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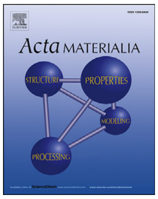

Full length article

Microstructural effects on damage evolution in shocked copper polycrystals

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ABSTRACT

Three-dimensional crystal orientation fields of a copper sample, characterized before and after shock loading using High Energy Diffraction Microscopy, are used for input and validation of direct numerical simulations using a Fast Fourier Transform (FFT)-based micromechanical model. The locations of the voids determined by X-ray tomography in the incipiently-spalled sample, predominantly found near grain boundaries, were traced back and registered to the pre-shocked microstructural image. Using FFT-based simulations with direct input from the initial microstructure, micromechanical fields at the shock peak stress were obtained. Statistical distributions of micromechanical fields restricted to grain boundaries that developed voids after the shock are compared with corresponding distributions for all grain boundaries. Distributions of conventional measures of stress and strain (deviatoric and mean components) do not show correlation with the locations of voids in the post-shocked image. Neither does stress triaxiality, surface traction or grain boundary inclination angle, in a significant way. On the other hand, differences in Taylor factor and accumulated plastic work across grain boundaries do correlate with the occurrence of damage. Damage was observed to take place preferentially at grain boundaries adjacent to grains having very different plastic response.

1. Introduction

Predicting the conditions that determine material failure is one of the most fundamental challenges in materials science. One important failure mechanism for ductile materials undergoing dynamic loading conditions is void nucleation, growth and coalescence [1–8]. In the first stage, void nuclei under appropriate driving forces reach a size large enough to become stable and eventually sustain growth. At this nucleation phase of damage the influence of the material's microstructure can be very strong. Growth occurs when the volume of stable voids increases driven by stress triaxiality [2], which reaches high values under the dynamic loading conditions considered in this work. Coalescence occurs when voids grow enough such that stress and strain concentrations in the surrounding material start overlapping and further increasing, promoting neighboring voids to join together [1]. It is at this stage in the process where ultimate failure of the material is initiated. The ability to predict the extent to which a given microstructure is vulnerable to damage nucleation and growth is relevant to the emerging field of computational materials design, to enable the discovery and development of new processes and/or materials with higher resistance to damage. The determination of whether or not voids will nucleate and grow in specific locations requires identifying which microstructural features promote or inhibit damage initiation.

Identifying potential microstructural features that influence damage requires knowledge of where damage develops within a microstructure under certain mechanical loading, and what is the micromechanical response at those locations. The use of non-destructive three-dimensional (3-D) imaging techniques such as near-field high-energy diffraction microscopy (nf-HEDM) [9–11] and X-ray tomography, before and after deformation is applied, is ideal so that comparisons to the pristine sample can be made. Micromechanical fields can be obtained performing full-field simulations with direct input from the 3-D image of the initial microstructure.

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There have been many investigations on the effect of various microstructure features on void formation within polycrystalline materials, although experimental constraints have often limited the scope of these studies. Field et al. [12], Diard et al. [13], Fensin et al. [8], and Yang et al. [14] analyzed multiple two-dimensional micrographs of damaged materials and found that damage preferentially occurred at interfaces with specific relationships to the principal loading directions, although the nature of the relationship depends on the type of loading (e.g. fatigue versus shock). The nature of the plastic response of the crystals vicinal to voids has also been associated with damage initiation by Wright et al. [15], Bieler et al. [16,17], Semiatin et al. [18], Escobedo et al. [19,20] and Yang et al. [14], although different authors often made an arbitrary choice of parameters to correlate with damage, and the number of void sites studied was limited. The factors most frequently used to quantify plastic response are Schmid factor and Taylor factor.

In this work we study damage initiated by shock loading [19–24]. For shocked fcc materials, there has been a special focus on understanding the effect of $\Sigma 3$ boundaries with $\{111\}$ boundary normals, which are variously known as coherent twin boundaries or annealing twins. Escobedo et al. [19], Fensin et al. [25] and Yang et al. [14] have shown, based on orientation maps of cross-sections, that $\Sigma 3$ boundaries tend to be resistant to void formation. Although this suggests a resistance to damage based solely on interface character, the results presented here implicate heterogeneous plastic deformation.

Shock loading is frequently applied in gas-driven plate impact experiments, which provide a controlled method of developing a shock wave of a certain magnitude and thus testing dynamic damage processes [19,26–28]. Void nucleation occurs as part of the process of spallation failure. As the compressive wave propagates through the material, it eventually reflects off the rear surface of the sample, opposite to the side of initial impact, and returns as a rarefaction wave. This rarefaction wave then interacts with a similar reflected wave coming from the contact side of the sample (originating from compression of the impact plate) to form a region of high tensile stress at the spall plane. Full spallation occurs when the sample separates into two pieces at the spall plane. When the tensile stress is high enough to nucleate voids but not high enough to cause coalescence and full spallation, incipient spallation occurs, which is particularly useful for investigating early stages of porosity evolution.

In this work, we utilize data from an experiment in which a polycrystalline copper sample was characterized with nf-HEDM and then subjected to incipient spall. The recovered sample was again orientation-mapped using nf-HEDM and X-ray tomography. Registration of the 3-D images before and after the experiment allowed the locations of the eventual void sites to be established within the image of the undeformed sample, as described in Section 2. In turn, the undeformed microstructural image was used as input of a full-field crystal plasticity Fast Fourier Transform (FFT)-based model [29,30] to simulate the micromechanical fields developed during the shock, as described in Section 3. In Section 4, we provide details of a novel technique for quantifying grain boundary and triple junction morphology directly from microstructural images, needed for subsequent analysis. In Section 5 we compare the predicted field distributions computed for the entire microstructure with those obtained only in the vicinity of regions developing porosity. This comparison allows us to assess the influence of different micromechanical fields on the occurrence of void nucleation and early growth, as discussed in Section 6.

2. Materials and methods

To investigate microstructural properties influencing damage initiation, this work utilizes the results of an experiment performed by Bingert et al. [31] and analyzed by Menasche et al. [32], whose goal was to obtain 3-D images of a material in which incipient spall occurred. In this experiment, a 99.997% pure polycrystalline copper sample was machined into a 1.2 mm diameter cylinder of height 2.42 mm. This sample was then characterized using nf-HEDM [33] over a height of 0.704 mm. The sample was machined down to a 0.725 mm tall piece centered about the characterized section. This sample was then embedded into two copper polycrystal radial momentum traps and impacted by a copper flyer plate at 300 ms^{-1}. The experimental setup involved placing the ringed sample onto the front of a pipe that was slightly larger in diameter than the HEDM characterized sample; thus when the target was impacted, the sample alone was stripped from the momentum trapping rings and soft-captured. The velocity was specifically selected such that the sample was recovered while causing incipient spall voids. The recovered sample was then characterized using both nf-HEDM and X-ray tomography. The end result was a pair of 3-D orientation maps of the same volume of the copper sample both before the experiment and after the plate impact had produced voids within the sample. Computed tomography also provided 3-D images of the porosity distribution. The tomography provided higher spatial resolution of the voids compared to the nf-HEDM image.

Menasche et al. [32] analyzed the experiment by mapping the voids characterized from the deformed sample onto the microstructure measured from the undeformed sample. First, a technique was developed to map the voids identified via X-ray tomography in the post-shocked sample to the corresponding nf-HEDM image. This was achieved by aligning larger-scale surface features present in both sample images. Next, the nf-HEDM images of the sample both undeformed and deformed were aligned with each other through the use of rotations and affine transformations. The purpose of this was to account for differences in sample alignment of the two measurements, as well as for the plastic deformation experienced by the sample as a result of the shock loading, which was on the order of a few percent in the spall plane region. This plastic deformation also made registration between the two nf-HEDM datasets more difficult because defect accumulation and crystal rotation results in larger uncertainty in crystal orientation. In more detail, the centers of mass of 1,800 grains were compared between the undeformed state and the post-shock state, of which approximately 1,000 were interior grains. The final result was that it was possible to identify certain regions within the nf-HEDM image of the undeformed sample as having developed voids in the deformed sample.

Using the orientation field of the undeformed sample obtained by Menasche et al. [32] as the input of a micromechanical simulation, this work analyzes the local response of the material in the regions developing porosity. A full-field crystal plasticity model that utilizes FFT to solve the micromechanical governing equations [29,30] is used to determine the local micromechanical fields under shock loading conditions, as described in the following section. Menasche et al. [32] found that (see Table 1) of the 485 measured voids, 332 occurred at grain boundaries. Of those 332 grain

Table 1
Distribution of voids at grain boundary features from Menasche et al. [32] and from this work.

Type of interface	Menasche et al.	This work
Total Voids	485	447
All Interface Voids	332 (68.5%)	308 (68.9%)
Grain Boundary Plane	196 (40.4%)	156 (34.9%)
Triple Junction	126 (26.0%)	99 (22.2%)
Higher-Order Interface	10 (2.1%)	53 (11.9%)