Tools for linking modeling and experiments to enable materials design at the mesoscale

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ABSTRACT

There have been substantial advances in modeling and simulation of microstructure in 3D. These have been accompanied by equally significant advances in characterization techniques, with serial sectioning, synthetic microstructure generation, and synchrotron radiation all contributing strongly. Image-based methods for solving elastic, viscoplastic and elasto-viscoplastic problems are now available to complement finite element methods. The image-based methods sidestep the difficulty of generating meshes that conform to 3D microstructures while preserving mesh quality. The resolution available permits many aspects of heterogeneity in deformation to be investigated. Materials can also be orientation mapped nondestructively in 3D thanks to penetrating radiation at synchrotrons, which permits microstructural evolution to be characterized. Synthetic microstructure generation now accounts for distributions of orientation, grain boundary character, and grain morphology, even fitting the tails of distributions. Software packages such as Dream3D substantially facilitate the exchange of 3D data between experimental systems and simulation programs. Examples of applications are drawn from a number of different projects including one on understanding the origins of void nucleation under dynamic loading.