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Microstructure Evolution in Heterogeneous Solids Experimental Characterization vis-à-vis
Numerical Simulation

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ABSTRACT

The internal structure or *microstructure* of heterogeneous solids plays a key role on their observed mechanical response. This *microstructure* is often a complex arrangement spanning several length scales. For example in polycrystalline metals, several nested structures can be identified, from the lattice structure (sub-nanometer range), to volumetric defects (nanometer), to dislocation structures (submicron), to grains (micron). Each of these structures imparts observable features in the mechanical response. These structures, however, do not remain frozen during the deformation process. On the contrary, they evolve giving rise to material history effects.

In this talk we examine an approach for incorporating into numerical simulations the interplay among the different structures and its effect on the mechanical response. In particular, we utilize a hierarchical multiscale modeling paradigm for threading the different scales. We show that the meticulous application of this paradigm renders truly predictive models of the mechanical behavior of ductile single and poly-crystals. The feat of this approach is that predictions from these atomistically informed models recover several of the macroscopic characteristic features of the available experimental data, without a priori knowledge of such experimental tests. This approach provides a procedure to forecast the mechanical behavior of material in extreme conditions where experimental data is simply not available or very difficult to collect.

A critical aspect in the development of predictive capabilities is validation, which includes not only the constitutive models but also the associated implementations and the overarching simulation approach. The validation process provides a measure of the quality of the predictions, which in turns allows for using these capabilities for quantifying the impact of uncertainties of the material properties and test conditions on the resulting macroscopic behavior. During this talk, we examine a multi-resolution validation approach for ductile oligo-crystals under tensile conditions, where both the evolution of sub-grain and supra-grain features are considered. In general we observe good agreement between simulations and experiment but also intriguing differences in the evolution of the surface roughness profiles. We also show that these validated simulations allow us to provide quantitative estimates of the effect of in-grain misorientation on the formation of localization bands.

BIOGRAPHY

Alberto Cuitino is presently a Professor of Mechanical and Aerospace Engineering at Rutgers University. He was a visiting professor in the Graduate Aeronautical Laboratories at the California Institute of Technology during 2000-2001. Dr. Cuitino received a Civil Engineering Diploma from the University of Buenos Aires, Argentina, in 1986, and a MS degree in Applied Mathematics and a Ph.D. degree in Solid Mechanics from Brown University in 1992 and 1994 respectively. His research interests include multiscale modeling, dislocation mechanics, fracture in metal single crystals, granular materials, mechanical behavior of solid foams and folding patterns in thin films. He is currently associated with the ASC Caltech Center for simulating the dynamic response of materials under extreme loading conditions. Cuitino is subject editor for Applied Mechanics of the Latin American Applied Research and he is in the editorial board of the International Journal of Plasticity.

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