



Grain size evolution during discontinuous dynamic recrystallization

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Grain size behaviour during discontinuous dynamic recrystallization in alloys is characterized by a theoretical approach that combines a novel thermostatics framework, with classical grain nucleation and growth formulations. Configurational effects from dislocation migration paths control microstructure variation via an entropic effect. An alternative approach for accounting for solute–drag effects is proposed. It is shown that the drag atmosphere linearly amounts to the atomic radius of solute atoms. The approach is validated for various deformation conditions in 20 single-phase metals.

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Discontinuous dynamic recrystallization (DRX) occurs during the hot deformation of low to medium stacking fault energy alloys. New grains are formed by strain-induced grain boundary motion once a critical shear strain γ_{DRX}^* is reached [1]. Dislocation-free grains then grow as deformation continues, by bulging into their surroundings and consuming the deformed regions [2]. Once steady state is achieved, a constant average grain size D_{ss} is reached; D_{ss} is shown to be independent of the average initial size D_0 [3]. However, D_{ss} is shown to be highly sensitive to the material's purity and solute concentration [4–6]. The objective of this work is to present a novel approach for describing grain size behaviour during discontinuous DRX at high temperatures in single-phase face-centred cubic (fcc) alloys.

A thermodynamic framework has been derived by the authors for predicting the dynamic recovery rate and average dislocation density ρ evolution at various temperatures and strain rates [7,8]. The evolution of the average dislocation subgrain size d_c has also been modelled by performing a balance between the energy produced by a dislocation forest and by the ordered material in the form of dislocation cells [9]: $d_c = \frac{\kappa_c}{\sqrt{\rho}} = \frac{12\pi(1-\nu)}{(2+\nu)} \left(1 + \frac{T\Delta S}{\mu b^3}\right) \frac{1}{\sqrt{\rho}}$, where ν is the Poisson ratio, μ is the shear modulus, b is the magnitude of the Burgers vector and ΔS is the entropy associated with the possible dislocation migration paths. The latter has been introduced to account for the energy loss due to

the different dislocation velocity configurations. The entropy equals:

$$\Delta S = k_B \ln \left(\frac{\dot{\epsilon}_0 + \vartheta}{\dot{\epsilon}} \right), \quad (1)$$

where $\dot{\epsilon}$ is the axial strain rate¹; $\dot{\epsilon}_0 = cb\rho_Y$ is a constant related to the speed of sound c , and ρ_Y is the dislocation density consistent with the yield point ($\rho_Y = (0.9\sigma_Y/\mu b)^2$ [8]); $\vartheta = 10^{13} \exp(-\frac{E_m}{RT})$ is the vacancy atomic jump frequency, and E_m is the vacancy migration energy. Details on the derivation and application of ΔS can be found elsewhere [7–9].

Once recovery and subgrain evolution have been obtained, the critical conditions for the onset of DRX can be described [8]: the strain energy to nucleate dislocation-free grains (being proportional to $\frac{1}{2}\mu b^2$, around the initial boundary length) equals the stored energy at subgrain boundaries ($\frac{1}{2}\mu b^3$), which is reduced by the dissipation (entropy) effects when grain boundary bulging occurs ($T\Delta S^2$), and from the fraction of dislocations in the subgrain interiors moving towards the walls ($\frac{1}{\kappa_c}T\Delta S$ [8]). From this balance, γ_{DRX}^* is obtained [8]:

$$\gamma_{DRX}^* = \frac{\frac{1}{2}\mu b^3 - \left(1 + \frac{1}{\kappa_c}\right)T\Delta S}{\frac{1}{2}\mu b^3}. \quad (2)$$

¹The shear (γ) and axial (ϵ) strains are directly related by the Taylor factor $\gamma = M\epsilon$, where $M = 3$ for the tested materials [8].

²Grain boundaries are considered to be formed by a dislocation arrangement, hence configurational effects from moving boundaries equal $T\Delta S$ [8].

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This equation represents the ratio between the effective activation energy to initiate grain boundary bulging, and the stored energy in the material. Thus, the activation energy for grain nucleation Q_{nuc} should be proportional to the numerator in the previous equation:

$$Q_{nuc} = \frac{1}{8} \left(\frac{1}{2} \mu b^3 - \left(1 + \frac{1}{\kappa_c} \right) T \Delta S \right), \quad (3)$$

where 8 is a geometric factor that accounts for the effective boundary sites where grain bulging occurs; this constant amounts to the subgrain surface area per unit volume of a subgrain, and has been considered to be in the range 1–10 [10,11]. By combining the previous results, the average dislocation density evolution and flow stress response (via ρ and d_c) during DRX have been described for several multicomponent systems [8].

The average grain size at a given shear strain (γ) is obtained by adding the size of the deformed (D_j^{Def}) and recrystallized (D_k^{Rex}) grains over the total number of grains N :

$$\bar{D} = \frac{\sum_{i=1}^N D_i}{N} = \frac{1}{N} \left(\sum_{j=1}^{N_0} D_j^{Def} + \sum_{k=N_0+1}^N D_k^{Rex} \right), \quad (4)$$

where N_0 is the number of deformed grains prior to recrystallization. N and D_i ($i = 1, \dots, N$) are dependent on γ ; in addition, $\bar{D} = D_0$ and $N = N_0$ for $\gamma \leq \gamma_{DRX}^*$. ($N^{-1} \sum D_j^{Def}$) represents an average deformed grain size, whereas ($N^{-1} \sum D_k^{Rex}$) defines an average recrystallized grain size D_{DRX} . D_{ss} is obtained before deriving the equations for \bar{D} and D_{DRX} .

A grain boundary moves in response to a difference in the free energy between adjacent grains, allowing atoms to move towards a preferred configuration [1,12]. This behaviour is promoted by a net driving pressure $P = \sum_i P_i$ induced on the boundary, where P_i accounts for different acting pressures. The average velocity \bar{v} for moving boundaries can be expressed by the product of the driving pressure and its mobility $M > 0$ [13]: $\bar{v} = MP$. Steady state is achieved when grains stop growing and \bar{v} is null, which occurs when $P = 0$. The driving force for grains to grow during DRX accounts for the energy variations as the grain size evolves. Such is composed by the contributions of: (1) the pressure available for grains to grow, P_1 , this term being proportional to the stored energy in dislocations $\frac{1}{2} \mu b^2 \rho$ [1]; (2) capillary pressure effects $-P_2$, due to grain size variations $\frac{\chi_{GB}}{D}$ [13,14], where χ_{GB} is the grain boundary energy; and (3) solute and/or impurity drag pressure $-P_3$, preventing further growth [12]. ρ and \bar{D} account for regions containing both deformed and recrystallized grains; however, P should include effects from recrystallized grains only. A term multiplying $\frac{1}{2} \mu b^2 \rho$ in (1) is introduced to account for the regions on the freshly nucleated grains: $\beta_1 d_c^2 \exp\left(-\frac{Q_{nuc}}{k_B T}\right) / \bar{D}^2$, where $\beta_1 d_c^2 \exp\left(-\frac{Q_{nuc}}{k_B T}\right)$ represents the effective area consuming dislocations by new grains, and β_1 is a constant related to the number of effective nucleation sites around subgrain boundaries. Another term multiplies $\frac{\chi_{GB}}{D}$ in item (2) to account for the effective length where capillary effects can take place;

this equals the ratio between the grain boundary perimeter of recrystallized grains and the total grain boundary perimeter³: $\sum_{j=N_0+1}^N \pi D_k^{Rex} / \sum_{i=1}^N \pi D_i = D_{DRX} / \bar{D}$ (Eq. (4)). On the other hand, classical solute-drag models are based on the assumption that a moving boundary drags a solute atmosphere that exerts a retarding force on it [12]. This force is defined in terms of the boundary velocity and solute concentration. Although they provide good qualitative agreement with experimental observations, it has been shown that they are limited in making real quantitative predictions [1]. An alternative approach is proposed by estimating the probability that a moving boundary will drag a number of impurity/solute atoms randomly located on its surroundings. This probability depends on the distortion atmosphere and the binding energy between impurity atoms and grain boundaries. Boundary-solute interactions will exhaust a fraction of the pressure available for further growth ($P_3 = pP_1$). If it is assumed that the boundary-drag atmosphere is $\alpha_{sol} b$ meter per solute atom, where α_{sol} is a dimensionless constant related to the distortion field induced around solute atoms and to the solute-boundary binding energy, the probability p that during recrystallization all boundaries will drag x_{sol} solute atoms during the whole process, where x_{sol} is the solute atom fraction, corresponds to an exponential distribution [15]: $p = 1 - \exp(-\alpha_{sol} b / \Lambda_{sol}) = 1 - \exp(-\alpha_{sol} x_{sol}^{1/3})$, where $\Lambda_{sol} = b / x_{sol}^{1/3}$ is the average solute spacing [16]. Finally, the driving pressure for grain growth during DRX becomes ($P = P_1 - P_2 - P_3 = (1 - p)P_1 - P_2$):

$$P = \frac{1}{2} \mu b^2 \rho \left[\frac{\beta_1 d_c^2}{\bar{D}^2} \exp\left(-\frac{Q_{nuc}}{k_B T}\right) \right] \exp\left(-\alpha_{sol} x_{sol}^{1/3}\right) - \left(\frac{\chi_{GB}}{D} \right) \frac{D_{DRX}}{D}. \quad (5)$$

If additional solute elements are incorporated into the alloy, then $\alpha_{sol} x_{sol}^{1/3}$ is replaced by $\sum_s \alpha_s x_s^{1/3}$, to account for the total drag effect from different elements. An impurity-drag term $\alpha_{imp} x_{imp}^{1/3}$ is included in the previous summation. When steady state is achieved, Eq. (5) is null, and the average and recrystallized grain sizes are constant $\bar{D} = D_{DRX} = D_{ss}$ and equal to:

$$D_{ss} = 340 \frac{\kappa_c^2 \mu b^2}{2 \chi_{GB}} \exp\left(-\sum_s \alpha_s x_s^{1/3}\right) \exp\left(-\frac{Q_{nuc}}{k_B T}\right), \quad (6)$$

where $\beta_1 = 340$ was found for all (20) modelled materials. An important aspect of this equation is that the entropy term in Q_{nuc} is the principal contribution to the temperature and strain-rate variations in D_{ss} . The model results for D_{ss} are compared against experimental measurements obtained from the literature for various metallic systems. The deformation conditions and impurity concentrations for the modelled materials can be found in the [supplementary material](#); α_{imp} values are also shown for each alloy family.

Additionally, α_s values were obtained for Ni alloys and steels. A linear relationship was found between α_s

³The average grain size is estimated from two-dimensional micrographs, hence the analysis defined in two dimensions.

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