

# Modelling Recrystallization of Nickel-Base Alloys

C. Sommitsch, W. Mitter, S. Kleber, Böhler Edelstahl GmbH & Co KG Kapfenberg (Austria)

## Introduction

In the last 15 years, several numerical models for the microstructure simulation of industrial processes, such as heat treatment or hot forming processes, have been developed. There are commercial FE-computing programmes available that can describe the evolution of the grain structure based on semi-empirical models (e.g. DEFORM<sup>TM</sup>-HT). However, such models cannot give a deeper insight into the real physical process because they do not consider the deformation history and the interaction of inhomogeneities (precipitations, solute atoms etc.) with moving large angle grain boundaries.

The present model<sup>1</sup> (1) simulates the grain structure development during and after hot deformation of nickel-base alloys. It considers normal grain growth and dynamic, postdynamic and static recrystallization and can be used for alloys with low stacking fault energy and thus recrystallization as the predominant softening process. A corresponding precipitation model is described elsewhere (1,2).

## Criteria for Recrystallization

During hot forming, the derivative of the dislocation density can be described (3) by the equation

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

taking the strain hardening and the recovery of dislocations into account, where  $\dot{\epsilon}$  is the strain rate,  $b$  the Burgers vector,  $l$  the mean free path of the dislocations,  $M$  the mobility of recovery and  $\tau$  the average energy per unit length of a dislocation.

A critical dislocation density is necessary in order to initiate dynamic recrystallization. The nucleus usually forms at pre-existing grain boundaries in the material, at least at higher strain rates (4). For an area that has just been recrystallized it is assumed that the dislocation density  $\rho_0$  generated by the preceding strain is reduced to a very low value.

Roberts and Ahlblom (5) developed a nucleation criterion, which is based upon the idea that during dynamic recrystallization, 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 recrystallization if the boundary is to migrate at the same velocity. The nucleation theory gives the net free energy change (5)

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

where  $\gamma_{GB}$  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:

---

<sup>1</sup> W. Mitter developed the analytical recrystallization model.

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

where  $m$  denotes the mobility of a moving high angle boundary and  $\rho_s$  the stationary dislocation density (5).

No real critical radius  $r_c$  exists unless  $\rho_0$  exceeds a critical value  $\rho_{cr}$ .

In the case of static recrystallization ( $\dot{\epsilon} = 0$ ), the dislocation density behind the boundary is zero, thus the dislocation energy is  $\tau\rho_0$ . Differentiation of the modified equation 2 leads to the classic Bailey and Hirsch (6) relationship:

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

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

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

where  $\tau\Delta\rho$  is the stored energy difference in the vicinity of the boundary,  $P_Z$  the Zener drag (7) and  $P_S$  the solute drag for high boundary velocities (8).

### Recrystallization Model

In the following it is assumed that nucleation will occur at the grain boundaries (in the grain boundary area  $F$ ) of the deformed material.  $F/f_0$  is the number of stable nuclei, which can be formed, where  $f_0$  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

$$Z(t) = Z_\infty (1 - \exp(-\alpha t)) \quad (6),$$

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

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

where  $d_{gb}$  is the ‘thickness’ of the grain boundary and  $K_\alpha$  is a constant factor.

During recrystallization, a grain boundary slips over the plane  $f_p$

$$f_p = \pi \left( r_0 + \int_0^t v dt \right)^2 - f_0 = \pi \left[ \left( \int_0^t v dt \right)^2 + 2r_0 \int_0^t v dt \right] \quad (8),$$

with the assumption that the grain boundary velocity depends on time. This can occur during the recrystallization process (equation 5) due to the precipitation of particles, changing temperature and strain rate.

The number of annihilated potential nuclei in  $f_p$  is  $\phi$

$$\phi(v,t) = \frac{f_p}{\pi r_0^2} = \left( \int_0^t \frac{v}{r_0} dt \right)^2 + 2 \int_0^t \frac{v}{r_0} dt \quad (9).$$

Because of this annihilation process, the constant factor  $Z_\infty$  in equation 6 becomes time dependent. Hence the number of nuclei can be calculated by

$$Z(t) = \int_0^t Z_\infty(\tau) \alpha d\tau \quad (10)$$

and the recrystallized fraction  $f$  is given by

$$f = Z(t) V_m \quad (11),$$

where  $V_m$  is the mean volume of the recrystallized grains.

Let us divide the time  $t$  into  $n$  steps ( $\Delta t = t/n$ ). The number of potential nuclei changes with each time step according to the following:

$i$	Number of potential nuclei $Z_\infty$
0	$Z_{\infty 0}$
1	$Z_{\infty 1} = Z_{\infty 0} - Z_{\infty 0} \alpha \Delta t - Z_{\infty 0} \alpha \Delta t \phi(v, \Delta t) = Z_{\infty 0} [1 - \alpha \Delta t (1 + \phi(v, \Delta t))]$
2	$Z_{\infty 2} = Z_{\infty 1} (\alpha, \Delta t, \phi(v, 2\Delta t)) [1 - \alpha \Delta t (1 + \phi(v, \Delta t))]$
3	$Z_{\infty 3} = Z_{\infty 2} (\alpha, \Delta t, \phi(v, 3\Delta t), \phi(v, 2\Delta t)) [1 - \alpha \Delta t (1 + \phi(v, \Delta t))]$
.	.
.	.
$n$	$Z_{\infty n} = Z_{\infty 0} \prod_{i=1}^n [1 - \alpha \Delta t (1 + \phi(v, i\Delta t))]$

(12),

where  $i$  is the time step number. Substituting with

$$N(t) = \prod_{i=1}^n \left[ 1 - \alpha \frac{t}{n} \left( 1 + \phi(v, i \frac{t}{n}) \right) \right] \quad (13)$$

leads to

$$Z_\infty(t) = Z_{\infty 0} N(t) \quad (14).$$

$N(t)$  is called the function of nuclei formation and  $Z_{\infty 0}$  is given by

$$Z_{\infty 0} = \frac{F}{f_0} = \frac{3}{D \pi r_0^2} \quad (15),$$

assuming a spherical grain and where  $D$  is the diameter of the unrecrystallized grains. The concomitant grain formation and growth, which are coupled with the annihilation of potential nuclei stop if  $Z_\infty(t)$  and  $N(t)$  become zero.

Calculating the growth of the recrystallized grains, it must be considered that the grains will touch with time and will form new, immobile boundaries. After this moment only a fraction of the boundary  $\Psi(f)$  will move, which is a function of the recrystallized volume fraction, where  $\Psi(1)$  has to be zero. Hence the following relationship can be defined

$$\psi(f) = 1 - \left( \frac{f - f_c}{1 - f_c} \right)^n S(f, f_c) \quad (16),$$

where  $f_C$  is the recrystallized volume fraction at the first contact time.  $S(f, f_C)$  is a switch function, where at  $f < f_C$ :  $S=0$  and  $f \geq f_C$ :  $S=1$ .

The derivations of the grain size distribution, the mean volume  $V_m$  and the mean dislocation density are given in detail in reference (1).

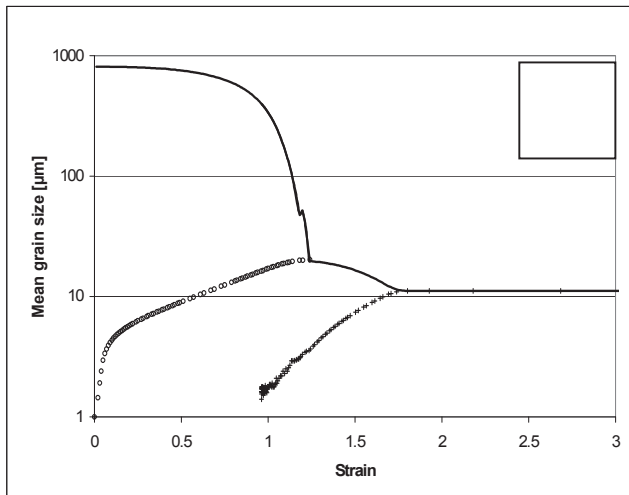
The nuclei of the second recrystallization cycle will form at the contact points of the grains of the first cycle. It seems to be suitable to set the number of the contact points in proportion to the fraction of the pinned grain boundary plane ( $1-\Psi$ ). The geometry of the grains is assumed to be 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

$$Z_C(t) = Z_1(t)6[1 - \Psi(f(t))] \quad (17),$$

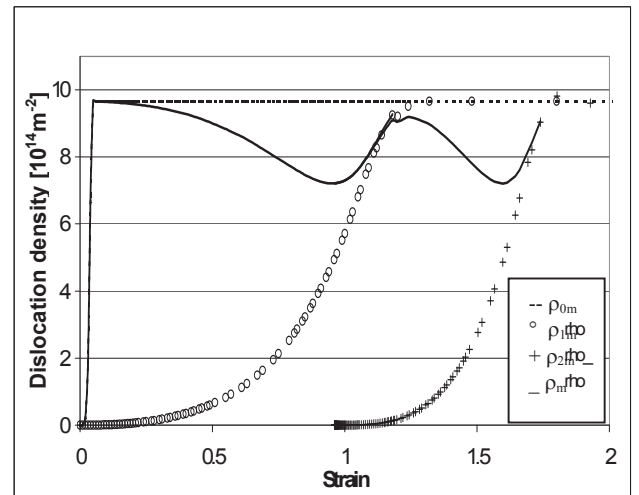
where the factor  $6=12/2$  follows from the fact that each contact point belongs to two adjacent grains. The total recrystallized volume fraction is assumed to be equal to the fraction of the first cycle because the second recrystallization front only exists within the recrystallized structure of the first generation.

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

$$D_m = D_{2m} f_2 + D_{1m} (f_1 - f_2) + D_0 (1 - f_1) \quad (18).$$



**Fig.1:** Development of the recrystallized mean grain size within the first and second cycle and the total mean grain size during dynamic recrystallization of Alloy 80A at a temperature of 1100°C and a strain rate of  $1 \text{ s}^{-1}$ . The initial grain size is  $800 \mu\text{m}$ .



**Fig.2:** Development of the dislocation density of the first and second recrystallization cycle as well as the mean dislocation density of Alloy 80A at a temperature of 1100°C and a strain rate of  $1 \text{ s}^{-1}$ .

The mean grain size of the first cycle ( $D_{1m}$ ) reaches a final value of  $20 \mu\text{m}$  after the completion of the first cycle at a logarithmic strain of approximately 1.2 in figure 1. The second cycle ( $D_{2m}$ ) starts at a strain of approximately 0.9 and reaches the final value of  $10 \mu\text{m}$  at a strain of 1.7. Hence the total mean grain size  $D_m$  reaches the final value of  $D_{1m}$  after the completion of the first cycle and  $D_{2m}$  after the completion of the second cycle.

The mean dislocation density of  $n$  recrystallization cycles (also taking into account the unrecrystallized structure with  $i=0$ ) results from

$$\rho_m = \sum_{i=0}^n \rho_{im} f_i \quad (19),$$

where  $\rho_{im}$  denotes the mean dislocation density within cycle  $i$ . For the calculation of the total mean dislocation density in the case of two cycles it has to be considered that all grains of the second generation lie within the first cycle structure. Hence it follows:

$$\rho_m = (1 - f_1)\rho_{0m}(t_e) + (f_1 - f_2)\rho_{1m}(t_e) + f_2\rho_{2m}(t_e) \quad (20).$$

In figure 2  $\rho_{0m}$  indicates the dislocation density in the unrecrystallized structure, which reaches a steady state value after exceeding the critical value for recrystallization.  $\rho_{1m}$  and  $\rho_{2m}$  are the mean dislocation densities of the first and second cycle respectively.  $\rho_m$  is the total mean dislocation density, which represents the flow curve.

In the case of postdynamic recrystallization the started recrystallization cycles will be finished while the dislocation density decreases due to recovery. The recrystallization front can stop if the temperature decreases to a level where the grain boundary mobility approaches zero, or if the former deformation (and therefore the driving force of recrystallization) was not strong enough for the grain boundary velocity to reach significant values. Also a retarding effect for recrystallization is the decrease of the nucleation exponent, and hence the number of nuclei, because of recovery processes (equation 7).

During classical static recrystallization only one recrystallization cycle can occur. Therefore the recrystallized grain size becomes dependent on the initial grain size. Smaller initial grain sizes force finer grains and faster recrystallization because of a higher density of nucleation sites. The influence of the former deformation on static recrystallization can be neglected for simulating hot forming processes because in most cases strain is high enough to initiate the nucleation of dynamic recrystallization. Different and sufficient strong deformations lead to for a relatively small variation in the start dislocation densities for dynamic recrystallization because of the typical shape of the flow curve for hot deformations. Thus there is a general problem distinguishing between static and postdynamic recrystallization in hot forming processes because nuclei even form at small deformations. Jonas et al. (9) formulate a “significant amount” of dynamic recrystallization being necessary in order that the following process of recrystallization be independent of the initial grain size and the strain. The extent of this amount would have to be measured by experiment. Obviously the number of dynamic nuclei would have to be sufficiently large and the nuclei would reach a growth advantage to suppress the following static nucleation.

### Numerical Model

Figure 3 shows a flow chart for the calculation of recrystallization during deformation. The nucleation conditions for recrystallization are obtained for a given temperature and strain rate by equation 3. If the dislocation density (equation 1) reaches a critical value, a first recrystallization cycle starts and  $Z$  nuclei with the critical radius  $r_{cr}$  grow with velocity  $v$  (equation 5). The number of grains per volume, recrystallized fraction, dislocation density and grain size describe the grain structure of each cycle. A second or higher recrystallization cycle is begun at the contact points of the grains of the current cycle. The global grain structure is described both by the distribution of the grain size and the mean dislocation density, which is in proportion to the flow stress. The global recrystallized fraction is assumed to be equal to the fraction of the first cycle.

In the simulation program, the number of recrystallization cycles are increased until a steady state grain size is reached. This will happen if the mean grain size of the following recrystallization cycle does not become smaller because only one grain per old grain is formed.

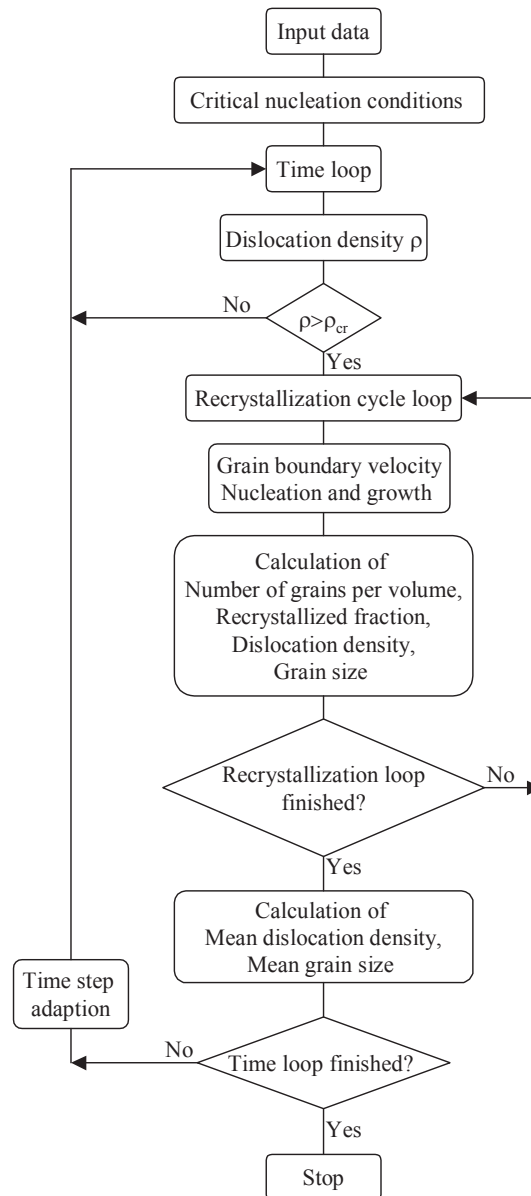


Fig.3: Flow chart of the numerical model for dynamic recrystallization.

### Experimental Details

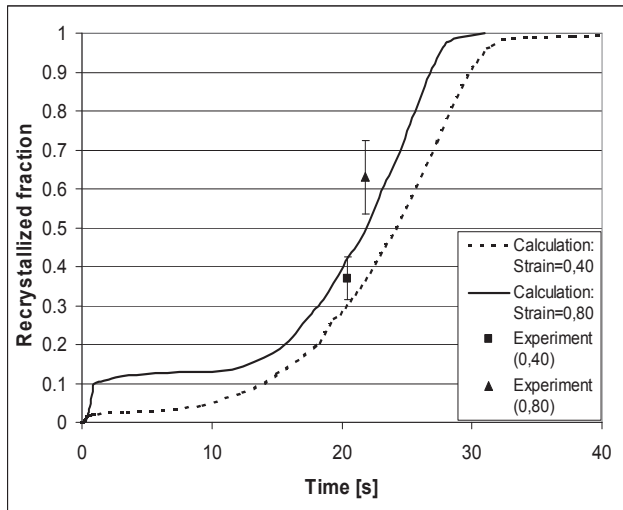
Experiments were performed to confirm the simulation of dynamic and postdynamic recrystallization on measured recrystallized fraction data. Samples of Böhler L306 VMR (Alloy 80A) were cut from hot rolled pieces, thus ensuring a completely recrystallized, fine-grained and homogeneous microstructure. Hot compression tests were carried out on a Gleeble 3800 testing system. Solution heat treatment was carried out at 1220°C for 60 seconds. The short annealing time was chosen to avoid grain growth. For the investigation of the dynamic recrystallization the specimens were cooled down to the test temperature and were compressed at different strain rates and temperatures. The investigation of the recrystallized fraction and grain size was done by an image analysis system.

The interrupted tensile tests (10-12) were carried out on a Gleeble 1500 system at a constant strain rate of  $1\text{s}^{-1}$ . Specimens were deformed by a strain of 1 and after a holding time, were deformed

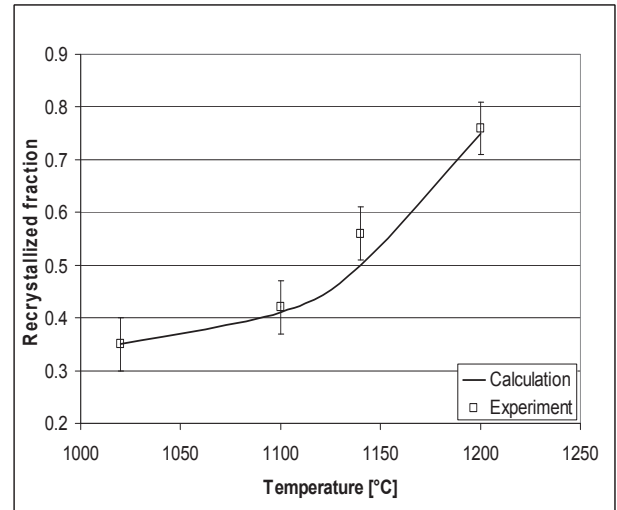
again to obtain a partially recrystallized fraction. Comparing the lower flow stress of the initial and the partially recrystallized material yields the postdynamic recrystallized fraction (11).

## Results

Figures 4 and 5 show calculated postdynamic and dynamic recrystallized fractions in comparison with measured data, which were obtained from interrupted tensile tests.



**Fig.4:** Postdynamic recrystallization of Alloy 80A at 1020°C. Comparison of calculations (this model) and experiments (12).



**Fig.5:** Dynamic recrystallization of Alloy 80A at 1100°C. Comparison of calculations (this model) and experiments (this work).  $\dot{\varepsilon} = 1 s^{-1}$ ,  $\varepsilon = 1$

In figure 4, the recrystallization velocity tends towards a lower value after the deformation because of the decreasing dislocation energy due to recovery. Shifting the recrystallization curves at the same temperature to the same starting point shows that postdynamic recrystallization does not depend on the applied strain. During deformation, the recrystallized fraction for a given strain and strain rate increases with temperature. The measured values fit well with calculations (figure 5).

## Conclusions

The described numerical procedure represents a general model for the simulation of the time-dependent grain structure during and after hot forming of nickel-base Alloys. A statistical approach was chosen for the description of the nucleation rate. The growth of recrystallization nuclei is modelled in an iterative manner. Currently, the model is embedded in a general microstructure model that is coupled to a commercial FE-computer program for the simulation of hot forming processes.

## References:

(1) Sommitsch, C.: Ph.D. Thesis, Institute for Materials Science, Welding and Forming, Graz University of Technology, Graz, 1999.

- (2) Sommitsch, C., Kozeschnik, E., Wasle, G., Buchmayr, B.: "A Precipitation Model for Multi-Component Multi-Phase Systems in Nickel-Base Superalloys", *J. Mater. Proc. Tech.*, to be published.
- (3) Sandström, R., Lagneborg, R.: *Acta Met.* 23, 1975, 387.
- (4) Sah, J.P., Richardson, G.J., Sellars, C.M.: *Metall. Sci.* 8, 1974, 325.
- (5) Roberts, W., Ahlblom, B.: *Acta Met.* 26, 1978, 801.
- (6) Bailey, A.R., Hirsch, P.B.: *Proc. R. Soc. A267*, 1962, 11.
- (7) Zener, C.: *T.M.S.-A.I.M.E.* 175, 1949, 175.
- (8) Cahn, J.W.: *Acta Met.* 10, 1962, 789.
- (9) Jonas, J.J., Maccagno, T., Yue, S.: *Phase Transformations during the Thermal/Mechanical Processing of Steels*, Hawbolt, E.B., Yue, S., (Eds.), The Canadian Institute of Mining, 1995.
- (10) Djaic, R., Jonas, J.J.: *J. of the Iron and Steel Inst.*, 04/1972, 256.
- (11) Tormo, J.O., Choquet, P.: *Physical Simulation of Welding, Hot Forming and Continuous Casting*, CANMET, Metals Technology Laboratories, Ottawa, 1988, III-35.
- (12) Bock G.: *Diploma Thesis*, Institute for Materials Science, Welding and Forming, Graz University of Technology, Graz, 1998.