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Comparison in 3D of Experiments on, and Simulations of Plastic Deformation of Polycrystals

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This talk will address various aspects of image processing relevant to the plastic deformation of metals. The motivation behind the talk is to point out that the current state of comparisons between experiments and simulations of deformation of polycrystalline materials reveals some interesting challenges [1]. Addressing first the image processing issues, EBSD [2] relies heavily on image transformations of the diffraction patterns in which there is useful information about electron energy. HEDM [3] also relies on thresholding of the diffractograms for peak identification and more sophisticated methods are slowly being introduced [4]. Computer simulation of the experiments in which materials are plastically deformed has been accomplished almost entirely with the finite element method. In the past few years, however, an image-based approach[5] that relies on the Fast Fourier Transform has started to be used because it offers a more efficient solution of the same equations (e.g. mechanical equilibrium) as the finite element approach. It is possible, for example, to import directly a measured 3D image from HEDM into the FFT simulation code and simulate with no need for the time-consuming step of creating a 3D mesh. Image-based approaches to simulation offer not only more efficient computation and data flow but they also prompt the development of more direct comparison at the level of the raw experimental data, which in this case is the set of diffraction images associated with each snapshot of the material.

Turning to the background 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 will be given for tensile tests on an interstitial-free sheet steel, using electron back-scatter diffraction (EBSD [2]), and for a pure copper, using High Energy Diffraction Microscopy (HEDM [3]). An alternative to the standard finite element method is to model the mechanical response on the image itself using a spectral method based on Fast Fourier transforms (FFT [5]). 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 [6]. Although correlations are found between hot spots and interfaces, special boundaries do not appear to play any role. Various measures of heterogeneity such as maps of grain average strain, Kernel Average Misorientation, Grain Orientation Spread, Intragranular Grain Misorientation and lattice reorientation can be used to make comparisons.

As one example of the type of image processing being applied, we discuss a tensile test carried out on a sample of pure copper with a diameter of approximately 1 mm, for which HEDM maps were measured before and after a strain of 6 %. Calculations were performed using a standard viscoplastic model for crystal plasticity embedded in a code, vpFFT, that solves the equations of stress equilibrium and strain compatibility in a periodic unit cell built from a two- or three-dimensional image of the material [5]. A standard constitutive equation relates the strain rate to the local (tensor) stress resolved onto each slip

system. For a given strain rate, the strain rate and stress fields and the corresponding effective stress are obtained iteratively. The code uses the Fast Fourier transform (FFT) to alternate between real and frequency spaces [3]. This permits convolution integrals to be replaced by point-wise tensor products (in frequency space), thus accelerating the computation. The initial state (annealed) of the material was used to instantiate the simulation and a cross-section near the center of the volume was used for comparisons. The change in lattice orientation, reduced to a magnitude, was computed for each point, Fig. 1(a), which reveals significant variations from grain to grain and within grains. The same pointwise lattice rotation was computed from the simulated result, Fig. 1(b). One advantage of using the lattice rotation is that it integrates changes over the strain interval, as compared, say, to computing orientation gradients. This comparison, as with others [1], shows only moderate agreement between experiment and simulation. The challenge to our understanding is therefore why crystal plasticity simulations give good results at the statistical level (e.g. texture development) but indifferent agreement at the local (grain) scale. The many contributions to this work are greatfully acknowledged [7].

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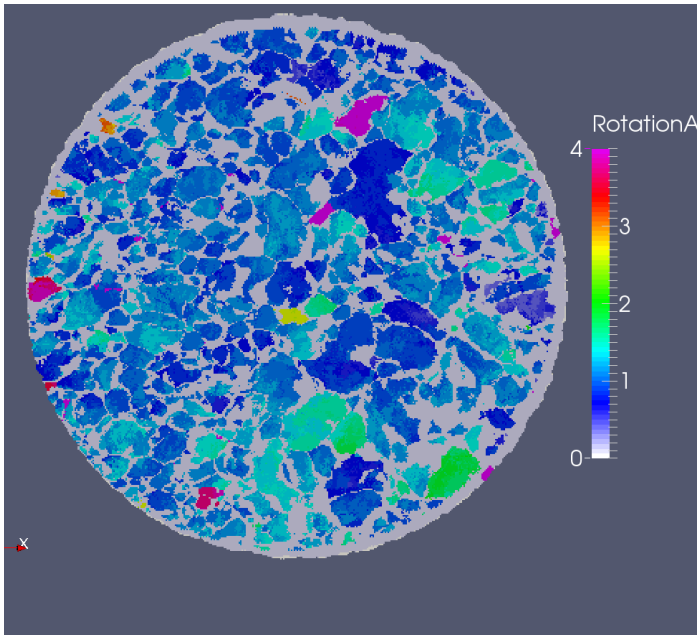

Fig. 1(a). Cross-section of specimen of pure copper, for which the magnitude of the lattice rotation (in degrees) has been computed pointwise between the initial state and after 6 % plastic strain in uniaxial tension. The diameter is approximately 1 mm.

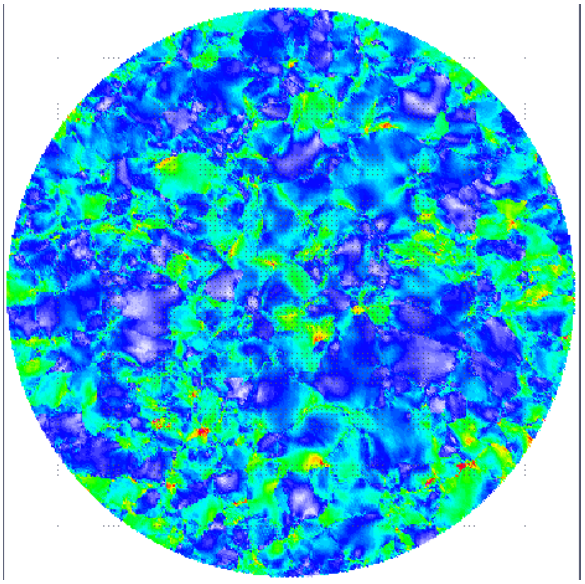

Fig. 1(b). The same cross-section as shown in 1(a) with the magnitude of lattice rotation between the initial state and after 6 % strain simulated with the vpFFT code.