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Strain hardening of crystalline materials

Edison A. Bonifaz[1*]

[1]*Colegio de Ciencias e Ingeniería - El Politécnico, Universidad San Francisco de Quito.*
Diego de Robles y Vía Interoceánica, Quito, Ecuador
[*]*Autor principal/Corresponding author, e-mail: edisonb@usfq.edu.ec*

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Abstract

To describe the work hardening process of crystalline materials in uniaxial deformation, a gradient-one-internal-variable model (GM1) constructed in the basis of the Kocks-Mecking model is proposed. The time and temperature dependence of flow stress is accounted via grain boundary migration, and the migration is related to annihilation of extrinsic grain boundary dislocations (EGBD's) by climb *via* lattice diffusion of vacancies at the triple points. To model the polycrystalline behavior of commercially pure nickel (from a composite point of view) by means of the finite element method, virtual specimens with dimensions in the range 3 - 25 *um* should be used.

Keywords. Dislocations, grain boundary, finite element method, polycrystalline behavior.

Resumen

Para describir el proceso de endurecimiento de materiales cristalinos en deformación uniaxial, un modelo de gradiente variable interna simple (GM1) construido en base del conocido modelo de Kocks-Mecking es propuesto. La dependencia en tiempo y temperatura de la tensión de flujo es considerada vía migración de bordes de grano, y la migración es relacionada al aniquilamiento de dislocaciones de borde de grano extrínsecas (EGBD's) mediante climb vía difusión de red de vacancias en puntos triples. Para modelar el comportamiento policristalino de níquel comercialmente puro (desde un punto de vista de un compuesto) por medio del método del elemento finito, probetas virtuales con dimensiones en el rango de 3–25 μm deberían ser usadas.

Palabras Clave. Dislocaciones, borde de grano, método de los elementos finitos, comportamiento policristalino.

Introducción

Ashby [1] showed that polycrystalline specimens, even in pure metals, deform plastically in a non-uniform way, so, the total dislocation density, ρ^T, defined as the sum of geometrically necessary dislocations ρ^G and statistically stored dislocations ρ^S can be used to represent polycrystalline flow stress at any strain by means of the following equation

$$\sigma = \sigma_0 + M\alpha Gb\sqrt{\rho}^T \qquad (1)$$

Here, σ_o considers the additive contribution from lattice resistance at zero temperature σ_p (Peierls or friction stress), and solution hardening stress from alloying elements σ_{ss}, i.e., $\sigma_0 = \sigma_p + \sigma_{ss}$,*M* is the average Taylor factor, which evolves in the process of straining, *b* is the magnitude of the Burgers vector, *G* an appropriate shear modulus and α a constant of order 0.3. Equation (1) is supported from the experimental observations carried out by Narutani and Takamura [2] and other investigators [3] [4] [5] , indicating that the flow stress is proportional to the square root of dislocation density ρ, irrespective of the grain size, amount of strain and test temperature. Ashby's total dislocation density ρ^T definition assume that the geometrically necessary dislocations, ρ^G, have no direct influence on the accumulation of the statistically stored dislocations ρ^S. The statistically stored dislocations are accumulated in the matrix of pure crystals during straining and are responsible for the normal 3-stage hardening [1] . On the other hand, the difference in crystallographic orientation between neighboring grains can be corrected by introducing geometrically necessary dislocations, which are introduced to accommodate the incompatibility of deformation between grains.

Thompson et al [6] have shown during straining that in-

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homogeneous deformation occurs adjacent to grain boundaries, leading to a concept of a harder 'mantle' close to the boundary and a softer 'core' in the grain interior. Furthermore, Li [7] has shown that grain boundaries can act as sources for dislocations and via TEM Murr [8] corroborated Li's proposal that grain boundary ledges act as sources for dislocations during straining. Therefore besides the intrinsic grain boundary dislocations, extrinsic grain boundary dislocations (EGBD's), can be formed during straining, giving the mantle of geometrically necessary dislocations adjacent to the grain boundary. It was also shown by Meyers and Ashworth [9] that shear stresses can exist initially at low strain levels in the grain boundaries, up to three times higher than the overall homogeneously applied stress. Therefore generation of dislocations would usually occur at grain boundary ledges, before sources operated in the grain interior. The flow stress in the boundary therefore is greater than the overall bulk value, this being the mantle and core proposal of Thompson et al. [6]

Previous research by our group has shown that 2.5 - 6 % strain give the highest Σ_{sp} values, where sigma is the reciprocal density of coincident sites. For these low strain values, it was proposed that strain levels around 2.5-6 % produce the mantle-core effect, whereas greater strains such as 9 and 12 % strains result in the flow stress of the core and mantle being approximately the same [10]. During subsequent heat treatment at these low strain values recovery process are underway and recrystallization does not occur, whereas at higher strain levels, depending on temperature, recrystallization may occur and new high angle grain boundaries form destroying the existing microstructure which is conducive to the formation of special boundaries.

During the annealing of lightly strained 316 stainless steel, Sangal and Tangri [11] showed, that the non-equilibrium grain boundaries formed by straining (EGBD's), can be transferred to an equilibrium state via grain boundary migration, and the migration is related to annihilation in the area of the grain boundary. The annihilation of the EGBD's is a function of temperature and time is given by the following equation [11] :

$$\rho^e = \frac{1}{\frac{1}{\rho^o} + \left\{ \frac{D_s G V \left[1 - 2\ln\left(\frac{r_o}{L}\right)\right]}{L(1-v)kT\ln\left(\frac{R_o}{r_o}\right)} \right\}} \qquad (2)$$

where ρ^o is the initial dislocation density, D_s is the self-diffusion coefficient, *V* is the atomic volume, *L* is the length of grain boundary, r_o is approximately equal to the Burger's vector, R_o is approximately equal to the half distance between triple points, *G* is the shear modulus and *t* is time. Note that at temperatures below the recovery process, $\rho^e \approx \rho^o$.

The Gradient one-internal-variable model (GM1)

This model is constructed on the basis of the following equations [12] :

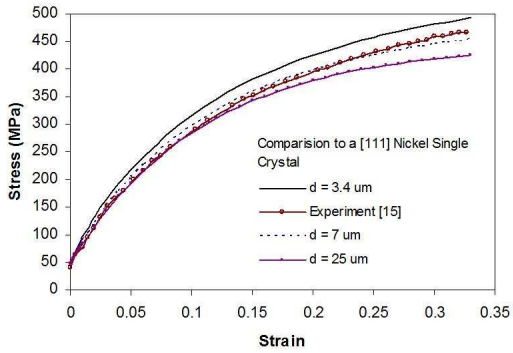

Figure 1: Experimental and calculated stress-strain curves for [111] single crystals. Model parameters: *M*=3, α=0.3, *b*= 2.52E-8 cm, *G*=116.5 GPa, =293 K, ρ^e =1E8 cm^{-2}, K_1=947000 cm^{-1} [2] , K_2=6.12 [2] , *d*=3.4, 7 and 25 *um*, σ_o = 21.8 MPa [13] .

$$\sigma = \sigma_0 + M\alpha G b\sqrt{\rho^S + \rho^G} \qquad (3)$$

$$\rho^S = \left[\frac{K_1}{K_2}\left(1 - e^{\frac{-MK_2\overline{\varepsilon}}{2}}\right) + \sqrt{\rho^e}e^{\frac{-MK_2\overline{\varepsilon}}{2}}\right]^2 \qquad (4)$$

$$\rho^G \approx \frac{\overline{\varepsilon}}{4bd} \qquad (5)$$

Here, $\overline{\varepsilon}$ represents the tensile equivalent strain and ρ^e is the dislocation density at time t. K_1 and K_2 characterize the processes of dislocation storage and concurrent dislocation annihilation by dynamic recovery, respectively [2] [14] . To validate the model, true stress-true strain curves for three grain sizes of nickel are shown in Fig. 1, as a comparison to a [111] crystal result.

The grain size diameter *d* = 7 *um* is shown to agree very well, while the grain sizes *d*= 3.4 *um* and *d* = 25 *um* agree reasonably well.

Conclusions

A gradient-one-internal-variable model constructed in the basis of the Kocks-Mecking model is proposed. If all of the above parameters are consistent with experimental observations, to model the polycrystalline behaviour of commercially pure nickel (from a composite point of view) by means of the finite element method, virtual specimens with dimensions in the range 3 - 25 *um* should be used.

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