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A MODEL OF DISCONTIUOUS DYNAMIC RECRYSTALLIZATION AND ITS APPLICATION FOR NICKEL ALLOYS (PREPRINT)

S. Lee Semiatin, Gilles Damamme, David Piot, and Frank Montheillet

Metals Branch
Metals, Ceramics and NDE Division

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S.L. Semiatin (AFRL/RXLMP)
Gilles Damamme (CEA-DAM)
David Piot and Frank Montheillet (École nationale supérieure des mines de Saint-Étienne)

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Air Force Materiel Command, United States Air Force

CEA-DAM, Centre Île de France, BP 12, F-91680 BRUYERES LE CHATEL CEDEX, FRANCE

École supérieure des mines de Saint-Étienne, Centre SMS; CNRS UMR 5146 158 cours Fauriel, F-42023 ST ETIENNE CEDEX 2, FRANCE

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14. ABSTRACT
A simple mesoscale model was developed for discontinuous dynamic recrystallization. The material is described on a grain scale as a set of(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 nuclea-tion of new grains. The model can be used to predict transient and steady-state flow stresses, recrystallized fractions, and grain-size distributions. A method to fit the model coefficients is also described. The application of the model to pure Ni is presented.

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dynamic recrystallization, grain boundary mobility, modeling, aerospace applications, superalloys, nickel–niobium alloys (Ni–Nb)

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A Model of Discontinuous Dynamic Recrystallization and Its Application for Nickel Alloys

Gilles Damamme[1,a], David Piot[2,b], Frank Montheillet[2,c], S. Lee Semiatin[3,d]

[1]CEA-DAM, Centre Île de France, BP 12, F–91680 BRUYERES LE CHATEL CEDEX, FRANCE

[2]École nationale supérieure des mines de Saint-Étienne, Centre SMS; CNRS UMR 5146
158 cours Fauriel, F–42023 ST ETIENNE CEDEX 2, FRANCE

[3]Air Force Research Laboratory, AFRL/RX, Wright-Patterson Air Force Base, OH 45433-7817, USA

[a]Gilles.DAMAMME@CEA.fr, [b]PIOT@EMSE.fr, [c]MONTHEIL@EMSE.fr,
[d]Lee.SEMIATIN@WPAFB.AF.mil

Keywords: dynamic recrystallization, grain boundary mobility, modeling, aerospace applications, superalloys, nickel–niobium alloys (Ni–Nb)**.**

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. A method to fit the model coefficients is also described. The application of the model to pure Ni is presented.

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 introduces a model of discontinuous dynamic recrystallization (DDRX) which describes microstructure evolution for a distribution of isotropic, spherical grains of various diameters, each with a dislocation density ρ which is the same for all grains of identical diameter [1,2]. Topological features treated elsewhere [1] are not considered here in order to simplify the approach.

Description of Grain Properties

When deterministic evolution equations (*i.e.*, with no stochastic terms) are used, all grains of a given age τ 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 τ. The following functions can then be introduced:

– the number of grains of age τ, $N(\tau,t)$ (number per unit volume and age time);

– the plastic strain within the grain $\varepsilon(\tau,t)=\int_{t-\tau}^{t}\dot{\varepsilon}(u)\,\mathrm{d}u$, in which the strain rate $\dot{\varepsilon}$ is assumed to be the same for each grain (per the classical Taylor isostrain crystal-plasticity assumption);

– the strain hardening of the grain as represented by its dislocation density $\rho(\tau,t)$ (length per unit volume);

– 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.*,

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

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.*,

$$\left(\partial D/\partial t\right)_\tau(\tau,t) = 2M\mathcal{T}\left[\bar{\rho}(t) - \rho(\tau,t)\right], \tag{2}$$

in which M is the grain boundary mobility and $\mathcal{T}$ 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,

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

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, $\mathrm{d}\rho/\mathrm{d}\varepsilon = \mathcal{H}(\rho)$, in which $\mathcal{H}(\rho)$ 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, $\mathcal{H}(\rho) = h - r\rho$; the Kocks–Mecking law, $\mathcal{H}(\rho) = h - r\sqrt{\rho}$; the power law, $\mathcal{H}(\rho) = H^{\nu+1}/\rho^{\nu}$. 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 [1-3].

(iii) Nucleation of new grains. The nucleation of new grains (age $\tau = 0$) is postulated to be proportional to the grain boundary surface $S(t)$ and is of the form $\left(\partial N/\partial t\right)_\tau(0,t) = f(\bar{\rho})S(t)$, where t is the current time and S is the grain surface area per unit volume; in practice, this latter function is specified as $f(\bar{\rho}) = k_{\mathrm{N}}\bar{\rho}^{p}$. 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 [3]. 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.

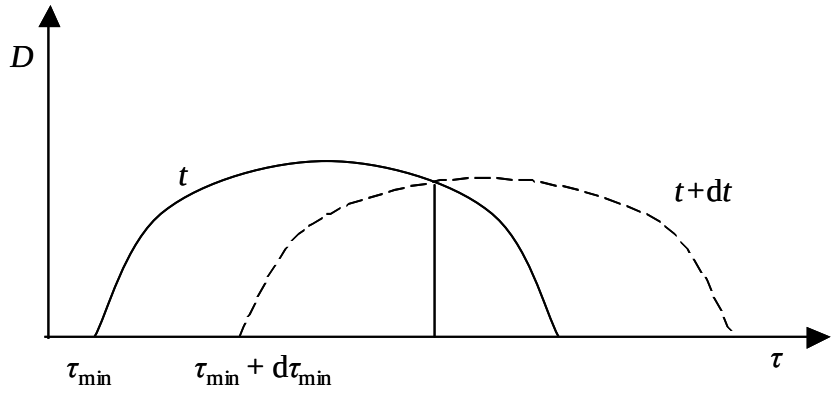

Figure 1. Schematic evolution of the grain size distribution in the DDRX model

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 constant (*i.e.*, independent of t), 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:

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

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

The steady-state distribution of grain size $g(D)$ associated with such a one-parameter distribution can be obtained from $g(D) = \left[\left(dD/dt\right)_{+}^{-1} - \left(dD/dt\right)_{-}^{-1}\right]/\tau_{\text{end}}$, in which τ_{end} is the lifetime of the grains and the indices + or – are associated with growing and decreasing grains, respectively. The above distribution necessarily tends to infinity when $D \to D_{\max}^{-}$. More precisely, a $g(D)$ equivalent is then proportional to $1/\sqrt{D_{\max} - D}$. Nevertheless, all average values that can be deduced from Eq. 4 (*e.g.*, the average grain size) do not necessarily have the same problem in their calculation. Moreover, such a behavior can be avoided by considering that the maximum diameter is likely to be not precisely defined due to variability in the material, *e.g.* variations in the hardening parameter h because of its dependence on crystallographic orientation.

Determination of the Model Parameters

For given strain rate and temperature, the model parameters are determined from stress–strain curves measured during mechanical tests, such as hot torsion tests, conducted at constant strain rate and temperature. After a pseudo-elastic initial domain, the initial grains strain harden before the influence of the newly generated grains becomes noticeable. For ε_{e}, $\sigma_{\text{e}} = \alpha\mu b\sqrt{\rho_0}$ where ρ_0 is the

initial value of ρ. The first part of the stress–strain curve can thus be used to fit the parameters involved in the definition of the strain hardening and recovery function $H(\rho)$; see (ii) and Fig. 2 for an example.

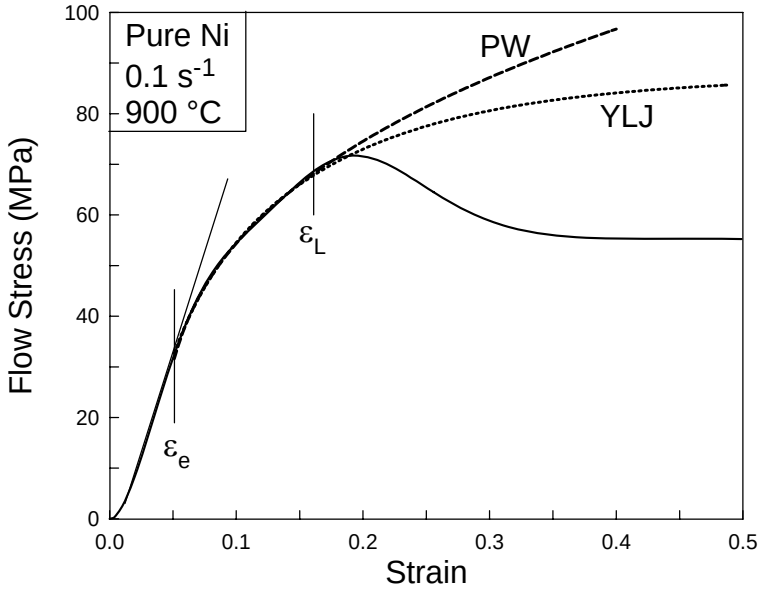

Figure 2. True stress–strain curve for pure nickel determined *via* torsion testing at 900 °C and 0.1 s^{-1} and model fits for the Yoshie–Laasraoui–Jonas (YLJ) and power-law (PW) equations using flow-stress data between ε_e and ε_L

In the second step of the fitting procedure, the nucleation parameter k_N and the grain boundary mobility M can be *analytically* derived from the steady state stress σ_s and the measured average steady-state grain size D_s using the power law for $H(\rho)$ [3], *i.e.*,

$$MT = (2\nu+3)(\nu+1)^{\nu+2}(\nu+2)^{-\nu-1}H^{\nu+1}\dot{\varepsilon}D_s(\alpha\mu b/\sigma_s)^{2(\nu+2)}, \tag{5}$$

$$k_N = \left(\left[3(3\nu+4)(3\nu+5)(\nu+1)^{\nu+2}H^{\nu+1}\dot{\varepsilon}\right]\Big/\left[8(2\nu+3)^2(\nu+2)^{\nu+1}D_s^2\right]\right)(\alpha\mu b/\sigma_s)^{2(p+\nu+1)}. \tag{6}$$

In the case of other formulations for $H(\rho)$, these values can still be used for M and k_N as rough estimates or initial guesses for performing inverse-method parameter identification.

Figures 3-5 present model predictions of the evolution (with strain) of flow stress, average grain size, and recrystallized fraction for the hot deformation of high-purity nickel. For the power-law (PW) and YLJ curves, the values of M and k_N were derived from Eqs 5 and 6 while they were optimized for the "best-fit" prediction. The fitted curves show reasonable agreement with the available data for pure nickel. Furthermore, the value of the exponent p in the nucleation equation can be tuned in the neighborhood of $p = 3$ to improve the agreement.

The model can also be used for more detailed predictions such as the grain size distribution, as illustrated in Fig. 6. As mentioned previously, the exact shape of this distribution can vary due to variations in the material parameters; the inclusion of local neighborhood effects (which would require a more complex model formulation) may also lead to different forms of the grain-size distribution that show more of resemblance to experimental observations.

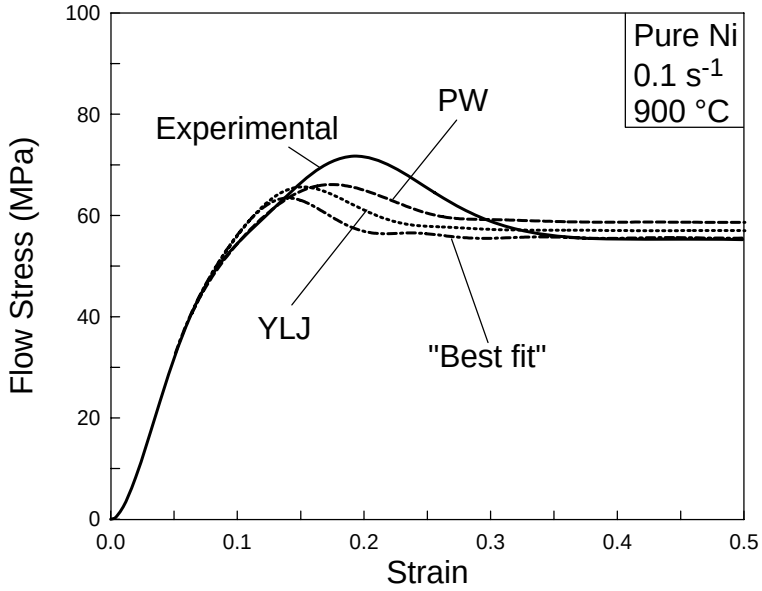

Figure 3. Comparison of predicted and measured flow stress of Ni deformed at 900 °C, 0.1 s^{-1}

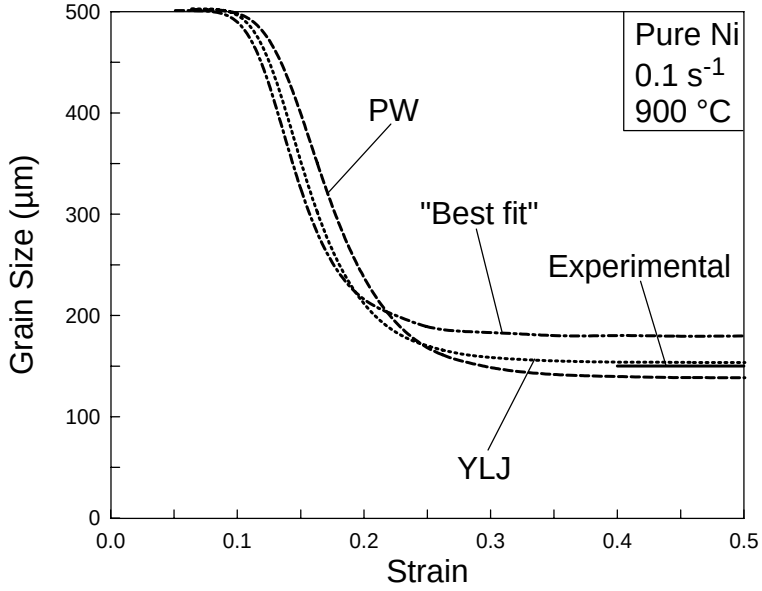

Figure 4. Predicted vs measured average (volume weighted) grain size of Ni (900°C, 0.1 s^{-1})

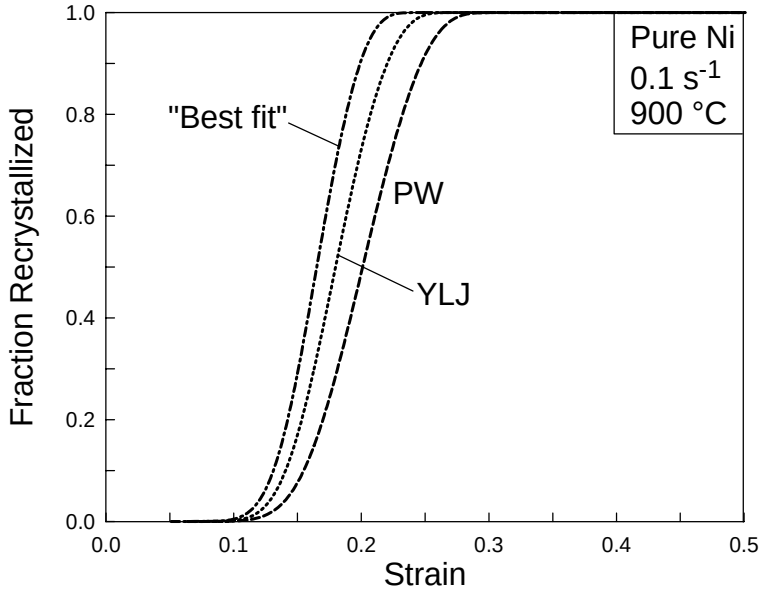

Figure 5. Predicted recrystallized fraction for pure nickel deformed at 900 °C and 0.1 s^{-1}

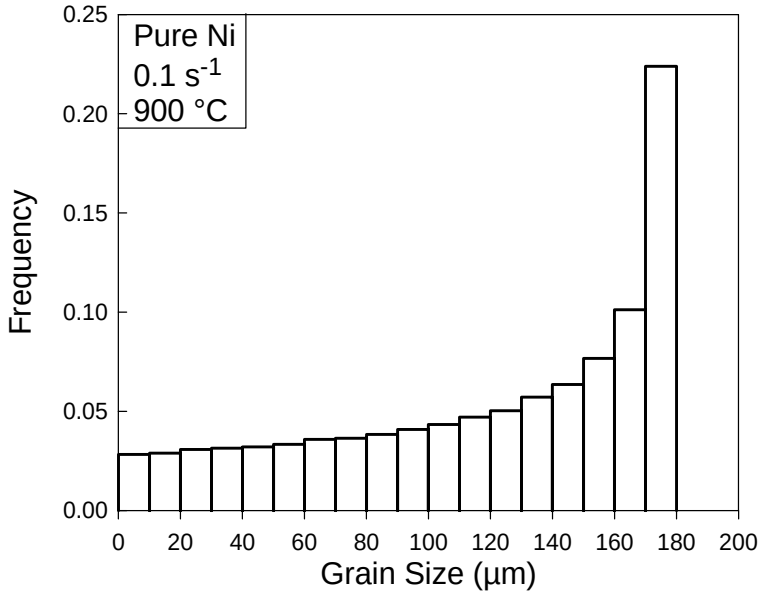

Figure 6. Predicted (YLJ equation) steady-state grain-size distribution for pure nickel deformed at 900 °C and 0.1 s^{-1}

Closing Remarks

The DDRX model can also be used for predicting the behavior of alloys during hot working. When sufficient data are available, it can be used in the same way as above for pure nickel. In the case of solid solution nickel–niobium alloys, for example, analytical descriptions of the strain hardening and dynamic recovery parameters have been established [4]. The grain boundary mobility and possibly the nucleation parameter are affected by solutes and second phase particles. The former effect has been addressed in a companion paper in this proceedings volume [5].

References

[1] J.P. Thomas, F. Montheillet and S.L. Semiatin: Metall. Mater. Trans. Vol. 38A (2007), p. 2095

[2] F. Montheillet, O. Lurdos and G. Damamme: Acta Mater. Vol. 57 (2009), p. 1602

[3] F. Montheillet and J.J. Jonas: Models of Recrystallization, *in* ASM Handbook, vol. 22, in press.

[4] D. Piot, F. Montheillet, S.L. Semiatin: *Rheological Behavior of Pure Binary Ni–Nb alloys*, in the present proceedings.

[5] F. Montheillet, G. Damamme, D. Piot, S.L. Semiatin: *Modeling Grain Boundary Mobility during Dynamic Recrystallization of Metal Alloys*, in the present proceedings.

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