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Hardening of pure metals by high-pressure torsion: A physically based model employing volume-averaged defect evolutions

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Abstract

A physically based model to predict the increment of hardness and grain refinement of pure metals due to severe plastic deformation by high-pressure torsion (HPT) is proposed. The model incorporates volume-averaged thermally activated dislocation annihilation and grain boundary formation. Strengthening is caused by dislocations in the grain and by grain boundaries. The model is tested against a database containing all available reliable data on HPT-processed pure metals. It is shown that the model accurately predicts hardening and grain size of the pure metals, irrespective of crystal structure (face-centred cubic, body-centred cubic and hexagonal close packed). Measured dislocation densities also show good correlation with predictions. The influence of stacking fault energy on hardening is very weak (of the order of -0.03 GPa per 100 J mol^{-1}).

Keywords: Severe Plastic Deformation (SPD); Dislocations; High-pressure torsion; Hardness; Grain size

1. Introduction

Severe plastic deformation (SPD) has attracted wide attention as a means of improving properties of metals and alloys, and especially improvements in strength have been targeted [1]. More than 20 years of research in SPD [1–3] has revealed that the strength increase in metals due to SPD is strongly dependent on the material, with strength increases in pure Al and Zn being very low (<30 MPa), whilst several pure metals with high melting temperature show very strong increases in yield strength (>500 MPa) [4,5].

In the present work we focus on high-pressure torsion (HPT), which is an SPD method that is particularly effective in terms of the speed at which high deformation can be introduced in materials [6]. The working principle of HPT is depicted in Fig. 1 (from Ref. [7]). Following extensive work in the field by a range of researchers, extensive data on the hardness and microstructure of HPT-processed metals and alloys are now available (e.g. [4–6,8–21]). Data on hardness increases due to HPT have been published for over 20 pure metals, and several of the factors influencing the hardness of HPT-processed pure metals have been investigated in some detail by Edelati and Horita [4,5]. Their work has indicated that these hardness values correlate to atomic bond parameters, stacking fault energy, specific heat capacity, specific latent heat of fusion, linear thermal expansion coefficient, activation energy for self-diffusion, melting temperature and shear modulus [5,22,23].

To fully exploit the capabilities of SPD we need quantitative models that are able to predict the microstructure development during the process and predict the resulting mechanical properties based on processing and materials parameters [19,24–28]. In particular, it is important to establish which SPD processed metals possess the combinations of properties (for instance strength, density, cost) that are most attractive for application in devises and structures. However, little attention has been given to establishing a model for strengthening and grain refinement that

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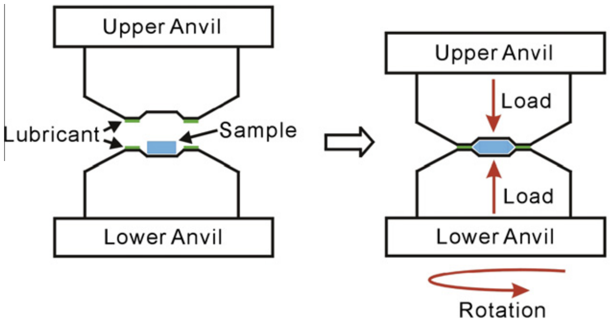

Fig. 1. The principle of high-pressure torsion (from Ref. [7]).

predicts the differences between different metals. In the present work we aim to derive a physically based model which captures the data on hardness increment and grain refinement of pure metals due to HPT. We focus our attention on computationally efficient approaches that are based on volume-averaged dislocation generation and annihilation, and volume-averaged grain boundary creation. This means in practice that we follow classical approaches to strengthening (e.g. [29–32]) and recovery [33], and include recent insights in the relation between dislocation generation and grain size [19,28]. We aim to show that these can explain published data on material dependence of hardening and grain size for HPT-processed pure metals.

2. A physically based model

2.1. Overview

To provide a physically based model for the hardness of HPT-processed pure metals we construct a model that takes account of the main aspects of hardening and recovery, focusing particularly those aspects that cause the differences between the various metals.

It has been shown in a range of publications that the strengthening of pure and commercially pure metals due to SPD processing is generally caused by dislocation hardening and grain boundary strengthening (e.g. [19,34,35]). In the present work we incorporate both strengthening mechanisms.

2.2. Dislocation generation and thermally activated dislocation annihilation

To obtain expressions for the total dislocation line length involved in dislocation strengthening and grain size strengthening we proceed as follows. We define L_{gen} as the total cumulative dislocation line length generated during the deformation processing. We consider that dislocations are retained in the grains, subsumed in grain boundaries (existing or new ones) [19,36] or annihilated within the grain [37]. We consider that the annihilation can be described through a temperature- and material-dependent annihilation fraction, f_{an}, i.e.:

$$L_{\mathrm{gb}} + L_{\mathrm{ig}} = (1 - f_{\mathrm{an}})L_{\mathrm{gen}} \tag{1}$$

where L_{ig} is the total dislocation line length of dislocations stored in the grain and L_{gb} is the total dislocation line length of dislocations that have moved to grain boundaries and have become part of the grain boundary (they are "subsumed" in the grain boundaries [19,28]). We consider that the effective width of grain boundaries can be ignored (this is further discussed in Section 5), hence

$$\rho_{\mathrm{ig}} = \frac{L_{ig}}{V} \tag{2}$$

where ρ_{ig} is the (average) dislocation density in the grain and V is the sample volume. We do not attempt here to model details of the mechanisms of partitioning of dislocations between grain and grain boundary. Instead, we assume that both L_{gb} and L_{ig} are effectively proportional to $(1 - f_{\mathrm{an}})$ L_{gen}, i.e. it is assumed that the L_{gb}:L_{ig} ratio is in good approximation constant for all the HPT-processed pure metals considered. (Consequently, f_{an} is the dominating factor determining the differences in L_{ig} between the pure metals; see below.) The influence of this assumption is further considered in Section 5. Similarly we do not attempt to include twinning or any other deformation induced defect creation in the model, i.e. we assume that if defects other than dislocations or grain boundaries are created they do not substantially alter predictions. (For discussions on the effect of vacancies see Section 5 and Refs. [37,38].)

Dislocation annihilation within grains can occur through several mechanisms. In particular, mutual annihilation of both screw and non-screw dislocations of opposite sign has been evidenced [39]. In the present work we approximate the rate of dislocation annihilation using the generic exponential relaxation function given by Nes [33]:

$$f_{an} = \exp(-t_p/\tau_1) \tag{3}$$

where t_p is the time available for the dislocation annihilation process, τ_1, is the time constant of the process. In his work, Nes showed that the latter exponential relaxation expression is a good approximation to the expression for network growth due to a range of processes [33].

The main temperature- and material-dependent factors of this annihilation process can be obtained from the model by Nes [33], which indicates that the time constant of the process, τ_1, is of the form

$$\begin{aligned}\tau_1^{-1} &= \frac{C_1}{RT} D_x(T) \exp\left(\frac{\alpha_3 \kappa_2 G b^3}{RT}\right)\\ &= \frac{C_1}{RT} D_{x,o} \exp\left(\frac{-E_{A,x} + \alpha_3 \kappa_2 G b^3}{RT}\right)\end{aligned} \tag{4}$$

where D_x is the self-diffusion constant during the (dynamic) recovery, $E_{A,x}$ is the activation energy for self-diffusion during the (dynamic) recovery, $D_{x,o}$ is the pre-exponential constant for self-diffusion during the (dynamic) recovery,