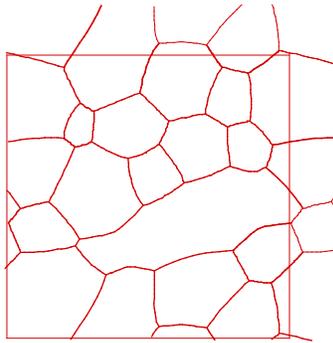
Multiscale Simulation of Polycrystalline Materials

Use grain growth as example to validate atomistic-mesoscale linkage

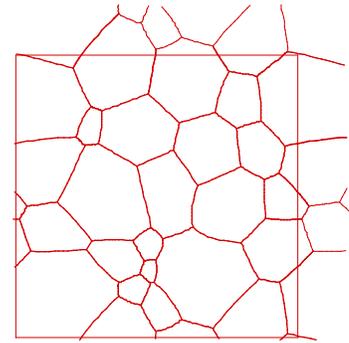
MD: $t = 2.89$ ns



meso with grain
rots.: $t = 2.47$ ns



meso with no grain
rots.: $t = 2.64$ ns



Newton's laws for atoms

*Dissipative dynamics for GBs based on virtual
power dissipation*

Comparison validates the correct transfer of insights into growth mechanisms and of grain-boundary parameters obtained from the MD simulations into the mesoscale simulation approach based on dissipative dynamics.

Performers: A. Haslam, D. Moldovan, V. Yamakov, D. Wolf, S. Phillpot, ANL, and H. Gleiter, FZ Karlsruhe