Comparisons of 3D Experiments and Simulations on Plastic Deformation of Metals

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The aim of this presentation is to point out that the current state of comparisons between experiments and simulations of deformation of polycrystalline materials reveals some interesting challenges. Addressing first the experimental sources of data, High Energy Diffraction Microscopy (HEDM) takes advantage of the high energy monochromatic x-rays available at third generation sources. Computer simulation of plastic deformation experiments has been accomplished almost entirely with the finite element method. In the past few years, however, an image-based approach that relies on the Fast Fourier Transform (FFT) offers a more efficient solution of the same equations (e.g. mechanical equilibrium) as the finite element approach. Thus one can, for example, take a measured 3D image from HEDM with thousands of grains and import it directly into the FFT simulation code. Such image-based simulations enable substantially more complex microstructures to be simulated than has been standard practice.

Turning to the underlying scientific issues, polycrystal plasticity is akin to deformation of a composite in which each grain has different properties by virtue of its anisotropic response to loading. It is important to demonstrate that we can validate crystal plasticity simulations in order to relate damage initiation such as cracks and voids to extreme values in stress, for example, as they relate to microstructural features such as triple lines. Specific examples of the use of HEDM will be given for tensile tests on pure copper and zirconium, and fatigued nickel-based superalloy. In general, both experiments and simulations show that hot spots in stress or elastic energy density occur close to grain boundaries, triple lines and quadruple points. Whether strain or orientation is used, however, comparisons of the full fields show significant differences despite at the good agreement found at the statistical level. This suggests that all aspects of the simulations will require attention.

Returning to the multiscale aspects of the problem, at the engineering scale, there is a need to develop accurate, physically-based constitutive models for mechanical behavior. Especially for problems such as initiation of cracks and voids, there is an obvious need for accurate full field modeling so that extremes in stress, slip, strain etc. are understood. In the other direction, the uncertainty around the capability of mesoscopic crystal plasticity modeling provides motivation for validation with molecular dynamics (MD) and dislocation dynamics (DD) simulations of polycrystals. An introduction will be given to application of the FFT method for accelerating the DD method and enabling anisotropic polycrystals modeling.