



ELSEVIER

Contents lists available at ScienceDirect

Materials Letters

journal homepage: www.elsevier.com/locate/matlet

Inverse Hall–Petch effect in quasi- and nanocrystalline materials

K.A. Padmanabhan^{a,*}, Sriharsha Sripathi^a, H. Hahn^{b,c}, H. Gleiter^b^a School of Engineering Sciences and Technology & Centre for Nanotechnology, University of Hyderabad, Prof. C R Rao Road, Hyderabad 500 046, India^b Karlsruhe Institute of Technology (North Campus), Institute of Nanotechnology, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany^c KIT-TUD Joint Research Laboratory Nanomaterials, TU Darmstadt, Jovanka-Bontschits-Strasse 2, 64287 Darmstadt, Germany

ARTICLE INFO

Article history:

Received 13 June 2014

Accepted 25 June 2014

Available online 8 July 2014

Keywords:

Grain size softening/inverse Hall–Petch effect

Grain boundary sliding

Rate controlling process

Quasi-crystals

Nanocrystalline materials

ABSTRACT

Inverse Hall–Petch effect/grain size softening in quasi- and nanocrystalline materials at ambient/low temperatures is attributed to mesoscopic (\sim a grain diameter or more) grain/interphase boundary sliding controlled flow. Equations for estimating the free energy of activation for the rate controlling process, the free volume fraction present in a basic sliding unit and the average number of grain boundaries that align to form a planar interface during superplastic deformation are given in some of our earlier papers. These predictions are verified here using experimental data pertaining to one quasi- and two nanocrystalline systems. The agreement between the predictions and the experimental observations is satisfactory.

© 2014 Elsevier B.V. All rights reserved.

1. Introduction

In micro-mechanics [1] decreasing grain size has a similar effect as increasing temperature so far as creep effects in a material are concerned. Therefore, it is understandable that creep/superplastic effects are seen at room temperature in a high-temperature-melting material like palladium when its micro-structure is nanocrystalline [2]. Koch and Narayan [3] found fault with most of the experimental results in which inverse Hall–Petch (IHP) effect was reported because they noted that the samples used were not defect-free. According to them [3] only four sets of data demonstrated a genuine grain size softening/IHP effect.

Recently, a grain softening effect in an Al–Cu–Fe based nano-/quasicrystalline material was reported [4]. The experimental results (Fig. 3 of [4]) seem to suggest that the grain size dependence of hardness in the region in which the grain softening effect is observed follows IHP relationship, as suggested earlier [5,6]. Notwithstanding this, the authors have interpreted their results in terms of a model [7,8] in which the hardness varies as $\log(L)$ or L , where L is the average grain size, depending on the approximation used.

The present authors [5,6] presented an explanation for the occurrence of IHP effect by refining a model for mesoscopic grain

boundary sliding (mGBS) controlled flow in microcrystalline materials [9] to include the nanocrystalline range as well. The correlation of the flow stress with superplastic strain rates and the method of knowing the atomistic constants, estimating the free energy of activation for the rate controlling process, the threshold stress for the onset of mGBS and the free volume fraction present in a basic unit of sliding were details presented in later works [10–15]. In fact, [7,8] appear to have used an earlier paper of ours [16] extensively, which, like [7,8], deals with grain boundary sliding (GBS) controlled flow. For example, Eq. (2) of [7] becomes identical to Eq. (2) of [16] when it is noted that N_v in [7] is represented as N (the number of sites along the grain boundary at which atomic jumps take place aided by stress and temperature) in [16] and (Ab) [7] as γ [16]. (N_v and N are defined somewhat differently in the two papers, but the physical picture is very similar.) Post-1990, our model was improved upon significantly by introducing many microstructural details concerning the general high-angle boundaries [10–15] because by then the controversies regarding the structure of general high-angle grain boundaries had got settled and understanding in terms of the structural unit model had emerged [17–21].

In brief, in the model the rate controlling processes are assumed to be confined to the grain/interphase boundary regions. High-angle boundaries, along which boundary sliding is concentrated [22,23], are divided into atomic-scale ensembles that surround free volume sites present at discrete locations on the boundary characteristic of misorientation and the nature and magnitude of inter-atomic forces. Due to the presence of free

* Corresponding author. Tel.: +91 40 2313 4455.

E-mail addresses: kapse@uohyd.ernet.in, ananthaster@gmail.com (K.A. Padmanabhan).

volume, these ensembles possess a lower shear modulus compared with the rest of the boundary and hence constitute the basic units of sliding. Microscopic sliding caused by localized shear persists till it is rendered ineffective by steric hindrances like at a triple junction. For GBS to develop to a mesoscopic scale, two or more grain boundaries need to align to form a plane interface, which by further interconnection with other similar plane interfaces will lead to large scale sliding till it gets stopped by an insurmountable barrier like an extra-large grain or a coarse precipitate. This plane interface formation process, brought about by dislocation emission from grain boundaries or diffusion, both of which are regarded as faster than GBS in the model, gives rise to a long-range threshold shear stress, τ_0 , which has to be overcome for mGBS to set in. Free energy minimization and the possibility of the applied stress doing maximum work in this configuration (principle of maximum work) are the reasons for plane interface formation. A mathematical analysis that assumes that the basic sliding unit is of oblate spheroid shape of base diameter ($5a_0$) and height ($2.5a_0$), where a_0 is the inter-atomic distance in the boundary region (\sim equal to the atomic diameter) and that the grain shape is rhombic dodecahedron, leads to Eqs. (1a) and (1b). From bubble raft experiments, the work of Argon [24] and MD simulations [20,21], the free volume fraction inside the basic sliding oblate spheroid is taken in a first order approximation as ~ 0.10 for all superplastic systems.

$$\dot{\gamma} = \frac{2W\gamma_0\nu}{L} \sinh\left(\frac{(\tau - \tau_0)\gamma_0 V_0}{2kT}\right) \exp\left(-\frac{\Delta F_0}{kT}\right) \quad (1a)$$

$$\Delta F_0 = \frac{1}{2}(\beta_1 \gamma_0^2 + \beta_2 \varepsilon_0^2) GV_0 \quad (1b)$$

In Eqs. (1a) and (1b), $\dot{\gamma}$ is the strain rate, W the average grain boundary width ($= 2.5a_0$), γ_0 the free volume fraction present in the basic unit of sliding present in the grain boundaries, which will approximately be equal to the shear strain (dependent on the material; the method of determining it has been given), ν the thermal vibration frequency ($= 10^{13} \text{ s}^{-1}$ or $(kT/h) \text{ s}^{-1}$, with h the Planck constant), τ the applied shear stress, V_0 the volume of the basic sliding unit ($= (2/3)\pi W^3$), k the Boltzmann constant, T the temperature of deformation on the absolute scale, ΔF_0 the free energy of activation for the basic sliding event, G the shear modulus of the basic sliding unit, ε_0 the dilatational strain in a unit sliding event ($= \gamma_0/\sqrt{3}$), if von-Mises yield criterion is assumed) as the oblate spheroid is embedded in a solid matrix, $\beta_1 = 0.944 (1.59 - p/1 - p)$ and $\beta_2 = 4(1 + p)/9(1 - p)$. Where p is Poisson's ratio.

There are no adjustable constants in the analysis. ΔF_0 , and σ_0 , the only unknowns, are obtained directly from the experimental results. (Expressions are available for their theoretical estimation also—Eq. (1b) above and Eqs. (13) and (14) of [10]). The numerical procedures used to solve the transcendental Eq. (1a) with a view to comparing the predictions of the model with experimental findings are also available [10,11,15].

It is known that if von Mises yield criterion is assumed $\tau = H_V/3\sqrt{3}$, when H_V , the hardness of the material, is reported on the Vickers scale. How this relationship gets modified, if other yield criteria like Mohr–Coulomb are used, has also been explained [12,13]. Thus, one obtains Eq. (2) [5,6].

$$H_V = H_{Va} - \frac{m_2}{L} \sqrt{(L - L_0)} \quad (2)$$

here H_V is the measured (steady state) hardness, H_{Va} the hardness equivalent of the applied stress at the moment of load application, m_2 , a constant ($= G\sqrt{L_1}/C$), with C a conversion factor (from shear to hardness, $\tau = CH_V$; $C = 1/3\sqrt{3}$ for von Mises yield criterion), $L_0 (= 2W\sqrt{6})$ the grain size at which τ_0 falls off to zero and L_1 is

Table 1

Degree of fit for the three relations: $H_V \propto \ln(L)$, $H_V \propto L$ and $H_V \propto L^{-0.5}$.

System	L (nm)	H (GPa)	Correlation coefficient of H and		
			ln(L)	L	L ^{-0.5}
Al62.5 Cu2.5 Fe12.5 [4]	38.8	11.41	0.9487	0.9168	0.9623
	23.5	10.46			
	20.6	9.31			
	17.5	8.56			
Zn [25]	11.0	1.06	0.9942	0.9813	0.9979
	7.9	0.84			
	5.9	0.58			
Ni 18Fe [26]	13.9	6.15	0.7867	0.8064	0.7767
	12.7	5.70			
	11.0	5.71			

a convenient notation representing

$$L_1 = 3^{-0.75} 2^{15} N_{\text{pl}}^{-0.5} \frac{\gamma_B}{G\alpha_f} \quad (3)$$

with α_f a form factor (~ 1) and γ_B specific grain boundary energy and N_{pl} the number of grain boundaries that align to form a plane interface at a given value of L . (For obtaining numerical values for N_{pl} using Eq. (2), within a narrow grain size range N_{pl} is treated as independent of L . But in general N_{pl} is a strong function of grain size and temperature.) Using isothermal experimental hardness vs. grain size data reported and Eqs. (2) and (3), not only one can account for the IHP effect, but also predict the number of grains that align to form a plane interface.

In this paper the data presented in [4] and in [25,26] are re-analyzed.

The degree of fit, as determined by coefficient of correlation, for all the three expressions H_V vs. $\ln(L)$, H_V vs. L and H_V vs. $L^{-0.5}$ is very similar—Table 1. On this basis alone it is fair to say that both our approach [5,6] and that of Conrad and Narayan [7,8] account for the experimental results satisfactorily. This finding clearly underlines the dangers in preferring one atomistic mechanism over another merely based on gross correlations.

With reference to the preference of [4] for the model of Conrad and Narayan [7,8] the following observations are in order. (a) Figs. 4 and 5 of [4] suggest that the activation energy for the rate controlling process gets doubled when the same is determined by plotting H_V vs. L instead of H_V vs. $\ln(L)$. This observation is in conflict with the finding [7,8] that very similar activation energy for the rate controlling process result from both types of plots. (b) In the earlier analysis [7,8] the effective stress is taken as \sim the applied stress, i.e., the strain-rate sensitivity index, $m = 1.0$. But, in nanocrystalline materials at room temperature the value of m is in the range 0.02–0.08 [27,28]. In contrast, in our approach [5,6,9–15] the value of m can vary from a very low value to 1.0, depending on the difference between the applied stress and the threshold stress needed to give rise to mesoscopic boundary sliding. Our analysis [5,6,9–15] also suggests (a) a method of calculating the threshold stress, τ_0 (see Eqs. (13) and (14) of [10]) and (b) the strain rate of deformation in terms of the material and experimental parameters, including the free energy of activation, ΔF_0 —Eqs. (1a) and (1b).

In the papers taken up for analysis, the strain rate of the hardness test is not reported. According to [29] this lies in the range of $5 \times 10^{-2} \text{ s}^{-1}$ – $5 \times 10^{-4} \text{ s}^{-1}$. (It is not clear from [4] what value of strain rate was assumed, while determining the activation energy from their Figs. 4 and 5). By assuming that the strain rate range reported [29] is relevant for the results of [4,25,26], a free energy of activation for the rate controlling

Download English Version:

<https://daneshyari.com/en/article/1643752>

Download Persian Version:

<https://daneshyari.com/article/1643752>

[Daneshyari.com](https://daneshyari.com)