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MESOSCOPIC MODELING OF DISCONTINUOUS DYNAMIC RECRYSTALLIZATION: Steady-State Grain Size Distributions

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Abstract. A simple mesoscale model was developed for discontinuous dynamic recrystallization. The material is described on a grain scale as a set of N (variable) spherical grains. Each grain is characterized by two internal variables: its diameter and dislocation density (assumed homogeneous within the grain). Each grain is then considered in turn as an inclusion, embedded in a homogeneous equivalent matrix, the properties of which are obtained by averaging over all the grains. The model includes: (i) a grain boundary migration equation driving the evolution of grain size *via* the mobility of grain boundaries, which is coupled with (ii) a dislocation-density evolution equation, such as the Yoshie–Laasraoui–Jonas or Kocks–Mecking relationship, involving strain hardening and dynamic recovery, and (iii) an equation governing the total number of grains in the system due to the nucleation of new grains. The model can be used to predict transient and steady-state flow stresses, recrystallized fractions, and grain-size distributions. The effect of the distribution of grain-boundary mobilities has been investigated.

Introduction

During the thermomechanical processing of superalloys, dynamic recrystallization controls microstructure evolution and thus important aspects of the mechanical behavior in service. For instance, grain boundary migration plays an important role because it is one of the main phenomena controlling the final grain size. The present paper returns to a model of discontinuous dynamic recrystallization (DDR_X) presented at Thermec'2009 Berlin [1]. This mesoscale model was already validated in terms of mean values but grain size distributions looked rare and in this paper, the effect of the distribution of grain-boundary mobilities is described.

Description of Grain Properties

When deterministic evolution equations (*i.e.*, with no stochastic terms) are used, all grains of the same age have undergone identical evolution and therefore have the same diameter D and dislocation density ρ . Hence, all properties of the grains in the model are one-parameter distributions, and each grain is characterized by its age. The following functions can then be introduced:

- at time t , the number of present grains nucleated at the instant τ , $N(\tau, t)$ (number per volume unit);
- the plastic strain within the grain $\varepsilon(\tau, t) = \int_{\tau}^t \dot{\varepsilon}(u) du$, in which the strain rate $\dot{\varepsilon}$ is assumed to be the same for each grain (using the classical Taylor homogeneous strain crystal-plasticity assumption);
- the strain hardening of the grain as represented by its dislocation density $\rho(\tau, t)$ (length per volume unit);

– the grain diameter $D(\tau, t)$.

A number of constraints connect the various functions; *e.g.*, the overall volume is constant at all times, *i.e.*,

$$\forall t, \quad \frac{\pi}{6} \int_0^t N(\tau, t) D^3(\tau, t) d\tau = 1. \quad (1)$$

Evolution of Grain-Property Distributions

Several mechanisms contribute to the evolution of grain-property distributions:

(i) Grain boundary migration. A simple grain boundary migration law, based on differences in strain hardening between adjacent grains, or more specifically between a specific grain and the equivalent homogeneous matrix, is assumed, *i.e.*,

$$\left(\frac{\partial D}{\partial t}\right)_\tau(\tau, t) = 2MT[\bar{\rho}(t) - \rho(\tau, t)], \quad (2)$$

in which M is the grain boundary mobility and T is the line energy of the dislocations. Such a form and the introduction of the average dislocation density $\bar{\rho}$ are justified by using an average over the matrix surrounding the grain.

Because plastic deformation occurs without volume change, $\bar{\rho}$ must be a surface weighted average,

$$\bar{\rho}(t) = \int_0^t \rho(\tau, t) N(\tau, t) D^2(\tau, t) d\tau / \int_0^t N(\tau, t) D^2(\tau, t) d\tau. \quad (3)$$

As a consequence of grain size evolution, “old” grains (which have large dislocation densities) decrease in diameter and eventually disappear. They are replaced by new ones as described in section (iii) below.

(ii) Strain hardening. Strain hardening and dynamic recovery are assumed to be described for each grain by the same equation, $d\rho/d\varepsilon = H(\rho)$, in which $H(\rho)$ can depend on temperature as well as on strain rate (in the same way for each grain).

Several forms of strain hardening and dynamic recovery law can be used, *e.g.*, the Yoshie–Laasraoui–Jonas law, $H(\rho) = h - r\rho$; the Kocks–Mecking law, $H(\rho) = h - r\sqrt{\rho}$; the power law, $H(\rho) = H^{v+1}/\rho^v$. In each case, the various parameters are temperature and strain-rate dependent.

A variant exists which takes into account the additional softening due to grain boundary migration; but this law is then no longer a local one because it also depends, *via* the grain boundary migration velocity, on the *average* dislocation density [2–4].

(iii) Nucleation of new grains. The nucleation of new grains ($t = \tau$) is postulated to be proportional to the grain boundary surface $S(t)$ and is of the form $(\partial N/\partial t)_\tau(\tau = t, t) = f[\bar{\rho}(t)]S(t)$, where t is the current time and S is the grain surface area per unit volume; in practice, the latter function is specified as $f(\bar{\rho}) = k_N \bar{\rho}^p$. The exponent of the Derby relationship between grain size and stress is related to the exponent p ; the unique integer value for p compatible with experimental Derby exponent is 3 [4]. In the present work $p = 3$ is assumed, although p could be fitted for specific sets of data.

Using the above equations, the change with time of the grain-size and other distributions are determined as shown schematically in Fig. 1.

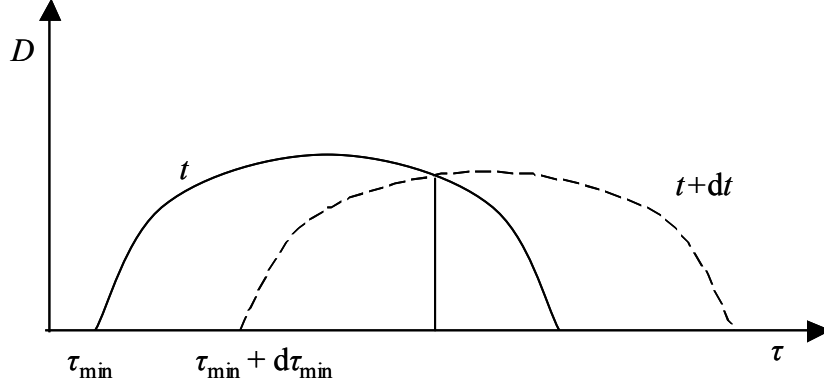


Figure 1. Schematic evolution of the grain size distribution in the DDRX model

The flow stress σ associated with this grain-size distribution is assumed to be given by $\sigma = \alpha\mu b\sqrt{\bar{\rho}}$.

Steady-State Behavior

When the material is strained at a constant strain rate and temperature, a steady state is obtained after some time (or strain) during which new grains continuously replace old ones.

The distribution $N(\tau, t)$ is then $N(t - \tau)$ (*i.e.* steady state) and the diameter distribution is a function of the average dislocation density according to a specific equation (which depends only on $\bar{\rho}$, the dependence on $\dot{\varepsilon}$ and temperature being implicitly included in $\bar{\rho}$). Under such a steady-state condition, Eq. 2 can be integrated to give:

$$D(\varepsilon, \bar{\rho}) = 2MT \left[\bar{\rho}\varepsilon - F(\varepsilon, \bar{\rho}) \right] / \dot{\varepsilon}, \quad (4)$$

in which $F(\varepsilon)$ is the strain hardening and dynamic recovery potential, defined by $\rho(\varepsilon) = (\partial F(\varepsilon, \bar{\rho}) / \partial \varepsilon)_{\bar{\rho}}$.

The determination of model parameters from rheological experiments and grain size measurements was deeply analyzed in [1]. It is worth to note that grain-boundary mobility and nucleation parameter are expressed as closed forms from the steady-state stress and the average of the steady-state grain size [4].

Steady-State Grain Size Distribution

The steady-state distribution of grain size $g(D)$ associated with such a one-parameter distribution can be obtained from $g(D) = \left[(dD/dt)_+^{-1} - (dD/dt)_-^{-1} \right] / t_{\text{end}}$, in which t_{end} is the lifetime of the grains and the indices + or - are associated with growing and decreasing grains, respectively. The above distribution patently tends to infinity when $D \rightarrow D_{\text{max}}^-$ in which D_{max} is the maximal grain diameter ($D = D_{\text{max}}$ trivially implies $dD/dt = 0$) when the grain is in the middle of its life (in fact when $\rho = \bar{\rho}$). More precisely, $g(D)$ is simply derived as in [5] with some additional assumptions:

$$g(D) = \frac{1}{2\sqrt{D_{\text{max}}(D_{\text{max}} - D)}}. \quad (5)$$

This analytical distribution is presented in Fig. 2a with its histogram counterpart from the numerical implementation, very close to the analytical result, confirming the coherency between both analytical and numerical methods despite the unusual obtained shape of the distribution.

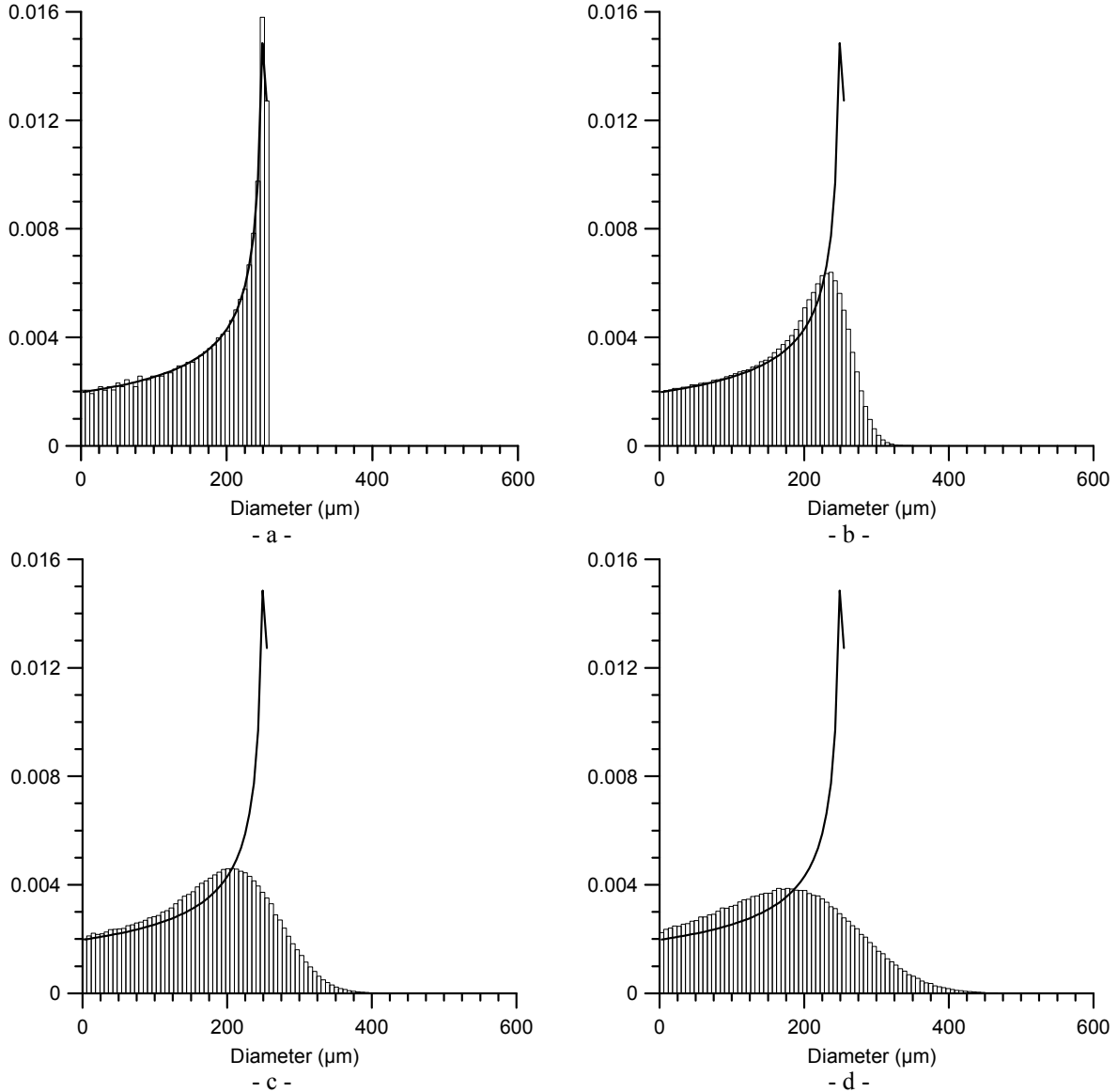


Figure 2. Grain-size histograms (6 μm -width class) in the DDRX model for pure nickel at 900 $^{\circ}\text{C}$ strained at 0.1 s^{-1} – M coefficient of variation: **0 (a), 10 % (b), 20 % (c), 30 % (d)** – Continuous line is the analytical solution for fixed M value as in the (a) case, final drop is due to the partial last class (252–258 μm , maximal diameter about 255.5 μm)

If any model parameter (impacting the maximal grain diameter) is now distributed, the grain-size distribution is altered by convolution with the newly induced D_{max} distribution (principally among other interactions). In [5], the effect of the distribution of the strain hardening parameter (related to Taylor factor) was studied. The present paper focuses on the effect of an M -distribution introduction. As this mean-field model does not account for any topological features, it can be useful to artificially integrate them using such M -distribution because grain boundary velocities are clearly affected by local surroundings and not only mean fields.

So, at nucleation of each grain, a certain mobility M is now affected to the new grain following a Gaussian distribution centered on the previous average value. Figure 2 compares 4 coefficients of variation (spread is thus characterized by the *ratio* standard deviation over mean): 0, 10 %, 20 %, and 30 %. In such a way, grain-size distributions are clearly smoothers and look more like grain-size measurements with a few larger grains.

Before validating this encouraging result, it is necessary to check the weak influence of the M -distribution on average (over grains) outputs of the model such as flow stress (see Fig. 3a), mean grain size or recrystallized fraction (see Fig. 3b).

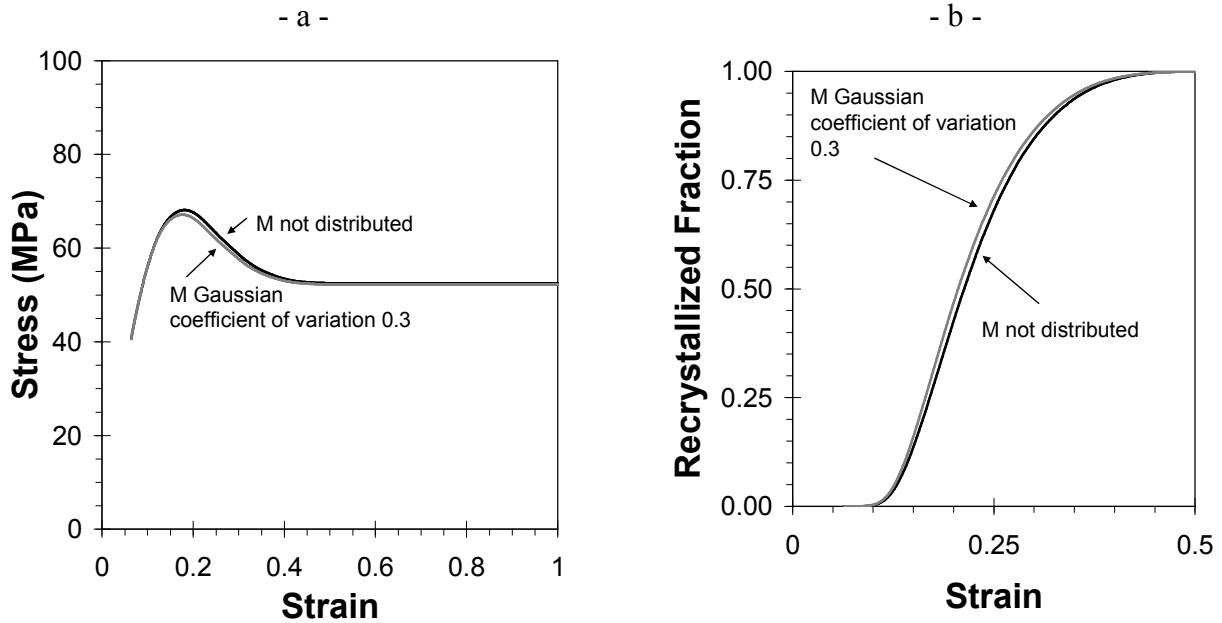


Figure 3. Comparisons between not distributed and Gaussian distributed grain-boundary mobility in terms of flow stress (a) and recrystallized fraction (b)

It can be concluded that, as expected, the effect of introducing an M -distribution leads to variations, with respect to mean field values, that can be neglected.

Usually grain size distributions are characterized by microscopy on a plane leading to a distorted distribution (less probability to see small grains and smaller appearing grains). In order to simulate these effects, the distribution of the apparent equivalent diameter on a 2D metallographic plane was computed from the 3D real diameter distribution located in Fig. 2d (M coefficient of variation: 0.30) and it is shown in Fig. 4. Let be $\mu_r(i)$ and $\mu_a(i)$ the number of grains in the class I , *respectively*, of the real 3D diameter (per volume unit) and the apparent 2D equivalent diameter (per area unit). The apparent diameter histogram is built using the relationship:

$$\mu_a(i) = \sum_{j=i}^k \mu_r(j) \Delta \left[\sqrt{j^2 - (i-1)^2} - \sqrt{j^2 - i^2} \right], \quad (6)$$

in which Δ is the class width. The apparent diameter histogram clearly looks like typical metallographic characterizations.

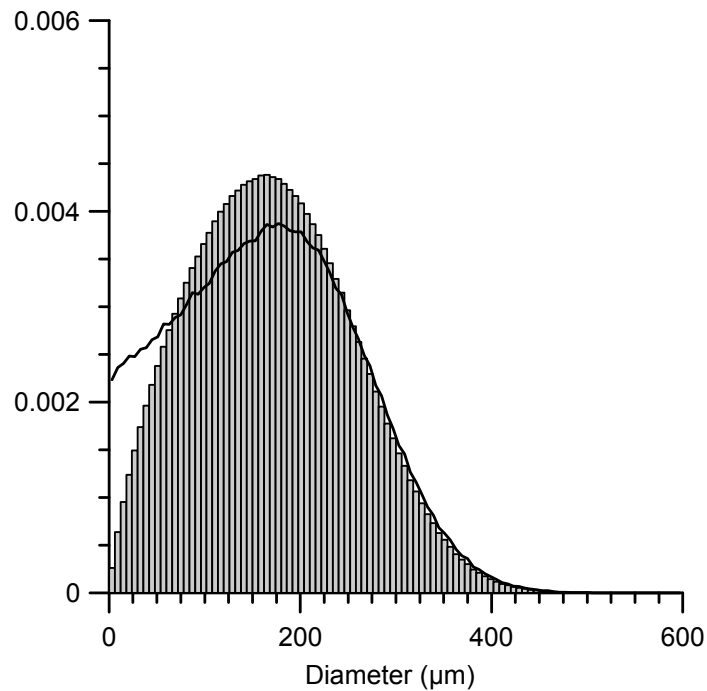


Figure 4. Histogram of apparent equivalent diameter (metallographic) obtained from the 3D real diameter of grain-size distribution in continuous line (M -coefficient of variation 0.3)

Closing Remarks

The mean field model of DDRX is a powerful tool to predict the material behavior during dynamic recrystallization, particularly the steady state behavior in terms of averages over the grains (flow stresses, mean size, recrystallized fraction,...). For distributed properties, such as grain-size distribution, the model fails with fixed parameters but it can be successful if some model parameters (*e.g.* grain boundary mobility) are also reasonably distributed in comparison to neighborhood effects in the aggregate.

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