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A model for strain hardening, recovery, recrystallization and grain growth with applications to forming processes of nickel base alloys

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ABSTRACT

An ensemble of *n* spherical grains is considered, each of which is characterized by its radius r_i and by a hardening variable a_i . The hardening variable obeys a Chaboche-type evolution equation with dynamic and static recovery. The grain growth law includes the usual contribution of the grain boundary energy, a term for the stored energy associated with the hardening variable, and the Zener pinning force exerted by particles on the migrating grain boundaries. New grains develop by recrystallization in grains whose stored energy density exceeds a critical value. The growth or shrinkage of the particles, which restrain grain boundary migration, obeys a thermodynamic/kinetic evolution equation. This set of first order differential equations for r_i , a_i and the particle radius is integrated numerically. Fictitious model parameters for a virtual nickel base alloy are used to demonstrate the properties and capabilities of the model. For a real nickel alloy, model parameters are adjusted using measured stress-strain curves, as well as recrystallized volume fractions and grain size distributions. Finally the model with adjusted parameters is applied to a forming process with complex temperature-strain rate histories.

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1. Introduction

If a metal is deformed at high temperature, the energy stored in the form of dislocation structures can be released by recovery processes, i.e. rearrangement and annihilation of dislocations, and/ or by recrystallization, i.e. the nucleation and growth of more or less defect-free new grains. A quantitative understanding of the mechanisms is helpful to achieve a desired microstructure (usually a small grain size with a mono-modal size distribution) in technological forming processes.

Doherty et al. [\[1\]](#page--1-0) summarize the knowledge of the 1990s on the material science of recrystallization in an exhaustive review. Classical papers describe the kinetics of recrystallization by equations relating recrystallized volume fraction to time or strain (Kolmogorov $[2]$, Johnson and Mehl $[3]$, Avrami $[4]$, Sellars $[5]$, Humphreys [\[6\]\)](#page--1-0). Sommitsch et al. [\[7\]](#page--1-0) apply this approach to study recrystallization and grain growth in a new nickel base alloy Allvac 718Plus under typical hot forming conditions. Also Lü et al. [\[8\]](#page--1-0) evaluate their experimental results on the annealing of a coldrolled Fe–Mn–C alloy in terms of the Kolmogorov–Johnson–Mehl– Avrami model. Lin et al. [\[9\]](#page--1-0) present a finite element study of the

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<http://dx.doi.org/10.1016/j.msea.2016.04.015> 0921-5093/© 2016 Elsevier B.V. All rights reserved. stress/strain distribution and the microstructural evolution in 42CrMo steel during a hot upsetting process using the Avrami equation.

In a review article, Hallberg $[10]$ summarizes the progress in modelling techniques beyond the classical approaches. Recently the cellular automata method has become popular [\[11,12\]](#page--1-0). In conjunction with a crystal plasticity model it provides not only detailed information on grain sizes, but also on crystallographic texture [\[12\]](#page--1-0). Schäfer et al. [\[13\]](#page--1-0) use cellular automata for the simulation of recrystallization and recovery in an Al–Fe–Si alloy during annealing after cold rolling and compare the results with experiments.

The present paper pursues a similar approach as Montheillet et al. [\[14\]](#page--1-0) and Bernard et al. [\[15\]](#page--1-0). There are, however, significant differences, some of which are explained in connection with the description of the model below. In [\[14,15\]](#page--1-0), as well as in the present paper, a set of n spherical grains is considered, each of which is characterized by two state variables, viz. the grain radius r_i and the hardening variable a_i . In the spirit of mean field theory each grain grows in competition with an average of all other grains, rather than with its actual neighborhood. The formation of new grains by recrystallization is described by a phenomenological rate equation.

Precipitates play an important role, since they can pin grain boundaries thus retarding grain growth. Hence the precipitation and dissolution of particles is also included in the present model. Compared to the classical models, which are based on explicit

γ

dependencies of the recrystallized volume fraction on time (or strain), the present model, which is based on evolution equations for the state variables, is more flexible in describing complex loading and temperature histories; and it provides grain size distribution functions. Other than the present model, cellular automata take the individual neighborhood of grains into account, but they are computationally much more demanding.

2. The model equations

2.1. Evolution of the hardening variable

The hardening variable a_i is taken from the Chaboche model, which is used here in a slightly modified form involving the hyperbolic sine function

$$
\dot{\varepsilon} = \dot{\varepsilon}_1 \sinh[(\left(\sigma_i - a_i - \sigma_{M,i}\right)/K)^m].\tag{1}
$$

The plastic strain rate, *ε*, is assumed to be the same in all grains ̇ (Taylor assumption), σ_i is the stress in grain *i*, $\dot{\varepsilon}_1$, *K* and *m* are model parameters; $\sigma_{M,i}$ is the temperature-dependent yield stress at zero strain; it includes precipitation hardening by the Orowan mechanism (the second term in Eq. 2 below) and the Hall–Petch effect (the third term):

$$
\sigma_{M,i} = (\sigma_y + \alpha_{0r}Gb\sqrt{P\rho} + k_y/\sqrt{2r_i})(1 - \tanh\frac{T - \tau_1}{\tau_2})/2.
$$
\n(2)

The Orowan stress contains the shear modulus G, the Burgers vector b, the number density of precipitates P and the precipitate radius $ρ$, which evolves according to [Eq. \(8\)](#page--1-0). The dimensionless factor α_{0r} is expected to lie in the range 1–3; however, it is set equal to zero in the examples shown below; k_y is the constant of the Hall–Petch relation; σ_{γ} , τ_1 und τ_2 are parameters. The hyperbolic-tangent describing the temperature dependence is purely empirical.

The hardening variable obeys the evolution equation

$$
\dot{a}_i = h\dot{\varepsilon} - R_{dyn}a_i\dot{\varepsilon} - R_{stat}a_i^3/(1 + \beta a_i^2) + (a_i/h)\partial h/\partial T\dot{\mathbf{I}}.
$$
\n(3)

Here *h* is the initial hardening rate, R_{dyn} and R_{stat} are model parameters for dynamic and static recovery, respectively, and the last term guarantees thermodynamic consistency under variable temperature conditions. The usual form of the static recovery term is recovered for large $β$. Montheillet et al. [\[14\]](#page--1-0) and Bernard et al. [\[15\]](#page--1-0) use "dislocation density" instead of the hardening variable and omit the last two terms in Eq. (3).

2.2. Macroscopic stress

The macroscopic stress is calculated as the volume average of the stresses in the grains, $\sigma = \sum \sigma_i r_i^3 / \sum r_i^3$, where σ_i is obtained from Eq. (1).

2.3. Stored energy

In the grain growth and recrystallization model described below, the hardening variable serves to calculate the stored energy density in a grain, $a_i^2/(2h)$ according to $[16]$. The stored energy drives recrystallization and favors the growth of grains with low stored energy.

2.4. Evolution of the grain size

The grain radius obeys the evolution equation

 $\dot{r}_i = MF_i$ (4)

with the temperature dependent grain boundary mobility M and the driving force F_i . The driving force contains contributions from the specific grain boundary energy, *γ*, from the stored energy density, $a_i^2/(2h)$, and from the Zener pinning force exerted by precipitate particles, F_{pin} (Eq. 7 below)

$$
F_i = \frac{-\gamma/r_i - a_i^2/(2h)}{1 + \theta r_i^2} + \lambda \mp F_{pin}
$$

if $abs(\frac{-\gamma/r_i - a_i^2/(2h)}{1 + \theta r_i^2} + \lambda) > F_{pin}$ (5a)

$$
F_i = 0 \text{ if } abs(\frac{-\gamma/r_i - a_i^2/(2h)}{1 + \theta r_i^2} + \lambda) \le F_{pin}
$$
 (5b)

The sign in Eq. $(5a)$ is chosen such that the pinning force reduces the amount of the driving force. The Lagrange multiplier *λ* ensures the conservation of volume expressed by $\sum_{i=1}^{n} r_i^2 \dot{r}_i = 0$. This leads to a nonlinear equation for λ , which can be solved numerically by the *regula falsi* method. For $F_{\text{min}}=0$ the equation for λ becomes linear and can readily be solved analytically. The term $1/(1+\theta r_i^2)$ in Eqs. (5a) and (5b) is introduced to capture the fact that grain coarsening seems to be retarded considerably at large grain sizes in the nickel base alloys considered below. For $\theta = 0$ and $a_i = 0$, the usual form of the grain growth law as proposed by Hillert [\[17\]](#page--1-0) is recovered.

Montheillet et al. [\[14\]](#page--1-0) neglect the term −*γ*/*ri* in Eqs. (5a) and $(5b)$, so that ordinary grain coarsening cannot be modelled. Bernard et al. [\[15\]](#page--1-0) mention the pinning force, but do not provide equations for its evolution. An advantage of the model in [\[15\]](#page--1-0) is that it is a two-site model, allowing a distinction between the effective neighborhoods of recrystallized and non-recrystallized grains.

2.5. Recrystallization

The recrystallization process is described phenomenologically by an equation for the rate at which recrystallized volume develops in grain *i*

$$
\dot{V}_{RX,i} = Br_i^2(a_i^2 - a_{crit}^2)/(2h) \quad \text{if } a_i \ge a_{crit}. \tag{6}
$$

According to Eq. (6) only grains with a sufficiently high stored energy, *i.e.* with $a_i \ge a_{\text{crit}}$, can recrystallize; for $a_i < a_{\text{crit}}$ is $\dot{V}_{RX,i} = 0$; *B* is a temperature dependent kinetic parameter. The factor r_i^2 is motivated by the idea that the number of nucleation sites scales with the grain surface, since recrystallization occurs mainly at grain boundaries. For nucleation in the bulk, r_i^3 should be used.

Montheillet et al. [\[14\]](#page--1-0) and Bernard et al. [\[15\]](#page--1-0) use different phenomenological expressions for the recrystallization rate. In [\[14\]](#page--1-0) the recrystallized volume in a time step depends on the dislocation density averaged over all grains. However, it appears to be more plausible to assume that grains with a high stored energy can recrystallize independently of the state of the other grains, as it is assumed in the present paper.

2.6. Pinning force

Assuming a statistical distribution of spherical particles with radius ρ and number density P the pinning force is (see e.g. [\[11\]](#page--1-0))

$$
F_{\rm pin} = 2\pi\alpha\rho^2\gamma P,\tag{7}
$$

where α is used as an adjustable parameter to account for the fact that particles are often located preferentially on grain boundaries rather than being homogeneously distributed in the grains.

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