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Influence of dislocation–solute atom interactions and stacking fault energy on grain size of single-phase alloys after severe plastic deformation using high-pressure torsion

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Abstract

Several pure metals (magnesium, aluminum, iron, cobalt, nickel, copper, zinc, palladium and silver) and single-phase Al–Mg, Al–Ag, Al–Cu, Cu–Al, Cu–Zn, Pd–Ag, Ni–Fe and Ni–Co alloys were processed by severe plastic deformation using high-pressure torsion (HPT). The steady-state grain size was decreased and hardness increased by alloying in all the systems. It was shown that the dominant factor for extra grain refinement by alloying was due to the effect of solute–matrix atomic-size mismatch and modulus interaction on the mobility of edge dislocations. For the selected alloys, unlike pure metals, the grain size was almost insensitive to the melting temperature, and like pure metals, no systematic correlation was established between the grain size and stacking fault energy (chemical interaction) or between the grain size and valence electrons (electrical interaction). The presence of a power-law relation, with $n \approx 0.56$, between the hardness normalized by the shear modulus and grain size normalized by the Burgers vector signified the large contribution of grain boundaries to the hardening. The contribution of the solid-solution effect to the total hardening appeared to be <15%.

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1. Introduction

Severe plastic deformation (SPD) processes such as high-pressure torsion (HPT) and equal-channel angular pressing (ECAP) are effective for producing ultrafine-grained (UFG) materials [1–4]. For all SPD methods, the grain size decreases with increasing strain at an early stage of straining but enters into a steady state at large strains, where the grain size remains unchanged with further straining. The steady-state grain sizes are characteristics of single-phase materials and they remain the same irrespective of the strain, pressure and initial microstructure [5]. Several theoretical models (e.g. [6–13]) and experimental works (e.g. [14,15]) have been developed to investigate the steady-state grain sizes, d_S. Most of these reports deal with pure metals, whereas little is understood to date regarding the correlations between d_S and the physical parameters of alloys after processing by SPD.

This study is thus initiated with two main objectives: one is to investigate variations of d_S with respect to physical parameters such as melting temperature, diffusivity, valence electrons and stacking fault energy, as attempted earlier in Refs. [14,15] for pure metals; and the other is to

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examine the effect of dislocation–solute atom interactions on grain size and hardness.

2. Theoretical background

Among the models developed to predict d_S, a dislocation model developed by Mohamed has received much attention [10,11]. The model can be represented as:

$$\frac{d_S}{b} = A\exp\left(\frac{-\beta Q}{4RT}\right)\left(\frac{D_{P0}Gb^2}{v_0 kT}\right)^{1/4}\left(\frac{\gamma_{SFE}}{Gb}\right)^{1/2}\left(\frac{G}{HV_S}\right)^{5/4}, \qquad (1)$$

where b is the Burgers vector, A is a constant, $\beta \approx 0.04$, Q is the activation energy for self-diffusion, R is the gas constant, T is the absolute temperature, D_{PO} is the frequency factor for pipe diffusion, G is the shear modulus, v_0 is the initial dislocation velocity, k is Boltzmann's constant, γ_{SFE} is the stacking fault energy and HV_S is the steady-state hardness.

An earlier paper reported that d_S for pure metals is almost independent of γ_{SFE} as far as the data are evaluated at a given T/T_m (where T_m is the melting temperature) [15]. This finding indicates that the dominant parameters controlling d_S for pure metals are temperature and diffusion. As compared in Table 1, Mohammed's model also reaches a similar conclusion which is consistent with the experimental data taken from Ref. [15]. It is noted that since A and v_0 in Eq. (1) are unknown, the grain sizes in Table 1 were calculated as d_S normalized by d_S of Cu, d_S/d_S(Cu), using the parameters listed in Table 2. Several papers (e.g. [16,17]), however, reported that d_S for alloys can be given by a simplified form of Eq. (1):

$$\frac{d_S}{b} = B\left(\frac{\gamma_{SFE}}{Gb}\right)^{1/2}, \qquad (2)$$

where B is assumed to be constant and material independent. This relation suggests that the contribution of thermally activated processes, diffusivity and dislocation–solute atom interactions to d_S is negligible once the effect of γ_{SFE} is considered. Table 1 gives the normalized d_S values predicted using Eq. (2) for pure metals, indicating that the predictions are consistent neither with the experimental data nor with the values calculated by Mohamed's model. A question arises as to whether the significant decrease in d_S with alloying reported in different nanostructured alloys (e.g. [16–21]) is due to the decrease in γ_{SFE} or due to other matrix–solute atom interactions.

Table 1
Comparison between steady-state grain size after processing by HPT d_S, normalized by d_S for Cu, measured by experiments, calculated by Mohammed's model (Eq. (1)), and calculated as $d_S/b = B(\gamma_{SFE}/Gb)^{1/2}$ (Eq. (2)), where b is the Burgers vector, B is a material-independent constant, γ_{SFE} is the stacking fault energy and G is the shear modulus.

	d_S/d_S (Cu)		
Metal	Experimental (see Table 2)	Mohammed's model [10]	$d_S/b = B(\gamma_{SFE}/Gb)^{1/2}$
Zn	13.78	9.67	1.93
Al	5.13	7.97	2.76
Mg	2.70	2.44	3.11
Ag	1.30	0.58	0.84
Cu	1	1	1
Ni	0.65	0.30	1.32
Pd	0.59	0.75	2.12
Fe	0.54	0.48	1.52
Co	0.32	0.10	0.63

For alloys, solute atoms play a role in enhancing the shear stress required for dislocation movement, $\Delta\tau$, through several interactions: elastic interaction (atomic size mismatch between solute and matrix), modulus interaction (shear modulus mismatch between solute and matrix), electrical interaction (change in valence electrons per atom) and chemical interaction (change in stacking fault energy) [22]. Fleischer commented that the two latter interactions are less important once the effect of the two former interactions is considered. Fleischer's model can be given as follows [23]:

$$\Delta\tau = \frac{G\left|\varepsilon'_G - m\varepsilon_b\right|^{3/2}c^{1/2}}{\alpha}, \qquad (3)$$

where c is the concentration of solute atoms, $m = 3$ for screw dislocations and 16 for edge dislocations, $\alpha = 700$ for face-centered cubic (fcc) alloys, $\varepsilon_b = (\mathrm{d}b/\mathrm{d}c)/b$ is the atomic size mismatch and ε'_G is the modulus mismatch parameter given as:

$$\varepsilon'_G = \frac{\varepsilon_G}{1 + 0.5\varepsilon_G}, \qquad (4)$$

where $\varepsilon_G = (\mathrm{d}G/\mathrm{d}c)/G$ is the modulus mismatch. Fleischer showed that the solid-solution hardening in fcc alloys is controlled mainly by the interaction of solute atoms with screw dislocations [23]. Several papers, however, indicated that Fleischer's model may need some modification, especially when the concentration of solute atoms is high [24,25] or when the grains are on the nanometer scale [26]. Labusch suggested that the following relation holds better than Fleischer's model under experimental conditions [24]:

$$\Delta\tau = \frac{G\left[\varepsilon'^2_G + (15\varepsilon_b)^2\right]^{2/3}c^{2/3}}{\varphi}, \qquad (5)$$

where $\varphi = 550$ for fcc alloys. Contrary to Fleischer's model, Labusch suggested that solid-solution hardening in fcc alloys is controlled by the strong interaction of solute atoms with edge dislocations [24]. In the following, we examine whether Fleischer's and Labusch's models can be employed to explain the effect of solute atoms on grain size and hardness during HPT.

3. Experimental materials and procedures

Samples of several pure metals (Mg, Al, Fe, Co, Ni, Cu, Zn, Pd, Ag) and several single-phase fcc alloys (Al–Mg, Al–Ag, Al–Cu, Cu–Al, Cu–Zn, Pd–Ag, Ni–Fe, Ni–Co) were used in this study. Table 2 gives a list of materials

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