A DISLOCATION DENSITY MODEL FOR THE SIMULATION OF HOT FORMING PROCESSES

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Abstract

An advanced process model for the calculation of the microstructural evolution of nickel base alloys during a hot forming process helps to optimise the forming process and to achieve the desired microstructure. The simulation of the grain structure development during and after the forming process is based on a dislocation density model that is embedded in the FEM-program DEFORM™.

Keywords: Hot forming, Nickel-base Superalloys, Microstructure, Simulation, Recrystallisation, Modelling

Introduction

Integrated modelling and simulation describes the coupling of computer codes with the aim to bridge the scale gaps among different simulation levels. Microstructure simulations typically address three salient points [1]: first, they aim at improving our insight into the underlying physical principles that govern the nature of microstructure evolution at the various scales. This task falls into the domain of elaborating physically plausible structural evolution laws. Second, they provide quantitative microstructure-property relations. This point can be regarded as a contribution to identifying appropriate microstructural equations of state. Third, they allow us to investigate both of the aforementioned aspects at levels that are not amenable to experimentation or under conditions that have not yet been studied. The latter aspect is particularly important for introducing simulations in industry.

Depending of the scale of modelling there are a great variety of modelling approaches in the field of materials science. Monte Carlo Simulations and Molecular Dynamics belong to the so called nanoscopic-microscopic scale simulation techniques that predict the microstructure from the atomic level to lattice defects ensembles below the grain scale. At the microscopic-mesoscopic scale Cellular Automata, Phase Field Kinetic Models, Vertex Models and Discrete Dislocation Statics and Dynamics are important representatives to describe lattice defect ensembles at the grain scale. Finally, Finite Element and Difference Methods and Polycrystal Elasticity and Plasticity Models represents the modelling approach at the mesoscopic-macroscopic scale.

The presented model [2,3] belongs to the latter type and can be classified as an advanced microstructure finite element model (microstructure mechanics). It simulates the grain structure development during and after hot deformation of nickel-base alloys. It considers normal grain growth and dynamic, meta-dynamic and static recrystallisation and can be used for alloys with low stacking fault energies and thus recrystallisation as the predominant softening mechanism.

For the model validation a comprehensive experimental program on a Gleeble 3800 testing system has been conducted [3,4]. A rolling step within the multi-line rolling mill of Boehler Edelstahl company was modelled for the Alloy 80A as an example of advanced microstructure integrated modelling at industrial scale.

Criteria for Recrystallisation

During hot forming, the derivative of the dislocation density can be described [5] by the equation

$$\frac{d\rho}{dt} = \frac{\dot{\varepsilon}}{bl} - 2M\,\tau\,\rho^2 \qquad (1),$$

taking the strain hardening and the recovery of dislocations into account, where $\dot{\varepsilon}$ is the strain rate, b the Burgers vector, l the mean free path of the dislocations, M the mobility of recovery and τ the average energy per unit length of a dislocation.
A critical dislocation density is necessary in order to initiate dynamic recrystallisation. The nucleus usually forms at pre-existing grain boundaries in the material, at least at higher strain rates [6]. For an area that has just been recrystallised it is assumed that the dislocation density ρ_0 generated by the preceding strain is reduced to a very low value.
Roberts and Ahlblom [7] developed a nucleation criterion, which is based upon the idea that during dynamic recrystallisation, the concurrent deformation reduces the stored energy difference (driving force) that effects migration of a high angle boundary. The driving force in the regions into which the reaction is proceeding must be higher for dynamic than for static recrystallisation if the boundary is to migrate at the same velocity. The nucleation theory gives the net free energy change [7]

$$\Delta G(r) = -\frac{4}{3}\pi r^3 \frac{\tau}{r}\int_0^r \left[\rho_0 - \rho(x)\right]dx + 4\pi r^2 \gamma_{GB} \qquad (2),$$

where γ_{GB} is the grain boundary energy per unit area, $\rho(x)$ the increasing dislocation density behind the boundary and r the radius of a spherical nucleus.
Maximising the net free energy change produces the critical nucleation conditions:

$$r_{cr}\tau\left[\frac{\rho_s}{3}\tanh\left(2\frac{M}{m}\frac{\rho_s}{\rho_0}r_{cr}\right) - \rho_0\right] + \left(\frac{\tau\,\rho_0 m}{3M}\right)\ln\left[\cosh\left(2\frac{M}{m}\frac{\rho_s}{\rho_0}r_{cr}\right)\right] + 2\gamma_{GB} = 0 \qquad (3),$$

where m denotes the mobility of a moving high angle boundary and ρ_s the stationary dislocation density [7]. No real critical radius r_{cr} exists unless ρ_0 exceeds a critical value ρ_{cr}. Substituting ρ in equation (1) with ρ_{cr} will give the critical time t_{cr} for a given strain rate.
In the case of static recrystallisation ($\dot{\varepsilon} = 0$), the dislocation density behind the boundary is zero, thus the dislocation energy is $\tau{\cdot}\rho_0$. Differentiation of the modified equation (2) leads to the classic Bailey and Hirsch [8] relationship:

$$r_{cr} = \frac{2\gamma_{GB}}{\tau\,\rho_0} \qquad (4).$$

The velocity of a high angle boundary during recrystallisation is the product of the boundary mobility, m, and the sum of the driving and dragging forces:

$$v = m\,\Delta P = m\left(\tau\,\Delta\rho - P_Z\right)P_S \qquad (5),$$

where $\tau\Delta\rho$ is the stored energy difference in the vicinity of the boundary, P_Z the Zener drag [9] and P_S the solute drag for high boundary velocities [10].

Figures (1) and (2) show the development of the critical dislocation density in Alloy 80A in dependence of the temperature (fig. 1) and of the strain rate (fig. 2), respectively.

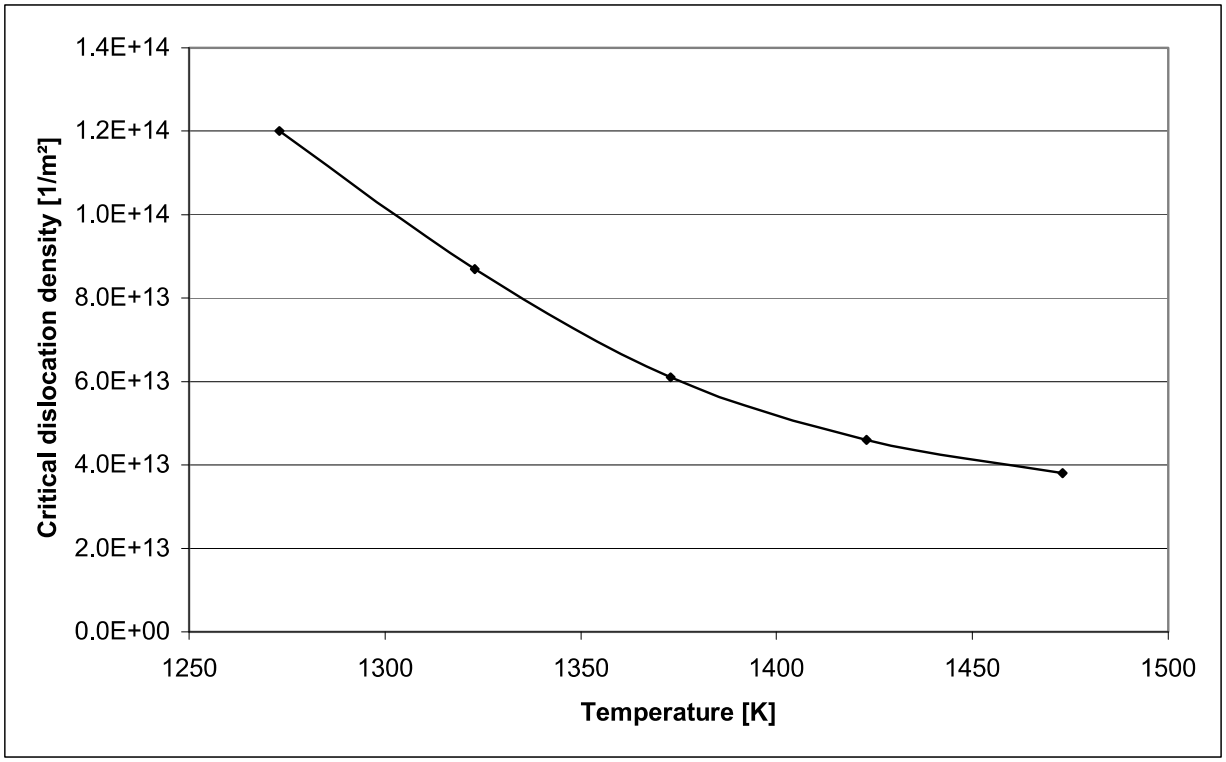

Fig.1. Critical dislocation density as a function of temperature of Alloy 80A at a constant strain rate of 1/s.

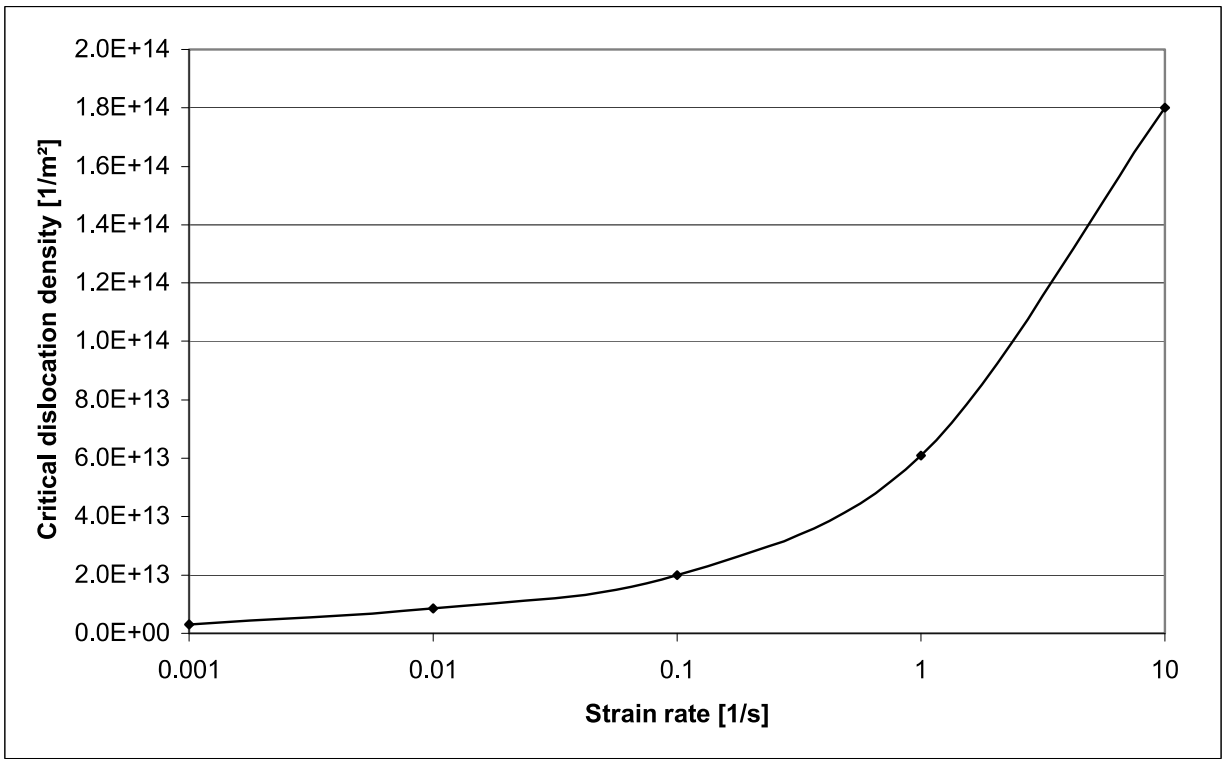

Fig. 2. Critical dislocation density as a function of strain rate of Alloy 80A at a constant temperature of 1373K.

Recrystallisation Model[1]

In the following it is assumed that nucleation will occur at the grain boundaries (in the grain boundary area F) of the deformed material. F/f_{cr} is the number of stable nuclei, which can be formed, where f_{cr} is the cross section area of a critical nucleus.

A statistical model where the number of nuclei per volume as a function of time is given by $Z(t)$ can describe the nucleation with time

$$Z(t) = Z_{\infty}\left(1 - \exp(-\alpha t)\right) \tag{6},$$

where Z_{∞} denotes the asymptotic number of nuclei per volume for $t \to \infty$ and α is an exponential variable. It results from preliminary calculations that α has to be in proportion to the gradient of the dislocation energy $\tau\rho/d_{gb}$:

$$\alpha = \frac{m\,\tau\,\rho_{cr}}{d_{gb}} K_{\alpha} \tag{7},$$

where d_{gb} is the 'thickness' of the grain boundary and K_{α} is a constant factor.

During recrystallisation, a grain boundary slips over the plane f_p

$$f_p(t) = \pi\left(r_{cr} + \int_{t_{cr}}^{t} v(t)\,dt\right)^2 - f_{cr} = \pi\left[\left(\int_{t_{cr}}^{t} v(t)\,dt\right)^2 + 2\,r_{cr}\int_{t_{cr}}^{t} v(t)\,dt\right] \tag{8},$$

with the assumption that the grain boundary velocity depends on time. This can occur during the recrystallisation process (equation 5) due to the precipitation of particles, changing temperature and strain rate.
The number of annihilated potential nuclei in f_p is ϕ

$$\phi(t) = \frac{f_p(t)}{\pi\,r_{cr}^{\,2}} = \left(\int_{t_{cr}}^{t} \frac{v(t)}{r_{cr}}\,dt\right)^2 + 2\int_{t_{cr}}^{t} \frac{v(t)}{r_{cr}}\,dt \tag{9}.$$

Because of this annihilation process, the constant factor Z_{∞} in equation (6) becomes time dependent. Hence the number of nuclei can be calculated by

$$Z(t) = \int_{t_{cr}}^{t} Z_{\infty}(\tau)\alpha\,d\tau \tag{10},$$

where the number of all potential nuclei $Z_{\infty}(0) = Z_{\infty 0}$ is given by

$$Z_{\infty 0} = \frac{F}{f_{cr}} = \frac{3}{D_u\,\pi\,r_{cr}^2} \tag{11},$$

assuming a spherical grain and where D_u is the diameter of the unrecrystallised grains. The concomitant grain formation and growth, which are coupled with the annihilation of potential nuclei stop if $Z_{\infty}(t)$ becomes zero.

Let us divide the time t into n steps ($\Delta t = t/n$). Therefore equation (10) can be written as

$$Z(t) = \sum_{i=0}^{n-1} \int_{t_{g,i}}^{t_{g,i+1}} Z_{\infty}(\tau)\alpha\,\Delta\tau \approx \sum_{i=0}^{n-1} Z_{\infty}(t_{g,i})\alpha\,\Delta t = \sum_{i=0}^{n-1} dZ(t_{g,i}) \tag{12},$$

[1] W. Mitter developed the analytical recrystallisation model.

where $t_{g,i}$ denotes the nucleation time of the i^{th} grain class. Thus each class is formed between the time steps $t_{g,i-1}$ and $t_{g,i}$ and contains $dZ(t_{g,i})$ nuclei.

This approximation corresponds to a step function . If we designate $dZ_i=dZ(t_{g,i-1})$ then

$$dZ(t_{g,i}) = dZ_{i+1} = \int_{t_{g,i}}^{t_{g,i+1}} Z_\infty(t)\,\alpha\,dt \approx Z_\infty(t_{g,i})\,\alpha\,\Delta t = Z_{\infty,i}\,\alpha\,\Delta t \qquad (12),$$

and therefore

$$Z_{\infty,n} = Z_{\infty,n-1}\left\{1-\alpha\,\Delta t\left[1+\phi_{n-1}(t_n)\right]\right\} - \Delta t\sum_{i=2}^{n} Z_{\infty,n-i}\,\alpha\left[\Delta\phi_{n-i}(t_n)\right] \qquad (13).$$

Figure (3) shows the calculated development of the density of nuclei as a function of the strain.

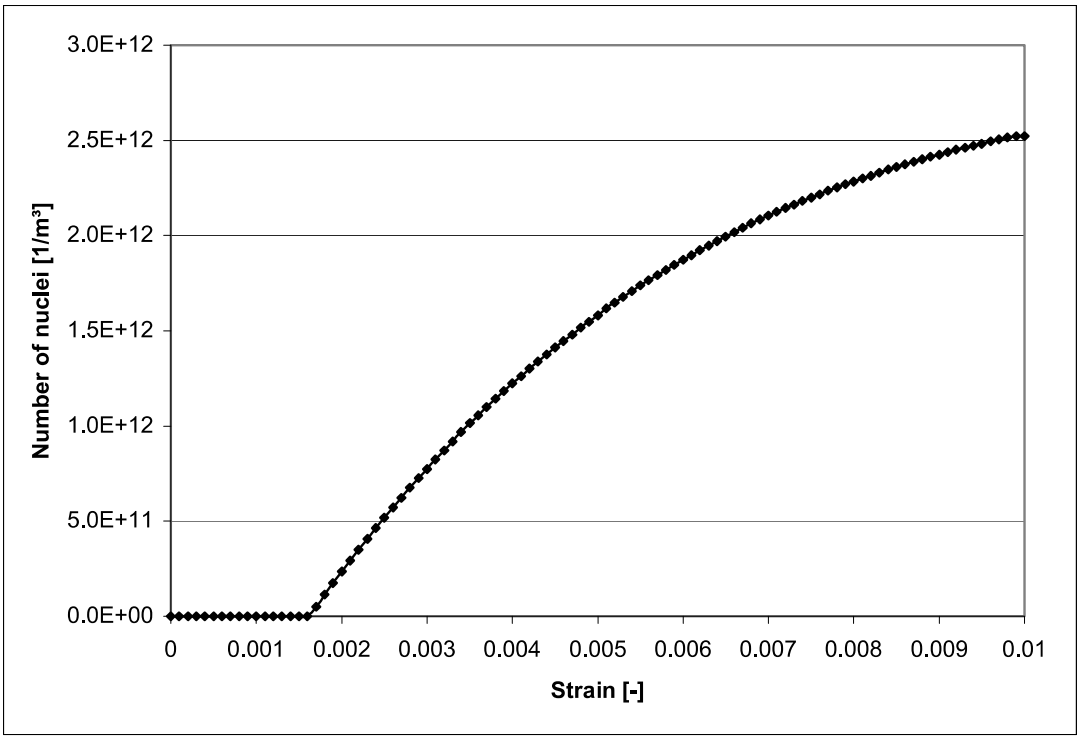

Fig. 3. Nuclei density at 1273K and at a strain rate of 0.1/s of Alloy 80A.

At the time step of observation t_b the size of a grain class can be determined by

$$D(t_{g,i},t_b) = 2\,r_{cr} + \int_{t_{g,i}}^{t_b} v(\tau)\,d\tau \qquad (14)$$

and the volume of this grain is

$$V(t_{g,i},t_b) = \frac{\pi}{6} D^3(t_{g,i},t_b) \qquad (15).$$

The very first grain class ($D(t_{cr},t)$) that is formed at the beginning of dynamic recrystallisation is represented in figure (4) where the first point marks the critical grain size $2\,r_{cr}$ ($1.6\mu m$).

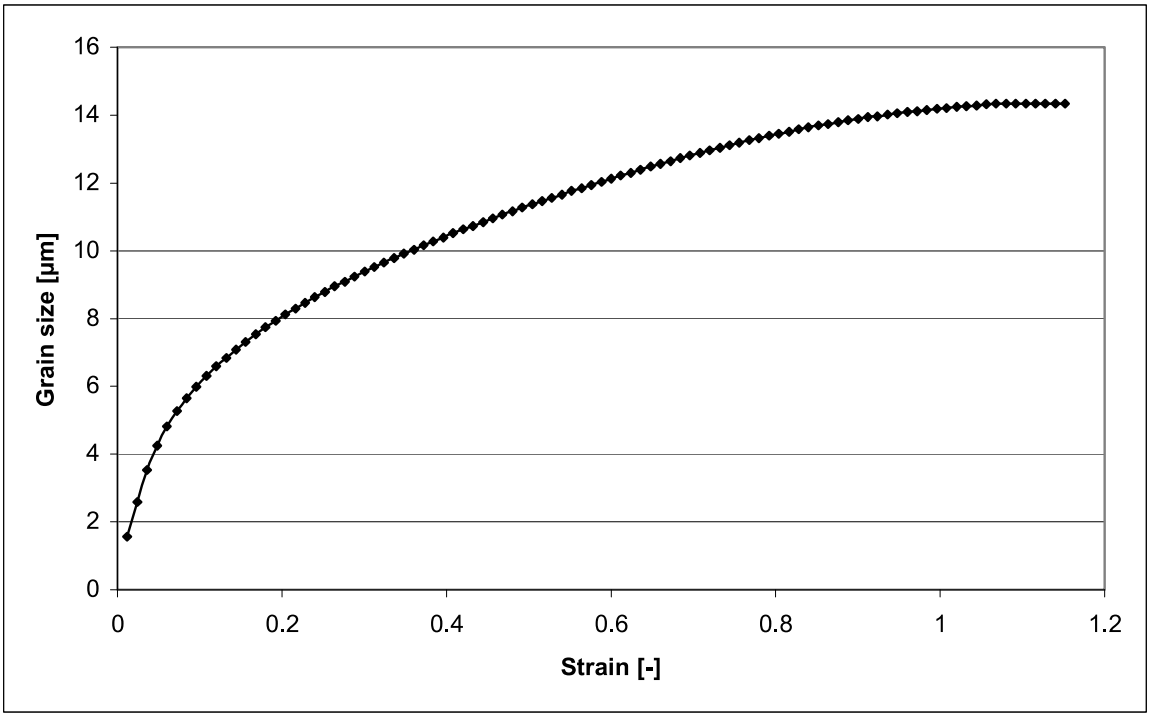

Fig. 4. Development of the size of a grain class *i* with time (Alloy 80A, temperature=1373K, strain rate=0.1/s).

$Z'(t_{g,i})\ dt_g$ grains are nucleated in the time interval $[t_{g,i}, t_{g,i}+dt_g]$. The volume of all grains which are nucleated within this time interval is $V(t_{g,i}, t_b)\ Z'(t_{g,i})\ dt_g$. The recrystallised fraction $f(t_b)$ at the time t_b is given by the sum over all nucleation times:

$$f(t_b) = \int_{t_{cr}}^{t_b} V(t_g, t_b)\, Z'(t_g)\, dt_g = \frac{\pi}{6} \int_{t_{cr}}^{t_b} D^3(t_g, t_b)\, Z'(t_g)\, dt_g \tag{16}.$$

The volume increase of a grain nucleated at the time t_g follows from equation (14)

$$dV(t_{g,i}, t_b) = \pi\, D^2(t_{g,i}, t_b)\, v(t_b)\, dt_b \tag{17}.$$

It must be considered that the growing grains touch with time. Therefore only a fraction of the boundary $\Psi(f)$ will move, where $\Psi(f)$ is a function of the recrystallised volume fraction and $\Psi(1)$ has to be zero. Hence the following relationship can be defined

$$\psi(f) = 1 - \left(\frac{f - f_C}{1 - f_C} \right)^n S(f, f_C) \tag{18},$$

where f_C is the recrystallised volume fraction at the first contact time. The exponent n is a constant factor and $S(f,f_C)$ is a switch function, whereat $f<f_C$: $S=0$ and $f \geq f_C$: $S=1$.
With $\Psi(f)$, the volume increase in equation (17) becomes

$$dV(t_{g,i}, t_b) = \Psi(f(t_b))\, \pi\, D^2(t_{g,i}, t_b)\, v(t_b)\, dt_b \tag{19}$$

and

$$V(t_{g,i}, t_b) = \frac{\pi}{6} D_u^{\,3} + \int_{t_{g,i}}^{t_b} \Psi(f(\tau))\, \pi\, D^2(t_{g,i}, \tau)\, v(\tau)\, d\tau \tag{20}$$

and

$$f(t_b) = \int_{t_g=t_{cr}}^{t_b} \int_{\tau=t_g}^{t_b} \Psi(f(\tau))\pi D^2(t_g,\tau)v(\tau)d\tau\ Z'(t_g)dt_g + \frac{\pi}{6}D_u^3\left[Z(t_b)-Z(t_{cr})\right] \quad (21).$$

Figure (5) show calculated dynamic recrystallised fractions in comparison with measured data. These data where determined by compression tests on a Gleeble 3800 testing system followed by a metallographical investigation. The partially recrystallised microstructure of a sample is depicted in figure (6).

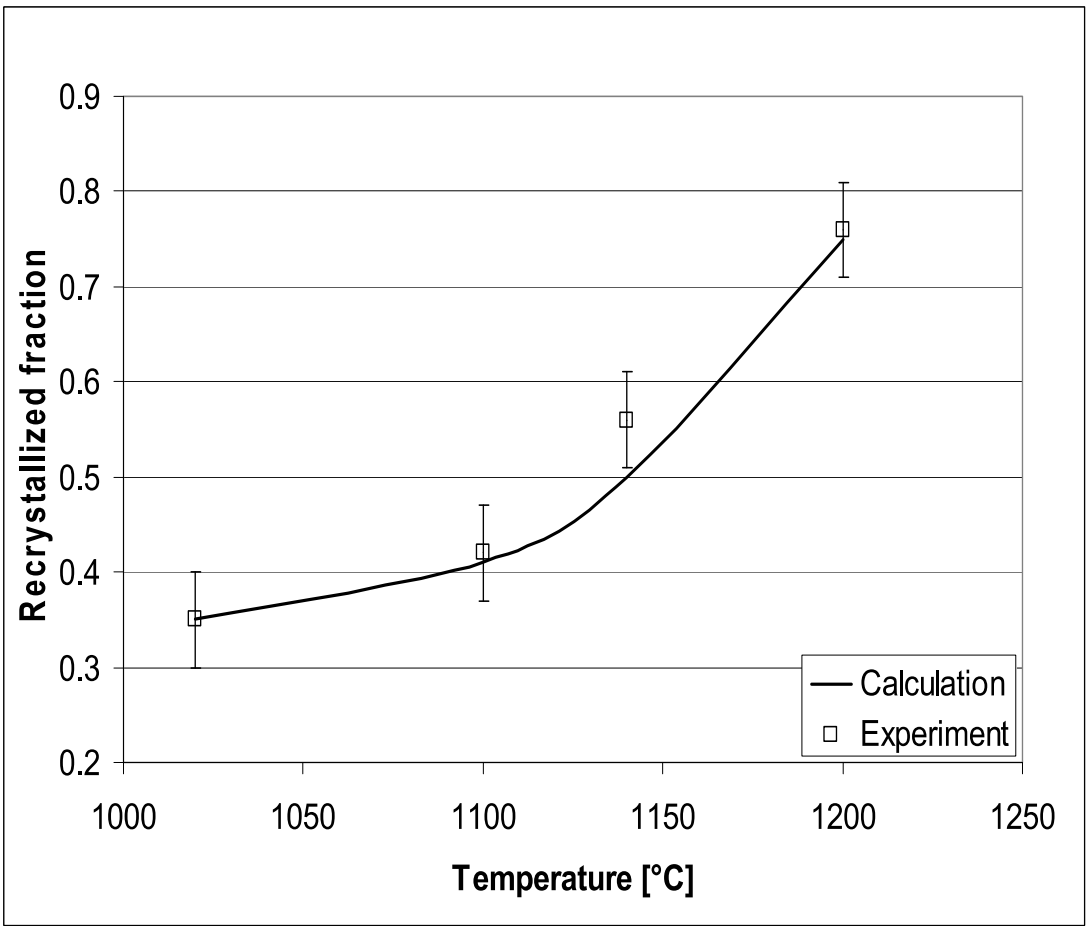

Fig. 5. Dynamic recrystallisation of Alloy 80A at a strain rate of 1/s and a strain of 1. Comparison of calculations (this model) and experiments [3,4].

The mean dislocation density $\rho_{m,i}$ within a recrystallised grain i can be obtained by the quotient of the dislocation length and the volume of the grain

$$\rho_{m,i}(t_b) = \frac{1}{V_i}\left[\int_{t=t_{g,i}}^{t_b} \rho(\varepsilon,t_b-t)\dot{V}(t)dt + \rho(\varepsilon,t_b-t_{g,i})\frac{4\pi r_{cr}^3}{3}\right] \quad (22).$$

Summing up over all grains i give the mean dislocation density of the recrystallised fraction

$$\overline{\rho}(t_b) = \int_{t=t_{cr}}^{t_b}\left[\int_{\tau=t}^{t_b} \rho(\varepsilon,t_b-\tau)\dot{V}(\tau)d\tau + \rho(\varepsilon,t_b-t)\frac{4\pi r_{cr}^3}{3}\right] Z_\infty(t)\alpha(t)dt \quad (23)$$

and the mean dislocation density of the whole structure

$$\overline{\rho}_{ges}(t_b) = \overline{\rho}(t_b) + (1 - f(t_b))\,\rho_u(t_b) \tag{24}$$

where ρ_u is the dislocation density of the unrecrystallised fraction.

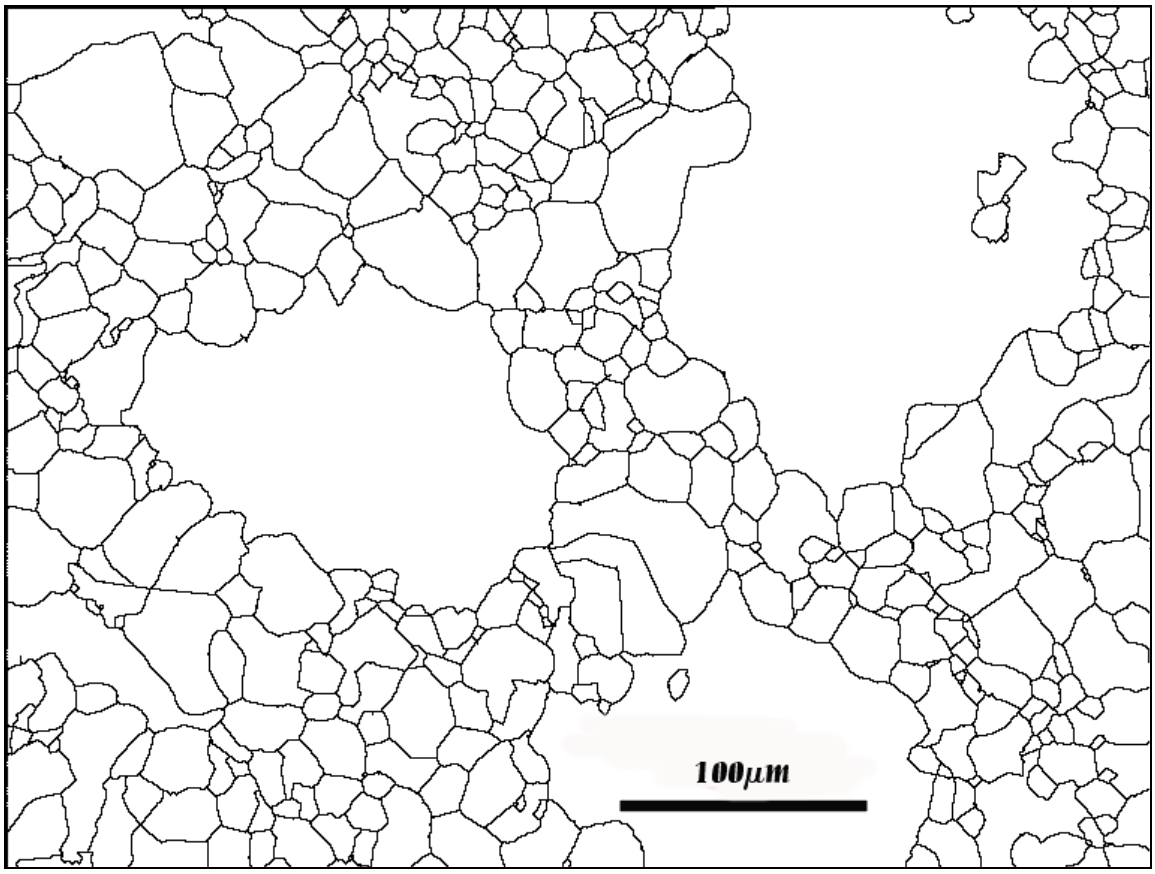

Fig. 6. Partially dynamically recrystallised sample of Alloy 80A. (strain rate: 1/s; strain: 1; temperature: 1373K).

The nuclei of the second recrystallisation cycle will form at the contact points of the grains of the first cycle. It seems to be suitable to set the number of the contact points in proportion to the fraction of the pinned grain boundary plane (*1-Ψ*). The geometry of the grains is assumed to be a pentagondodecahedron, hence the maximum number of contact points on a grain is *12*. The number of contact points per volume Z_C as a function of time can be defined as

$$Z_C(t) = Z_1(t)\,6\left[1 - \Psi(f(t))\right] \tag{25},$$

where the factor *6=12/2* follows from the fact that each contact point belongs to two adjacent grains. The derivations of the recrystallised fraction and the mean dislocation density of the second cycle are given in detail in reference (2).

The total recrystallised volume fraction is assumed to be equal to the fraction of the first cycle because the second recrystallisation front only exists within the recrystallised structure of the first generation.

There are several possibilities to describe the mean grain size D_m for all grain size classes (all recrystallisation cycles). A simple but demonstrative method is (here for two cycles):

$$D_m = D_{2m} f_2 + D_{1m}(f_1 - f_2) + D_u(1 - f_1) \tag{26},$$

where the indices 1 and 2 denote the number of recrystallisation cycle, and D_{im} is the mean grain size of the i^{th} recrystallisation cycle (D_{1m} in figure (7)) and D_u the mean grain size of the unrecrystallised grains.

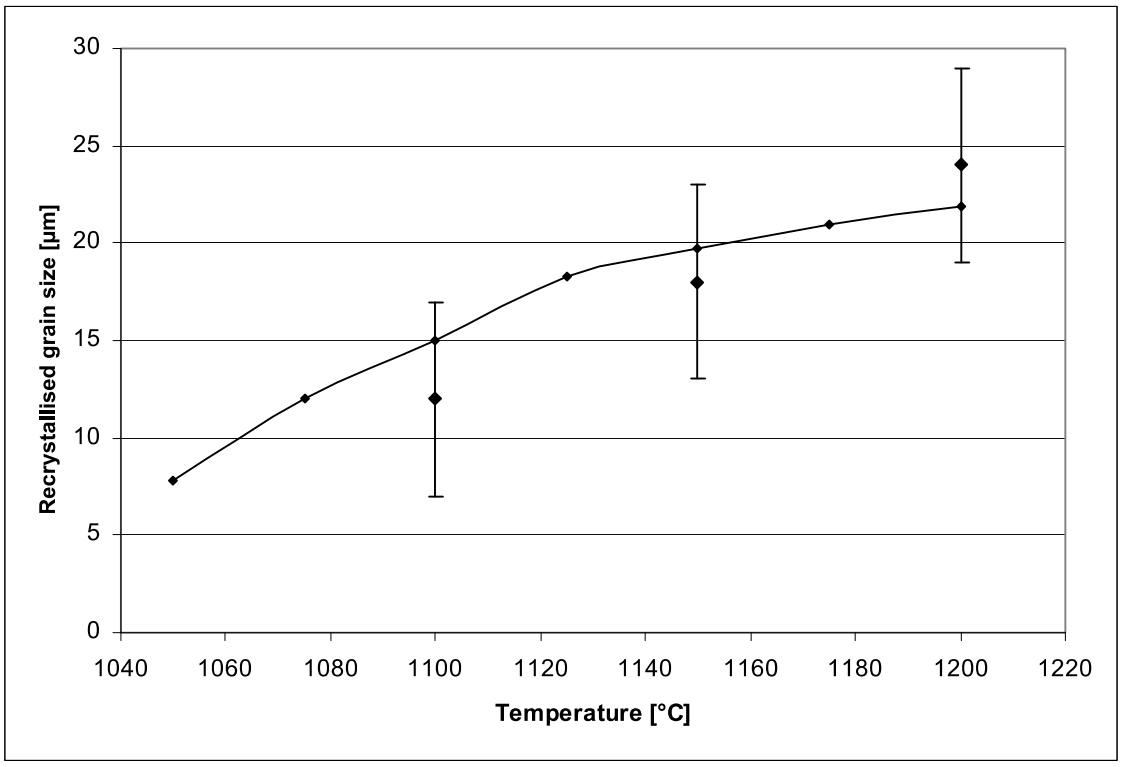

Fig. 7. Dynamic recrystallisation of Alloy 80A at a strain rate of 1/s: Mean recrystallised grain size. Comparison of calculations (this model) and experiments (error bars) [3,4].

Example

In the following one example using this model for hot rolling of slabs made of the Alloy 80A (fig. 8) is given (initial temperature: 1180°C, initial grain size: 500µm).

In the 45° direction of compression a maximum of strain is concentrated and hence the critical strain for recrystallisation is reached first in this area. The dislocation density in fig. (8d) represents the recrystallised grains only. If this dislocation density locally reaches the critical conditions for recrystallisation, a second cycle will start.

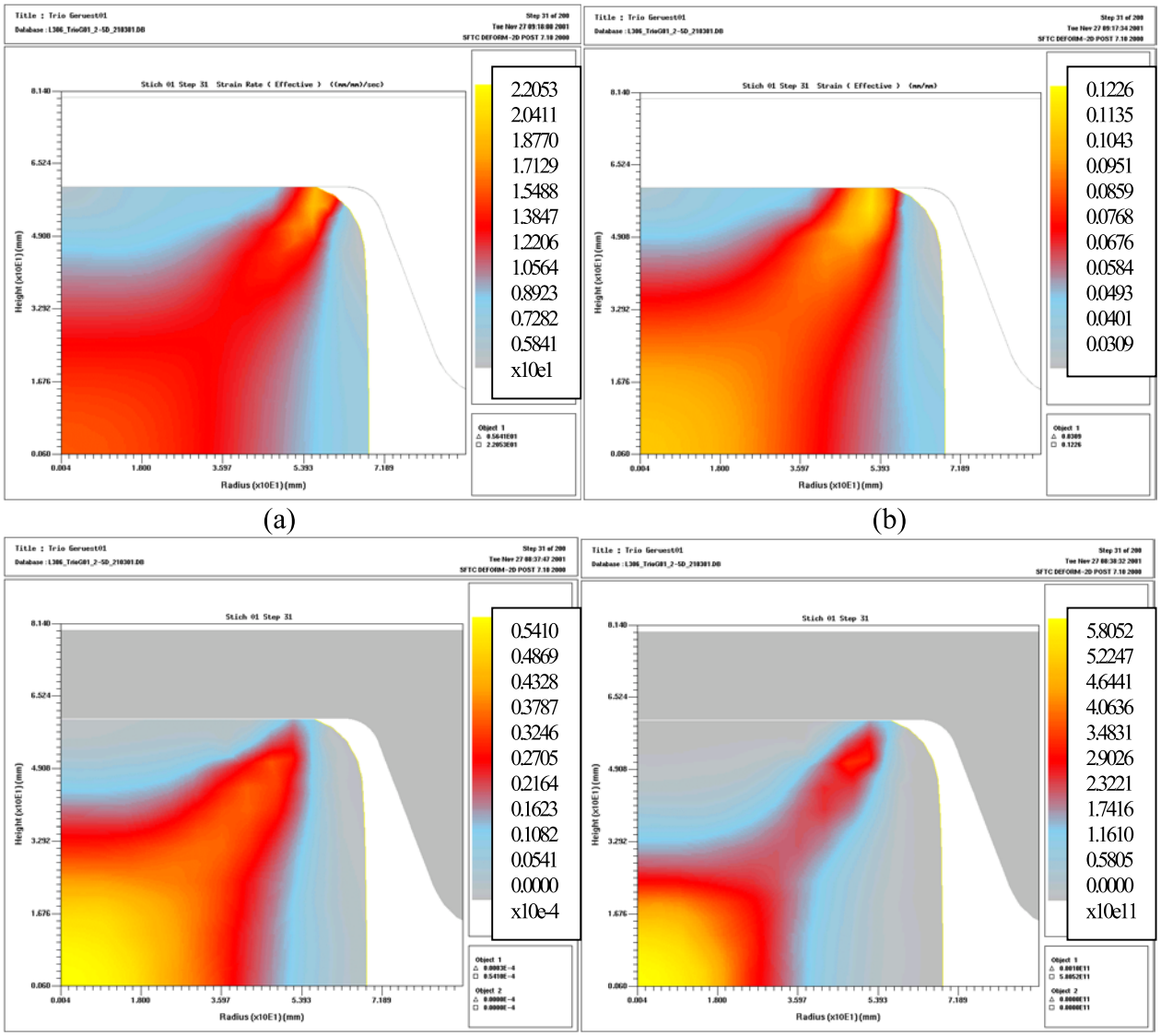

Fig. 8. Symmetrical quarter of a section of a rolling slab during the rolling pass: (a) strain rate [1/s]; (b) strain; (c) fraction of recrystallisation (eq. 21); (d) dislocation density of the first recrystallisation cycle (eq. 23).

Conclusions

An advanced microstructure model that is coupled with a commercial finite element program can describe the grain structure development during hot forming processes at industrial scale. The dislocation density is used as a state variable and predict the onset of recrystallisation when reaching the critical conditions. The size of the recrystallised grains depends on the number of nuclei and the velocity of the moving large angle grain boundaries. If the dislocation density of the recrystallised grains reaches the corresponding critical strain for recrystallisation, a second recrystallisation cycle will start at the contact points of the recrystallised grains of the first cycle. When the deformation stops the initialised recystallisation cycles will be continued if the thermo-kinetic conditions are sufficient. In the field of industrial hot forming processes, such models are used to optimise the deformation procedure and to predict the final microstructure.

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