Research Article

Giuseppe Napoli and Andrea Di Schino*

Statistical modelling of recrystallization and grain growth phenomena in stainless steels: effect of initial grain size distribution

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Abstract: Modelling and simulation of recrystallization, grain growth, and related phenomena are important tools for the fundamental understanding of microstructural evolution that takes place during the annealing and thermomechanical processing of steel. It is also important for the prediction of engineering properties. In this paper, the evolution of mean grain radius and the recrystallized volume fraction of steel was modelled using the statistical theory of grain growth originally developed by Lücke [1] and here integrated to take into consideration the effect of recrystallization. In particular, the effect of one free input parameter (initial distribution of grain radii) of the model is analysed without taking into account the textures effect.

Keywords: Grain growth, stainless steel, modelling

1 Introduction and description of the model

Grain size and chemical composition deeply affect the mechanical properties of steel and in recent years much efforts have been made to exploit the effect of these variables to improve mechanical and other properties of steels, these include: yield strength, ductility, fatigue behaviour, weldability, creep, and corrosion resistance [2–9].

Recrystallization and grain growth are others aspect relevant to the mechanical properties of steel and there is a need for models which will predict the effect of the processing parameters on the materials that are produced [10–12]. The modelling may be divided into two gen-

eral categories [13]. There are micro models such as Monte Carlo simulation [14], cellular automata [15], molecular dynamics, vertex model [16] and the phase-field model [17] which aim to treat individual problem such as deformation or annealing. There are also coupled models which may involve two or more models in an attempt to simulate large scale industrial process but this kind of model has a lack of information about the initial deformed condition [18]. In this paper an analytical model is reported, that can predict most of the characteristic of microstructural evolution (*i.e.* grain size and grain size distribution) combining a recrystallization model that works simultaneously with a grain growth model (based on Hillert model and further developed by Abbruzzese and Lücke) [18–20]. The goal of the micro model is to generate snapshots of the evolving microstructure with time and the local and ensemble properties of the microstructure may be determined from these snapshot.

As it is well known from the basics of metallurgy theory, the driving force of primary recrystallization is the driving force of primary recrystallization is for the most part related to the system tendency to eliminate the deformation energy introduced by cold working. During the heat treatment, it occurs a release of the deformation energy that activates the movement of dislocation and sub-grain boundaries thus restoring a dislocation free microstructure. Once all the dislocation is eliminated and a complete recrystallized structure is created in the material, the larger grains begin to growth at the expenses of the smaller grains (secondary recrystallization).

As concerns grain growth, the statistical model is based on the assumption of [21]:

- Super-position of average grain curvatures in individual grain boundaries.
- Homogeneous surroundings of the grains. As a first approximation is assumed that for each grain v the individual neighbourhood of N_v individual grain can be replaced by a surrounding obtained by averaging over a neighbourhood of all grains of the same radius R_v . Since then all grains of the same radius

*Corresponding Author: Andrea Di Schino: Dipartimento di Ingegneria, Università di Perugia, 06125 Perugia;
Email: andrea.dischino@unipg.it

Giuseppe Napoli: Dipartimento di Ingegneria, Università di Perugia, 06125 Perugia

would have the same surrounding, also their growth rate would be equal. This means that all grains could be collected in classes characterized by their radius and that the behaviour of only different classes has to be considered, instead of single grains.

- A random array of the grains namely the probability of contact among the grains is only depending on their relative surface in the system.

The integration of all the above assumptions in the model leads to the following final form of the grain growth rate equation:

$$\frac{dR_i}{dt} = M \sum_j \left(\frac{1}{R_j} - \frac{1}{R_i} \right) \frac{n_j 4\pi R_j^2}{\sum_j n_j 4\pi R_j^2} \quad (1)$$

Where:

R_i [cm] – Radius of grain belonging to class i

R_j [cm] – Radius of grain belonging to class j

n_i – Total number of grains in class i

n_j – Total number of grains in class j

Where $M = 2m\gamma$ is again the boundary diffusivity and in our case study m was evaluated according to the Stokes-Einstein relationship [22]:

$$m = \frac{D}{k_B T} = \frac{D_0}{k_B T} e^{\frac{-\Delta E}{k_B T}} \quad (2)$$

Where:

D [cm/s] – Diffusion coefficient

k_B [erg/K] – Boltzmann constant

ΔE [erg/mol K] – Activation energy

T [K] – Annealing temperature

D was chosen proportional to the diffusion coefficient of Fe in Fe- γ .

To describe the recrystallization process integrated with the grain growth, it is necessary to propose an extended growth equation that allows to analyse contemporarily and continuously the evolution of free nuclei in the matrix passing through partially impinged grains up to full contact. An “influence mean radius” that allow to evaluate the fraction of surface in contact between different grain [18] was introduced.

The final equation for recrystallization and grain growth can therefore be written as:

$$\begin{aligned} \frac{dR_i}{dt} = m \left[\left(\frac{Gb^2}{3} \Delta\rho - \frac{2\gamma}{R_i} \right) \sum_j^{i^*} p_j \right. \\ \left. + m\gamma \sum_{j=i^*}^{n_c} p_j \left(\frac{1}{R_j} - \frac{1}{R_i} \right) \right] \quad (3) \end{aligned}$$

Where:

G [dyne/cm²] – Shear modulus

b [cm] – Burger’s vector

$\Delta\rho$ [cm⁻²] – Difference of dislocation density for the deformed material and the recrystallized material.

Thanks to the previous equations, a calculus program that can predict the evolution over time of the grain size distribution, has been developed. The constitutive equation of plastic deformation has been introduced in the model to further reduce the free input parameters [23]:

$$\epsilon = \rho b L \quad (4)$$

Where:

ξ – Deformation of material (Reduction rate)

b [cm] – Burger’s vector

L [cm] – Free path of dislocation nuclei

2 Results

2.1 Effect of the initial grain distribution

One of the free input parameters of the statistical model is the initial grain size distribution. Three different distribution have been investigated: lognormal, normal and a uniform distribution (see figure 1). For the simulation, the other free input parameters namely, the reduction rate of steel, the total number of deformation nuclei and the dislocation density, have been maintained constant in the range values typical of industrially deformed steels.

Table 1: Input parameters used in the statistical model

ϵ [reduction]	N_{tot} [cm ⁻³]	$\Delta\rho$ [cm ⁻²]	T [° C]
0.80	8.59e9	1.99e11	1100

The lognormal distribution is very important in the description of natural phenomena because numerous natural growth processes are driven by the accumulation of many small percentage changes [24]. Normal (or Gaussian) distribution is a continuous probability function very common and thanks to the central limit theorem when independent random variables are added (like grain dimension), their sum tends toward a normal distribution even if the original variables themselves are not normally distributed [25]. Unlike a normal distribution with a hump in the middle, a uniform distribution has no mode and every outcome is equally likely to occur and was tested as a case limit [26].

Figure 1: Initial grain size distribution

A simulation of an annealing process of 300 seconds at $T=1100^{\circ}\text{C}$ resulted in a mean grain radius obtained from the uniform distribution bigger than the log-normal and normal distribution (respectively 29.25% bigger and 43.74%) and the difference for the three trends begin after the complete recrystallization of steel as can be seen in figure 2. The difference between the-log normal and normal distribution is less pronounced and the log-normal distribution leads to a 20 % larger grain.

Figure 2: Mean radius over time for three different grain size distribution

With regards to the recrystallized volume fraction, all the three simulation leads the complete recrystallization at the same time (approximately at 4.5 second), as is shown in figure 3. The recrystallized volume fraction in figure 3 was calculated based on the same input parameters as in figure 2.

Figure 3: Recrystallized volume fraction, for the first seconds of simulation, for the three different distribution

3 Conclusion

Results from a recrystallization and grain growth model based on statistical assumption have been discussed here. In particular, the effect of the initial grain radii distribution has been analyzed. Results show that:

- Final mean radius size is bigger for the uniform distribution than the log-normal and normal distribution;
- The mean radius is almost the same size for the three different distribution before the complete recrystallization;
- The complete recrystallization occurs at the same time for isothermal annealing process (even for different distribution).

The potential of this approach is a general purpose tool for thermo-mechanical treatment result prediction.

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