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# Physical Modelling of Recrystallization and Grain Growth in Steels: Analysis of Free Parameters

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**ABSTRACT**

The mechanical properties of steels are strongly affected by grain size and chemical composition variations. Many industrial developments have been carried out both from the point of view of composition variation and grain size in order to exploit the effect of these variables to improve the mechanical proprieties of steels. It is also evident that recrystallization and grain growth are relevant to the mechanical properties of steels, thus suggesting the necessity of mathematical models able to predict the microstructural evolution after thermo-mechanical cycles. It is therefore of primary importance to study microstructural changes, such as grain size variations of steels during isothermal treatments through the application of a mathematical model, able in general to describe the primary recrystallization and grain growth in metals. This paper deals with the recrystallization and grain growth modelling of steels based on the statistical theory of grain growth originally developed by Lücke[1] and here integrated to take into account the effect of recrystallization and Zener drag effect. A general continuity equation is proposed describing in continuous way recrystallization and grain growth phenomena without taking into account textures effect. The effect of input parameters is analyzed.

**Key-words:** Grain growth, Recrystallization, Stainless steel, Computer simulation.

## INTRODUCTION

Grain growth after primary recrystallization is described as taking place in two different forms, either in form of continuous grain growth ("normal") or in form of discontinuous grain growth ("secondary recrystallization"). In the development of this area two stages can be distinguished. In the first stage simple and mostly qualitative interpretations of grain growth have been given. For continuous grain growth, Beck[2] predicted an increase of the average grain diameter with time as $t^{1/2}$ which was practically never found. The second stage of the development of this area is characterized by more sophisticated approaches. Hillert[3] transferred the statistical treatment of Ostwald ripening of precipitates to grain growth according to the Lifshitz-Slyozov-Wagner theory[4-5]. Moreover, Hunderi and Ryum[6] introduced a deterministic model considering individual boundaries and describing the change of size of the individual grains by an extremely large set of differential equation (one for each grains) which they solved numerically. Finally,Abbruzzese[1] developed further the Hillert model by calculating a critical radius that was only postulated by Hillert [3]. The main novelty of Abbruzzese study was to use discrete grain size classes which reduce significantly the numbers of differential equations (one for each class) and thus to the possibility to calculate numerically the evolution of the grain size distribution. In recent years the Monte-Carlo simulation was widely used to simulate grain growth including also the case of Zener drag[7]. Hesselbarth and Gobel used, with success, a method named cellular automata in simulation of the theory of Johnson-Mehl-Avrami-Kolmogorov and other successful mesoscale simulations for micro structural evolution including front tracking model[8], vertex model[9] and phase

field model[10]have been developed. While analytical models, such as Abbruzzese and Lücke, predict all the characteristics of micro structural evolution (i.e., grain size and grain size distribution), the goal of mesoscale computational simulations is rather different: to generate snapshots of the evolving microstructure with time. Using the computational version of metallography, both local and ensemble properties of the microstructure may be determined from these snapshots.

**Description of the model**

A mathematical model able to simulate simultaneously recrystallization and grain growth phenomena is described in this paper. The driving force for primary recrystallization in metals is mainly related to the reduction of the deformation energy (dislocations) introduced by cold working. Heat treatment activates the movement of dislocations and sub-grain boundaries allowing the release of the deformation energy and thus restoring a "dislocation free" microstructure. Under further heat treatment, grain growth activated by boundary energy reduction is the dominant process[7]. In this approach, recrystallization nuclei are considered pre-existing and homogeneously distributed in the deformed microstructure.

As far as concerns grain growth, the statistical model, originally developed by Abbruzzese and Lucke[1], is based on the assumptions of:

- Super-position of average grain curvatures in individual grain boundaries. A grain *v* is characterized by a volume *V*, is assumed to growth at the expense of a neighbouring grain μ with a rate:

$$\left(\frac{dV_v}{dt}\right)_\mu = M s_{v\mu}\left(\frac{1}{R_\mu} - \frac{1}{R_v}\right) \quad ...(1)$$

Here the "radius" $R_v$ of a grain v is defined according $V_v = 4\pi {R_v}^3/3$. $S_{v\mu}$ is the area of contact between the two grains *v* and *μ*, and m, γ and *M=2m* γ represent respectively, the mobility, the tension and the diffusivity of the grain boundary *vμ*. By taking into account all *Nv* neighbours of this grain one obtain for all its total growth rate:

$$\frac{dR_v}{dt} = \frac{1}{4\pi {R_v}^2}\frac{dV_v}{dt} = \frac{M}{4\pi {R_v}^2}\sum_{\mu=1}^{N_v} s_{v\mu}\left(\frac{1}{R_\mu} - \frac{1}{R_v}\right) \quad ...(2)$$

With *v=1,2....$N_G$* and $N_G$ being the total number of grains, this expression represent a system on $N_G$ differential equation for the unknown $R_v(t)$. However, because of the large numbers of grains $N_G$ and thus a large number of equation is necessary to obtain a significant simulation, this leads to a great computational difficulties. Therefore, with the second and third simplifying assumptions will be easy to overcome these difficulties:

- 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 would have the same surrounding, also their growth rate would be equal. This means that then 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. In the following these classes will be denoted by the indices *i, j…*$N_s$ being the total number of classes. From the mathematical point of view the simplifcation consists in replacing in Equation (3) the individual contact area $s_{v\mu}$ by averaged area $a_{ij} = A_{ij}/n_j$ , $n_j$ is the total number of grains in class *j* and $A_{ij}$ is the total area of contact between the two classes *i* and *j*. Then, it follow that:

$$\frac{dR_i}{dt} = \frac{M}{4\pi {R_i}^2}\sum_{j=1} a_{ij}\left(\frac{1}{R_j} - \frac{1}{R_i}\right) \quad ...(3)$$

- A random array of the grains namely the probability of contact among the grains is only depending on their relative surface in the system. In this case the area of a grain of the class *i* is divided between the neighbouring grains of the class *j* inproportion to the individual surface area:

$$a_{ij} = 4\pi R_i^2 \frac{n_j 4\pi R_j^2}{\sum_j n_j 4\pi R_j^2} \quad ...(4)$$

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

$$\frac{dR_i}{dt} = M\sum_j\left(\frac{1}{R_j}-\frac{1}{R_i}\right)\frac{n_j 4\pi R_j^2}{\sum_j n_j 4\pi R_j^2} \quad ...(5)$$

Where $M = 2m\gamma$ is again the boundary diffusivity and in our case study *m* was evaluated according to the Stokes-Einstein relationship[11]:

$$m = \frac{D}{k_B T} = \frac{D_0}{k_B T} e^{\frac{-\Delta E}{k_B T}} \quad ...(6)$$

Where D is the diffusion coefficient, KB is the Boltzmann constant, ΔE is the activation energy of the process and T is the annealing temperature. D was chosen proportional to the diffusion coefficient of Fe in Fe-γ.

According to Zener[7], particles cause inhibition of grain boundary motion which can be considered as a retarding forces acting homogeneously along the moving boundary and has a similar behaviour of a frictional forces. In order to apply this description to grain growth phenomena has to be taken into account the magnitude of this force PZ. In fact, for a small external driving force P no motion of the boundary takes place. Only if external force surpasses a maximum force $I_{Z0}$ the particles can exert, the boundary moves, but with a net driving force $\Delta P=P-I_{Z0}$. This lead to three ranges for this net force acting on boundary[12]:

$$\begin{aligned}&\Delta P=P-I_{Z0} \text{ for } P> I_{Z0}\\ &\Delta P=0 \text{ for } I_{Z0} < P< I_{Z0}\\ &\Delta P=P+I_{Z0} \text{ for } -I_{Z0}> P\end{aligned} \quad ...(7)$$

For the maximum Zener force $I_{Z0}$ the will be used the usual expression where $f_p$ is the volume fraction and $r_p$ is the mean radius of the particles; β is a proportional constant in the range of 0.75-1.

$$I_{Z0}=\beta\gamma(f_p/r_p) \quad ...(8)$$

With equation (7) and (8), one obtains the net force $\Delta P_{ij}$ in the three ranges:

$$\begin{aligned}&\Delta P_{ij}(I) = \gamma\left(\frac{1}{R_j}-\frac{1}{R_i}-I_{Z0}\right) && \frac{1}{R_j} > \frac{1}{R_i}+I_{Z0}\\ &\Delta P_{ij}(II) = 0 && \frac{1}{R_i}+I_{Z0} > \frac{1}{R_j} > \frac{1}{R_i}-I_{Z0}\\ &\Delta P_{ij}(III) = \gamma\left(\frac{1}{R_j}-\frac{1}{R_i}+I_{Z0}\right) && \frac{1}{R_j} < \frac{1}{R_i}-I_{Z0}\end{aligned} \quad ...(9)$$

Therefor the growth rate for each class i can be derived as:

$$\frac{d\,R_i}{dt} = M\left[\begin{aligned}&\psi_I\cdot\left(\frac{1}{R_C^I}-\frac{1}{R_i}\right)+\psi_{III}\cdot\left(\frac{1}{R_C^{III}}-\frac{1}{R_i}\right)\\&-(\psi_I-\psi_{III})\cdot I_{Z0}\end{aligned}\right]$$

Where:

$$\psi_\lambda = \frac{\sum_\lambda \varphi_j R_j^2}{\varphi_j R_j^2} \quad ...(11)$$

$$\frac{1}{R_c^\lambda} = \frac{\sum_\lambda \varphi_j R_j}{\sum_\lambda \varphi_j R_j^2} \quad ...(12)$$

To describe the recrystallization process integrated with the grain growth, it is necessary to propose an extended growth equation that allows to contemporarily and continuously analyse the evolution of free nuclei in the matrix passing through partially impinged grains up to full contact. Was introduce an “influence mean radius” that allow to evaluate the fraction of surface in contact between different grain [13].

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

$$\frac{dR_i}{dt} = m[(\frac{Gb^2}{3}\Delta\rho-\frac{2\gamma}{R_i})\sum_{j=1}^{i^*-1} v_j] + \gamma\left[\psi_I\cdot\left(\frac{1}{R_C^I}-\frac{1}{R_i}\right)\right.$$

$$\left.+\psi_{III}\cdot\left(\frac{1}{R_C^{III}}-\frac{1}{R_i}\right)-(\psi_I-\psi_{III})\cdot I_{Z0}\right] \quad ...(13)$$

Where G is the shear modulus of the material, b is the Burger vector, ρ is the dislocation density, $\Delta\rho=\rho d-\rho r$ is the difference between the dislocation densities in the deformed and in the recrystallized material. The dislocation density ρ was considered proportional to the cold reduction rate and the initial numbers of nuclei N is a free parameter of the model that change in relations to reduction rate. The criterion for identifying the critical class is obtained by defining an average influence volume, and consequently an influence radius Rm, calculated as follows:

$$V_M = \frac{1}{N_T} - \sum_{i=1}^{n}\frac{n_i v_i}{N_T} = \frac{1}{N_T}(1-F_V) \quad ...(14)$$

$N_T$ is the numbers of grain per $cm^3$ , $F_V$ is the recrystallized volume fraction and viis the volume of the grain of the class and $n_i$ is the number of grains of volume $v_i$ . $R_m$ varies from $(3/(4\pi N_T)^{1/3})$ to zero when all the grain are in contact. Then $R_m$ parameter define an index i* that discriminates the class over which all the grains are in contact[13].

## RESULTS and DISCUSSIONS

### Annealing temperature effect

One of the free input parameters of the model is the annealing temperature deeply influencing the mobility parameters m and consequently affecting the grain size and the recrystallized volume fraction. Four temperatures, ranging from 700°C to 1100°C, have been investigated and reduction rate ε, dislocation density Δρ and the number of nuclei N was maintained constant. The effect of annealing temperature on grain size is reported in Figure 1. Results show that the mean radius size decreases with decreasing temperature because due to a decrease of the mobility parameters from 3.16e-11 erg/cm2 at 1100°C to 3.23e-14 erg/cm2 at 700°C, according to Equation 6. Results also show that a minimum temperature of 700°C is required in order to activate grain growth.

Also, the recrystallized volume fraction (Figure 2), reach for the two temperatures 1100°C and 1000°C the unitary value respectively in 13 seconds and 49 second and for the other two temperatures this value is never reached.

**Table 1: Dislocation density and initial number of nuclei used as input parameters in the simulations**

| Cold reduction grade ε | Δρ | N |
|---|---|---|
| 40% | 3 x$10^{10}$ $cm^{-2}$ | 4x$10^{9}$ $cm^{-3}$ |
| 60% | 5 x$10^{10}$ $cm^{-2}$ | 7x$10^{9}$ $cm^{-3}$ |
| 80% | 1 x$10^{11}$ $cm^{-2}$ | 1x$10^{10}$ $cm^{-3}$ |

### Reduction rate effect

For industrial purposes and for the statistical model, the reduction rate is one of the most important parameters and in Table 1 the different values used for the computer simulation are shown. The effect of reduction has been exploited by varying the reduction rate ε (at constant temperature equal to 1110°C) jointly to the dislocation density, according to Table 1.

The simulation results confirm that if cold reduction is varied from 40% to 80%, mean radius increase about 4%. This could be explained considering that higher values of deformations introduce in the structure more deformation micro-cells (nuclei *N*) that could increase less their size due to the excessive proximity of neighboring nuclei.

### Zener drag effect

Three different value of Zener parameter has been tested maintaining temperature (T=1100°C), reduction rate (ε=80 %) and dislocation density (Δρ=1x$10^{11}$ $cm^{-2}$) fixed. The comparison between the mean radius curve (over time) obtained by grain growth simulation without Zener effect and the other curves are shown in Figure 4. At the highest Zener parameter Iz=1000 a reduction of the maximum

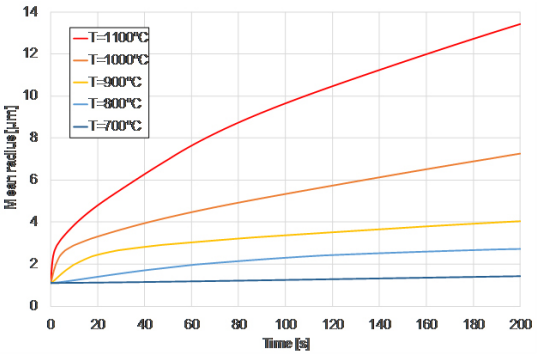


**Fig. 1: Mean radius over time for four different annealing temperature**

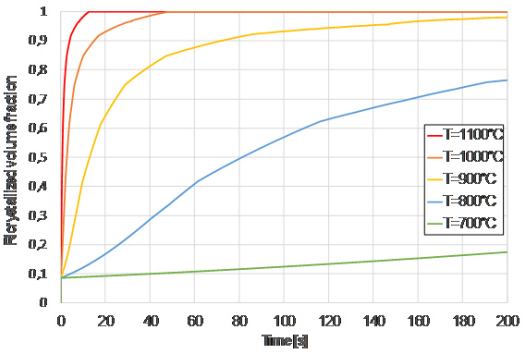


**Fig. 2: Recrystallized volume fraction over time for four different temperatures**

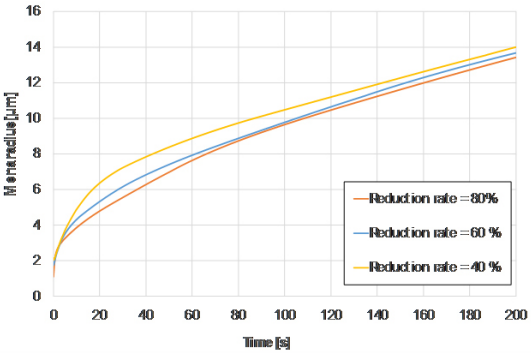


**Fig. 3: Mean radius over time for three different reduction rate**

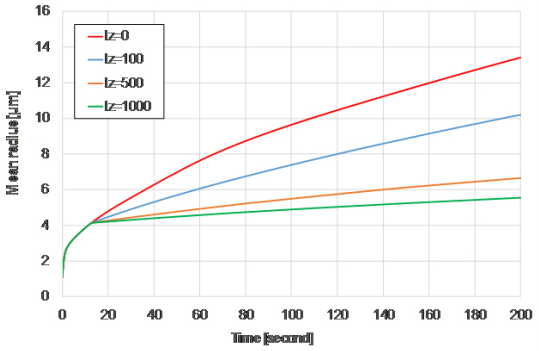


**Fig. 4: Mean radius over time for three different values of Zener parameter**

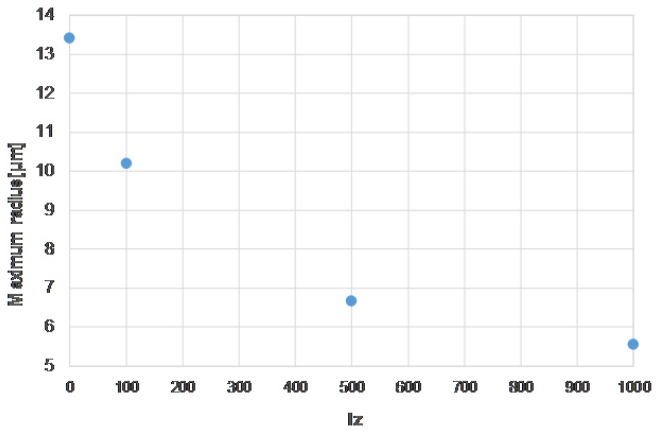


**Fig. 5: Maximum mean radius in relation with different Zener parameters**

mean radius is clearly visible and is equal to 41.39 % and in Figure 5 the maximum mean radius values in relation with Zener parameter are reported.

## CONCLUSION

Results from a recrystallization and grain growth model based on statistical assumption have been here discussed. In particular, the effect of the annealing temperature, dislocation density and Zener parameter have been analyzed. Results show that:

- mean radius size decreases with decreasing temperature because due to a decrease of the mobility parameters;
- mean radius increase about 4% with cold reduction variation in the range 40% to 80%;
- the model is able to take into account Zener effect.

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