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Dislocation density-based finite element analysis of large strain deformation behavior of copper under high-pressure torsion

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Abstract

The paper is concerned with large strain deformation behavior of metallic materials as exemplified by copper under high-pressure torsion (HPT). To that end, the evolution of microstructure was considered in terms of a dislocation density-based constitutive model embedded in a finite element code. The variation of the specimen geometry, the hydrostatic pressure state, the equivalent strain and the dislocation density were examined by numerical simulations. The concurrent variation of the average dislocation cell size, which was identified with the emerging new grain size of the material, was also traced. The simulated results for the dislocation density and the grain size were shown to be in good agreement with the experimental data for commercial purity copper. It was concluded that the dislocation density-based constitutive model is well placed as a tool for describing and predicting the evolution of microstructure during severe plastic deformation, particularly HPT, using the finite element method.

Keywords: High-pressure torsion; X-ray synchrotron diffraction; Dislocation density; Finite element method; Hydrostatic pressure

1. Introduction

Ultrafine-grained (UFG) and nanocrystalline (NC) materials have been extensively investigated due to their excellent and unique multifunctional properties as well as their high strength [1]. Severe plastic deformation (SPD) processes, such as equal channel angular pressing (ECAP) [2], accumulative roll-bonding (ARB) [3], high-pressure torsion (HPT) [4–6] and twist extrusion (TE) [7–9], have received much attention as a group of top-down techniques to manufacture bulk UFG and NC materials [10–13]. In order to understand and fully utilize these SPD processes, which are often very complex, it is necessary to analyze plastic deformation behavior of materials theoretically, and the finite element method (FEM) offers itself as a suitable platform for that.

In the past, FEM simulations of the SPD processes were performed with the purpose of analysis and optimization of the SPD processing variables and prediction of the mechanical and microstructural characteristics of the SPD processed samples. For example, for ECAP, the effect of processing parameters, such as die geometry [14–18], material properties [19–21] and initial sample geometry

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[22], on the plastic deformation behavior was reported in the literature in a great deal of detail. Such specific phenomena as the occurrence of a corner gap in strain hardening materials [23] and recurrent shear banding in strain softening materials [24] could be uncovered by FEM analyses. By contrast, only a limited number of researchers have looked at the effects of the material characteristics [25] and the processing variables, such as the coefficient of friction [26], temperature [27], pressure [28], die geometry [28] and dead metal zone [29], on the HPT behavior by employing FEM analysis. To date, not much can be found in the literature on the simulations of the evolution under HPT of such material related variables as the grain size, grain misorientation, texture, dislocation density and twin volume fraction.

In general, simple continuum-based FEM simulations of the SPD processes provide information on deformation geometry and solid mechanics variables, such as temperature, stress, strain and forming load. However, unlike the conventional metal forming processes, such as forging, rolling, extrusion and drawing, whose primary purpose is to control the shape and size of workpieces, the SPD processes aim at modifying the microstructures and the ensuing properties of the material. Therefore, the most important expected outcomes of FEM simulations of SPD processes are those providing information on the evolution of microstructural features (dislocation density, grain size, grain misorientation, etc.) on top of the mechanistic characteristics, such as stress, strain and strain rate. Baik et al. [30,31] successfully predicted the dislocation density and dislocation cell size after ECAP of pure Cu and Al using FEM simulations based on a dislocation density-based constitutive model. However, the reported HPT analyses using FEM computations are insufficient to fully understand the HPT process.

In this study, FEM analysis of the HPT process that employed a mechanism-based constitutive model for dislocation cell-forming materials [32] was carried out. The evolution of the workpiece shape, pressure state, stress and strain during HPT was investigated for HPT of commercial purity copper. Due to the microstructural underpinning of the constitutive model used, it was also possible to obtain information about the evolution of dislocation density and dislocation cell size as additional outputs of the simulations. The simulation results were verified experimentally by using synchrotron X-ray diffraction (XRD) measurements and transmission electron microscopy (TEM).

2. Numerical procedure

2.1. Dislocation mechanism based constitutive model

The dislocation cell based model employed in this work goes back to the seminal paper by Mughrabi [33], who introduced the two-phase approach underlying our modeling. Mughrabi's model predicts the occurrence of internal stresses (a back stress in the cell interiors and a forward stress in the cell walls) due to plastic strain incompatibilities between the cell wall and the cell interior "phases". Theoretically, these internal stresses should give rise to asymmetry of the XRD peaks for the HPT processed material. In this study, we used the synchrotron XRD with the resolution of $\Delta E/E = 2 \times 10^{-4}$ filtered by a monochromator. Almost no asymmetry is discernible in the $\{200\}$ and $\{311\}$ peaks, though. If the Mughrabi model is applicable and internal stresses are at play, the absence of peak asymmetry can only be rationalized if the magnitude of the internal stresses is small. A simple estimate shows that this is the case, indeed. According to Mughrabi's model [33], the back stress in the cell interior is given by $\sigma_c^{back} = fE\left(\varepsilon_c^p - \varepsilon_w^p\right)$, where E is the Young's modulus, ε_c^p and ε_w^p are the plastic strains in the cell interior and the cell walls, respectively, and f is the volume fraction of the cell wall "phase". The maximum difference in the plastic strains in the two "phases", as seen from the simulation results, was 1.75×10^{-4}, while the magnitude of f was continuously dropping from the initial value of $f_o = 0.25$, see Table 1. After one turn in the HPT process, this value dropped to a level close to $f_\infty = 0.06$, cf. Table 1, at least towards the rim of the sample, where the equivalent von Mises strain was of the order of 10, see Fig. 5. Hence, during the torsion stage of the process, the back stress would not exceed 1.16 MPa, which is negligible compared to the level of the applied equivalent stress (over 400 MPa, cf. Fig. 6b). Similar estimates apply to the forward stress in the cell walls.

The above argument explains why the expected asymmetry of the diffraction peaks stemming from the internal stresses was vanishingly small and could not be discerned, so that the predictions of the dislocation cell model pioneered by Mughrabi [33] and further extended by Estrin et al. [34] cannot be put in question on the basis of XRD data.

With this argument in mind, the three-dimensional version of the dislocation density-based constitutive model [32] successfully applied to ECAP [30,31] was also used in the present simulations of HPT. In this section, a brief

Table 1
Parameters of the constitutive model used in the simulations.

$\rho_w^{t=0}$ (m^{-2})	5×10^{13}
$\rho_c^{t=0}$ (m^{-2})	2.5×10^{13}
f_0	0.25
f_∞	0.06
$\tilde{\gamma}^r$	3.2
$\dot{\gamma}_0^r$ (s^{-1})	1
m	250
n	50
α	0.25
G (GPa)	47.4
b (m)	2.56×10^{-10}
K	10
α^*	0.065
β^*	0.012
k_0	9.2