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The effects of strain rate and grain size on nanocrystalline materials: A theoretical prediction

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ABSTRACT

The article describes a dislocation-based model for the coupling effects of strain rate and grain size on the mechanical behavior of nanocrystalline materials. Two important experimental findings about nanocrystalline materials are explained by the model: 1. the difference of the dependencies of strain rate sensitivity (SRS) on grain size between FCC and BCC nanocrystalline materials and 2. the abnormal dependency of activation volume on thermally activated stress. Our analysis shows that the strain rate-dependent behavior of nanocrystalline materials is mainly determined by the ratio between the activation volumes in grain and grain boundary regions.

1. Introduction

In the last thirty years, a vast set of constitutive relations have been proposed to describe the influences of strain rate and temperature on the deformation resistance of materials [1–3]. To further account for the grain size effects, an additional term $k_{HP}d^{-1/2}$ has been widely introduced into the description of deformation resistance, according to the Hall–Petch equation [4,5]. Here, d is the grain size and the Hall–Petch slope k_{HP} is usually regarded as a material constant, meaning that the effects of strain rate and grain size are not coupled in these models. However, in recent years, with the more and more intensive investigation of nanocrystalline materials, the roles of strain rate and grain size and their interdependence have attracted the interest of many researchers [6–8]. Blum and Zeng [9] pointed out that the strain rate sensitivity (SRS) of the flow stress σ, defined as $m = \partial \ln\sigma/\partial \ln \dot{\varepsilon}$, is relatively higher in nanocrystalline materials than that in materials with conventional grain sizes. The research of Wang [10] shown that although the SRS is almost independent of the strain rate $\dot{\varepsilon}$ for materials with conventional grain sizes, it is significantly affected by the strain rate for nanocrystalline materials. Wei [11], Gu [12], and Nyakiti [13] also demonstrated that the SRS is affected by the grain size. In more detail, the SRS increases with a decrease in grain size for FCC and HCP [14,15] nanocrystalline materials. On another hand, the work of Wei [16] demonstrated that for BCC nanocrystalline materials, the SRS prefers to decrease with the decrease in grain size. These results clearly shown that the effects of strain rate and grain size are coupled for materials with grain sizes reducing to nanoscale regime, and interestingly, the coupling effects of BCC and FCC materials are different. Besides the significant dependence of SRS on the grain size for nanocrystals, the dependence of apparent activation volume V_a on thermally activated stress σ_{th} has been found abnormal for FCC materials with nanoscale grain sizes [17]. It was revealed that V_a of nanocrystalline copper increases as the applied stress increases. This tendency is adverse to that of materials with conventional grain sizes, that V_a decreases with the increase in flow stress, as shown by Armstrong [18] and Gu [19,20].

The present paper is aimed at developing a dislocation-based model to investigate the coupling effects of strain rate and grain size on the mechanical behavior of nanocrystalline materials. The model is then used to account for the difference in the grain size dependencies between BCC and FCC materials. The abnormal dependence of apparent activation volume on thermally activated stress of FCC nanocrystalline materials can also be explained by the established model.

2. Theory

2.1. Grain size effect on dislocation gliding

The Orowan equation $\dot{\varepsilon} = \rho b v_{th}$ [21] has been widely used to study the strain rate-dependent behavior of materials with conventional grain sizes, in which the deformation mechanisms are dominated by the dislocation gliding in the grains. Here, ρ is the mobile dislocation density, b is the length of Burgers vectors, and v_{th} is the average speed of the thermally activated dislocation gliding. When the grain size

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decreases, the contributions of dislocation multiplication $\dot{\rho}$ to $\dot{\varepsilon}$ would be significant and this effect has been added in the modified Orowan equations by the subsequent researchers [5,22–25]. Recently, for modeling the behavior of nanocrystalline materials, Duhamel [17] introduced the grain boundary effect to modify the Orowan equation so as to account for the contributions of inter-granular behavior. Combining all the above-descried effects, the modified Orowan equation for materials can be written as:

$$\dot{\varepsilon}=\dot{\varepsilon}_g\left(1-\frac{\delta}{d}\right)+\upsilon\frac{\delta}{d}, \tag{1}$$

where the first term on the right side describes the contribution of dislocation gliding within the grain and the second term represents the contributions of grain boundary. δ is the thickness of grain boundary, d is the grain size, and υ is the frequency for dislocation emission from grain boundary. $\dot{\varepsilon}_g=\rho_g b v_{th}+\dot{\rho}_g bl$ is the strain rate caused by dislocation gliding and multiplication in the grain region [5,22], where ρ_g is dislocation density in grain region and l is the mean free path of dislocation glide. The term $\dot{\rho}_g bl$ represents the effect of dislocation multiplication and is significant when the evolution of dislocation density cannot be neglected. The term δ/d can be regarded as the volume fraction of grain boundary and $\upsilon\delta/d$ describes the effect of dislocation emission from grain boundary on strain rate.

The evolution of ρ_g has been widely investigated in the literature [26–28]. For nanocrystalline materials, the interaction of intra-grain dislocations with grain boundary is remarkable [29–32]. We therefore propose the following equations to describe the evolutions of dislocation densities in both grain and grain boundary by considering their interaction:

$$\begin{aligned}\dot{\rho}_g&=\left(\upsilon\rho_{gb}-\rho_g v_{th}\theta\frac{\delta}{d}\right)+\left(\kappa_3\frac{v_{th}}{bl}-\kappa_1\rho_g v_{th}\right),\\ \dot{\rho}_{gb}&=-\left(\upsilon\rho_{gb}-\rho_g v_{th}\theta\frac{\delta}{d}\right)-\kappa_2\rho_{gb}\upsilon,\end{aligned} \tag{2}$$

where ρ_{gb} denotes the dislocation density in grain boundary region and $\upsilon\rho_{gb}$ is the change of dislocation density caused by the propagation of dislocations from grain boundary into grain. $\theta(\delta/d)$ represents the volume ratio between grain boundary and grain in materials and $\rho_g v_{th}\theta(\delta/d)$ means the change of dislocation density by the propagation of dislocations from grain into grain boundary. Therefore, the term $\upsilon\rho_{gb}-\rho_g v_{th}\theta(\delta/d)$ describes the net increment of dislocation density in grain by the dislocation exchange between grain and grain boundary. $\kappa_1\rho_g v_{th}$ and $\kappa_2\rho_{gb}\upsilon$ correspond to the effects of dynamic recoveries in grain and grain boundary regions, respectively. $\kappa_3 v_{th}/(bl)$ represents the variation of dislocation density caused by the multiplication in grain region [33].

It was pointed out that as the plastic deformation develops, the mechanical behavior of nanocrystalline materials reaches a steady state where the deformation resistance is independent of the strain [9], which corresponds to $\dot{\rho}_g=0$ and $\dot{\rho}_{gb}=0$. By using Eq. (2), the steady dislocation densities ρ_{gs} for grain and ρ_{gbs} for grain boundary can be obtained as:

$$\rho_{gs}=\frac{1}{bl}\frac{\tilde{d}}{\tilde{\theta}+\tilde{\kappa}_1\tilde{d}},\quad \rho_{gbs}=\frac{\kappa_3 v_{th}\tilde{\theta}}{\upsilon bl\kappa_2\left(\tilde{\theta}+\tilde{\kappa}_1\tilde{d}\right)}, \tag{3}$$

where $\tilde{d}=d/\delta>1$, $\tilde{\kappa}_1=\kappa_1/\kappa_3$, and $\tilde{\theta}=\kappa_2(\theta/\kappa_3)/(1+\kappa_2)$ are dimensionless parameters. By using Eq. (1), the corresponding strain rate is:

$$\dot{\varepsilon}=\frac{v_{th}}{l}\frac{\tilde{d}-1}{\tilde{\theta}+\tilde{\kappa}_1\tilde{d}}+\frac{\upsilon}{\tilde{d}}. \tag{4}$$

Assuming both the average speed of the thermally activated dislocation gliding v_{th} and the grain-boundary emission frequency υ are dominated by thermal activation mechanisms, one can write v_{th} and υ by Arrhenius equation as

$$\begin{aligned}v_{th}&=v_0\exp\left(-\frac{G_d}{kT}\right),\quad V_d=-\frac{\partial G_d}{\partial\sigma_{th}},\\ \upsilon&=\upsilon_0\exp\left(-\frac{G_{gb}}{kT}\right),\quad V_{gb}=-\frac{\partial G_{gb}}{\partial\sigma_{th}},\end{aligned} \tag{5}$$

where G_d and G_{gb} are the activation energies for grain and grain boundary, respectively, V_d and V_{gb} are the corresponding activation volumes [34], k is Boltzmann constant, and $\sigma_{th}=\sigma-\sigma_{ath}$ is the thermally activated stress (σ_{ath} is the athermal stress which is independent of the strain rate and σ is the applied stress).

2.2. Grain size effect on strain rate sensitivity (SRS)

The strain rate sensitivity (SRS), defined as $m=\partial\ln\sigma/\partial\ln\dot{\varepsilon}$, can be obtained by combining Eqs. (4) and (5):

$$m=\alpha\left[1+(1-\beta)(\eta\gamma+\beta)^{-1}\right], \tag{6}$$

where $\eta=\tilde{d}(\tilde{d}-1)/(1+\lambda\tilde{d})$, $\alpha=kT/(\sigma V_d)$, $\gamma=v_{th}/(\tilde{\theta}\upsilon l)$, $\lambda=\tilde{\kappa}_1/\tilde{\theta}$, and $\beta=V_{gb}/V_d$ is the ratio between the activation volumes in the grain boundary and in the grain region. Since V_d is approximately proportional to σ_{th}^{-1} [35], α can be safely considered to be scarcely dependent on the applied stress σ when $\sigma_{ath}\ll\sigma_{th}$. The grain size effect is introduced to the SRS by parameter η. For $\tilde{d}\gg1$, Eq. (6) can be reduced to $m\approx\alpha=kT/(\sigma V_d)$, which is consistent with the conventional grain size condition, see, for example, [11,36–38].

The parameter β is critical to determining the grain size dependency of SRS, and β differs between FCC and BCC crystals. For FCC as well as HCP crystals, due to the closely packed crystal structures, the dislocations glide mainly by overcoming the thermal barriers of the solute atoms or pining dislocations [39], whereas for BCC crystals, the gliding resistance mainly comes from the formation the dislocation kinks [27]. These different types of thermal barriers results in a larger activation volume V_d in FCC crystals than that in BCC crystals. The activation volume in the grain boundary V_{gb} has the order of δb^2, which is usually a bit larger than V_d in BCC crystals. Consequently, for BCC materials, β is generally larger than 1, whereas for FCC crystals, $\beta<1$. Since $\tilde{d}>1$, the equation $\partial\eta/\partial\tilde{d}>0$ establishes. Therefore, according to Eq. (6), as the grain size increases, the SRS decreases for FCC materials ($\beta<1$) and increases for BCC materials ($\beta>1$). The results answer for the different experimental findings between FCC and BCC nanocrystallines [12–14].

It is worthy of pointing out that for BCC materials, when the grain size reduces to tens of nanometers, the deformation mechanism would be dominated by grain boundary-related behavior such as grain boundary sliding [32,40]. As a result, the activation volume of the grain boundary V_{gb} dramatically decreases and can be similarly described by Wu [41] as $V_{gb}=V_{gb0}(1+\xi d^{-3/2})^{-1}$, where V_{gb0} is the activation volume of the grain boundary for coarse-grained materials, and ξ is a model parameter. Therefore, $\beta=\beta_0(1+\xi d^{-3/2})^{-1}$ may reach a value less than 1, and for such a kind of BCC materials, the SRS increases with the decrease of grain size, as reported by Jang [40] and Wu [41].

2.3. Apparent activation volume

The apparent activation volume, defined as $V_a=kT(\partial\ln\dot{\varepsilon}/\partial\sigma_{th})$, is another parameter commonly used to characterize the strain rate-