Comparison of Mesoscale Finite Element Deformation Modeling With Measurements Using X-Ray Microscopy*

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ABSTRACT

The deformation of a nickel bi-crystal in uniaxial tension is simulated using a mesoscale finite element model, and the results are compared with corresponding experiments. The simulations make use of crystal plasticity to model the material constitutive response, and discretization of the bi-crystal with a large number of elements to capture the heterogeneous deformation of each grain. The simulations predict changes in the local orientation of each crystal during deformation, and the results are compared with experimental measurements of grain reorientations. The measurements are made using a polychromatic three-dimensional X-ray microscope, which provides in-situ spatially resolved orientation data at the sub-micron scale in individual grains during deformation of polycrystalline samples. Such detailed comparisons provide a valuable means to evaluate the capability of the crystal plasticity based finite element simulations to model the heterogeneous microstructure evolution during deformation of polycrystalline materials.

1. Introduction

It is well known that the deformation of metals, while seemingly homogeneous at the continuum scale, is an inherently heterogeneous process at the scale of individual grains. The variations in deformation among different grains are strongly influenced by the crystallographic orientations of the grains. Modeling the deformation of metals at the mesoscale has been accomplished in recent years by combining the explicit discretization of the microstructure using the finite element method with crystal plasticity theory to incorporate the anisotropy in the material constitutive response based on the crystal orientation [1]. In this paper we apply mesoscale finite element simulations to the deformation of a nickel bi-crystal in uniaxial tension, and compare the model predictions with corresponding experimental measurements of grain orientations made using a polychromatic three-dimensional X-ray microscope [2].

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2. Mesoscale Simulations and Experimental Measurements

The finite element discretization consisted of 80×20×20 hexahedral elements, with each crystal comprised of 40 elements along the direction of extension (x-axis). Material parameters for the crystal plasticity model were obtained by fitting a polycrystal model based on the Taylor mean field assumption to the stress-strain response for nickel. Initial orientations with appropriate spread in the two grains were assigned based on experimental data. The measurements were carried out using a polychromatic X-ray beam, and depth resolution was achieved using the differential aperture microscopy method developed by Larson et al. [2].

3. Results

The finite element mesh after deformation under uniaxial tension to a strain of 8% is shown in Fig. 1, along with the contours of the misorientation angle. The misorientation has been calculated for each element relative to its initial orientation, and therefore represents the change in orientation during deformation. It is evident from both the mesh distortion and the misorientation values that grain A has accommodated a larger share of the overall strain, with higher misorientation and greater heterogeneity, while grain B has deformed in more uniform fashion with relatively smaller change in orientation, as also seen from the deformed sample shown in Fig.1.

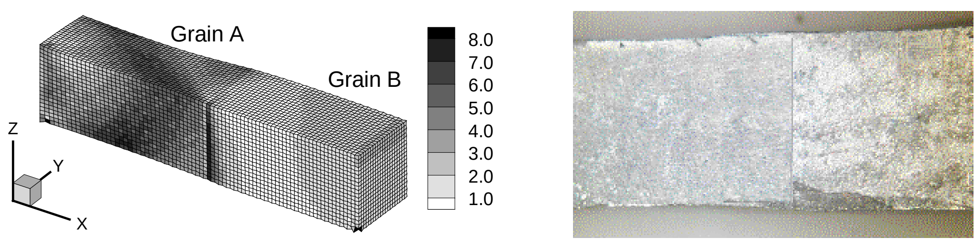

Figure 1: Deformed mesh showing misorientation in [°] from the initial orientation (left) and deformed sample from the experiment (right).

The experimental measurements of orientation after 8% tensile strain were taken at three locations along the z-axis at the grain boundary, and at distances of 5 and 10 µm from the grain boundary along the tensile axis in each grain. At each location, orientation data were measured at 1 µm intervals along the y-axis up to depths of 38 µm (or roughly halfway) into the sample. Results are presented as misorientation values calculated relative to the first orientation measured along the scan direction. Figure 2 shows the misorientations in grain A for points A-1 and A-2. Since the crystal plasticity model used in the simulations does not have an inherent length scale, the corresponding results from the mesoscale model are shown for elements at different distances from the grain boundary, at x=21, 36, 39 and 40, at z=10 for grain A. Since grain A is composed of 40 elements along the x-axis, x=21 is roughly halfway from the grain boundary to the end, and corresponds to a point in the grain interior, while x=40 is right next to the boundary. The experimental data show slightly higher misorientations developing at A-2, which is closer to the grain boundary, compared to A-1, although the difference in the range of values is not very large. The model predictions show a similar range of misorientations, especially through element 10 which is halfway into the sample, although locations closer to and further away from the grain boundary do not show much difference in the values.

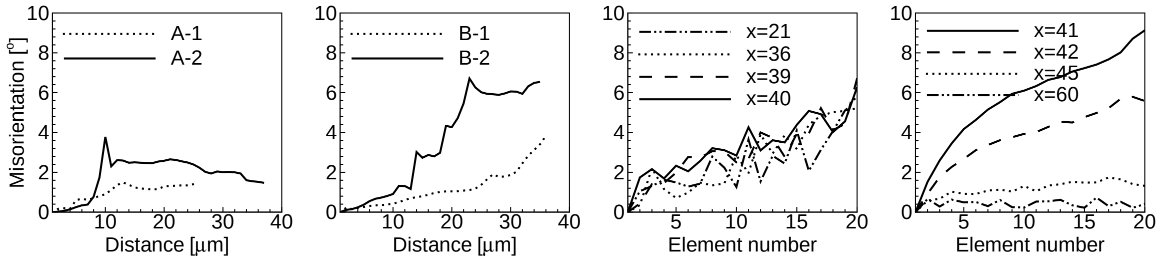

Figure 2: Misorientations along the scan direction relative to the first orientation from experiments (two left figures) and simulations (two right figures) for grains A and B.

Similar results on misorientation values are also shown in Fig. 2 for grain B. In this case, unlike for grain A, there is a larger difference in the misorientation values at the two locations, with the values at B-2, which is closer to the grain boundary, being much higher than the values at B-1. The simulation results in this case show a similar trend of higher misorientations closer to the grain boundary (x=41, 42) and much lower values further away (x=45, 60). The results indicate that the grain boundary has a stronger influence on the deformation of grain B than on grain A.

Comparisons of misorientation values along the scan lines in the two grains show that the model predictions match both the range and the overall trends in the experimental data. Further work is required in terms of measurements at more locations and at greater distances from the boundary, as well as more detailed modeling with higher mesh resolution near the grain boundary to capture the sharp orientation gradients as in grain B, to enable more meaningful comparisons between the simulations and the experiments.

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