MODELING OF STATIC RECRYSTALLIZATION IN ALLOYED AUSTENITE WITH ACCOUNT OF RECOVERY

[1]Alexander VASILYEV, [2]Semen SOKOLOV, [2]Dmitry SOKOLOV, [1]Alexandr ZISMAN

[1]*Peter the Great St. Petersburg Polytechnic University, Institute of Applied Mathematics and Mechanics, St. Petersburg, Russian Federation, vasilyev_aa@mail.ru*
[2]*PJSC Severstal, Cherepovets, Russian Federation, sok_s_w@mail.ru*

Abstract

To predict kinetics of static recrystallization with account of recovery and resulting grain size in alloyed austenite, a quantitative model is developed. Physically motivated, the model relates activation energy of the process with that of bulk self-diffusion. The known dependence of the latter on chemical composition of austenite solid solution, established previously, essentially simplifies the modeling. Employed empirical parameters have been fitted to relevant data covering a wide range of chemical compositions (12 steels) and sizes of recrystallized austenite grains. The model satisfactorily complies with experiments on steels whose apparent activation energy of recrystallization varies from 146.1 to 308.1 kJ/mol. It is notable as well that this performance has been achieved with no direct allowance for the pinning of grain boundaries by solute atoms (solute drag effect).

Keywords: Austenite, recrystallization, recovery, kinetics, modeling

1. INTRODUCTION

An important effect of static recrystallization on the austenite structure of hot rolled steels attracts a persisting interest [1-7]. To simulate this phenomenon, the Kolmogorov-Johnson-Mehl-Avrami (KJMA) equation is widely applied. Predictions by related models [1,2,4] satisfactorily comply with experiments at high temperatures in a wide range of chemical compositions where all alloying elements are completely dissolved in austenite. At the same time, the KJMA equation hardly enables allowance for the recovery phenomenon that precedes and accompanies the recrystallization and thus consumes its driving force. Several attempts [5] have been undertaken to formulate physically based models simultaneously involving the recrystallization and recovery. Although promising results are achieved in this way, quantitative models of this type should be refined in order to predict the effect of chemical composition on recrystallization kinetics in austenite of complexly alloyed steels.

According to physics of diffusional lattice rearrangements at moving boundaries of recrystallized grains, this energy should be comparable to that of grain boundary self-diffusion. The latter parameter, in turn, correlates with the energy of bulk self-diffusion (AESD). With allowance for the physically motivated correlation between AESD and the activation energy of recrystallization, we will presume proportionality of these parameters where the former depends on chemical composition of steel [7]. This presumption has been previously verified [8] by successful modeling of the normal grain growth in austenite of complexly alloyed steels.

The present paper formulates a model allowing for interacting processes of recrystallization and recovery. Empirical parameters of the model have been fitted to literature data as well as our experimental data on austenite recrystallization kinetics in steels of various compositions.

2. MODEL DESCRIPTION

We determine first the so-called extended recrystallized volume $X_{ext}(t)$:

$$X_{ext}(t) = N_{rex} \frac{4\pi}{3} \bar{R}_{rex}^3(t) \tag{1}$$

N_{rex} - volume density of nuclei, $\bar{R}_{rex}(t)$ - average radius of new grains in time t after they nucleated

To evaluate velocity $V_G^{rex}(t)$ of moving recrystallized grain boundaries, the following expression is used:

$$V_G^{rex}(t) = M_{GB}^{rex} P_{rex}(t) \tag{2}$$

$M_{GB}^{rex} \equiv M_{GB}^{rex}(T, Y_{AE})$ - recrystallized grain boundary mobility

T - absolute temperate

$Y_{AE} = \{y_C, y_{Mn}, y_{Si}, ...\}$ - set of average fractions of the sites of substitution and interstitial sublattices occupied, respectively, by the atoms of substitution alloying elements and carbon

$P_{rex}(t)$ - driving pressure (force) of recrystallization

With equation (1) kept in mind and the form-factor of the order of unity included in N_{rex}, the extended recrystallized volume takes the form:

$$X_{ext}(t) = N_{rex} \left(\int_0^t M_{GB}^{rex} P_{rex}(\tau) d\tau \right)^3 \tag{3}$$

The actual recrystallized volume fraction $X(t)$ is expressed in terms of $X_{ext}(t)$ as follows:

$$X(t) = 1 - \exp\left(-X_{ext}(t)\right) \tag{4}$$

An appropriate estimate for the driving pressure is:

$$P_{rex}(t) \cong 0.5 \mu b^2 \rho_d(t) \tag{5}$$

$\rho_d(t)$ - dislocation density, μ - shear modulus, b - Burgers vector magnitude

The distribution of dislocations in constitutive grains of a deformed polycrystal is generally non-uniform. Specifically, their density near grain boundaries significantly exceeds that in grain cores. Accordingly, for the dislocation density in equation (5) we use:

$$\rho_d(t) = \alpha_{d1} \bar{\rho}_d(t) \left(1 + \alpha_{d1}^{-1} \exp\left(-\alpha_{d2} X(t)\right)\right) \tag{6}$$

$\bar{\rho}_d(t)$ - average dislocation density calculated with allowance for recovery, $\alpha_{d1}, \alpha_{d2} > 0$ - empirical parameters

Based on the general dependence for the dislocation contribution to work hardening $\Delta\sigma(t)$, calculated here with allowance for recovery (see equations (11), (12)), we use expression:

$$\bar{\rho}_d(t) = \left(\frac{\Delta\sigma(t)}{\alpha_\rho M \mu b} \right)^2 \tag{7}$$

$M = 3.1$ - Taylor factor, $\alpha_\rho \approx 0.15$

The temperature dependence of the shear modulus is here evaluated according to [5].

As noted above, the model assumes nucleation of recrystallized grains at initial grain boundaries of austenite. Thus, according to [5], the volume density of such nuclei takes the form:

$$N_{rex} = \frac{\alpha_{rex}^* P_{rex}^2 (t = 0)}{D_{\gamma 0}} \tag{8}$$

$D_{\gamma 0}$ - average diameter of initial austenite grains, α_{rex}^* - empirical parameter

With α_{rex}^* including the geometrical factor of the order of unity in equation (8), we estimate the average grain size in the recrystallized structure as follows:

$$D_{rex} = N_{rex}^{1/3} \tag{9}$$

When considering recrystallized grains, mobility of their boundaries is treated like that in the normal grain growth [9]:

$$M_{GB}^{rex}\left(T; Y_{AE}\right) = M_0^{rex} \exp\left(\frac{S_{GG}^{rex}(Y_{AE})}{R_g}\right) \exp\left(-\frac{Q_{GG}^{rex}(Y_{AE})}{R_g T}\right) \tag{10}$$

$Q_{GG}^{rex}(Y_{AE})$ and $S_{GG}^{rex}(Y_{AE})$ - activation energy and entropy of the grain growth, M_0^{rex} - empirical parameter, R_g - gas constant

According to [8], activation entropy proportional to the corresponding energy will be treated with fitting parameter β_{GG}, i.e. $S_{GG}(Y_{AE}) = \beta_{GG} Q_{GG}(Y_{AE})$. Present model presumes that $Q_{GG}^{rex}(Y_{AE}) = \alpha_{GG}^{rex} Q_{SD}(Y_{AE})$, where $Q_{SD}(Y_{AE})$ is AESD in solid solution of complexly alloyed austenite calculated according to [7] and α_{GG}^{rex} is an empirical parameter.

According to [9], the recovery responsible for the material softening is ascribed first to gradual annihilation of dislocations, i.e. reduction of their density. This effect is expressed by:

$$\frac{d\Delta\sigma(t)}{dt} = -\frac{64\Delta\sigma(t)^2 v_d}{9M^3\alpha_\rho^2 E(T)}\exp\left(-\frac{U_{rec}}{R_g T}\right)\sinh\left(\frac{\Delta\sigma(t)V_{rec}}{k_B T}\right) \tag{11}$$

U_{rec} and V_{rec} - activation energy and activation volume of the recovery process, v_D - Debye frequency set to be 2 x 10^{12} s^{-1}, $E(T) = 2.6\mu(T)$ - Young modulus, k_B - Boltzmann constant

To integrate equation (11), the following initial condition is used:

$$\Delta\sigma(t = 0) = \sigma - \sigma_y \tag{12}$$

σ - deforming stress of austenite, dependent on temperature and plastic strain rate according to [7]

$\sigma_y \equiv \sigma_{0.2}$ - yield stress of austenite similarly calculated at its plastic strain of 0.2%

3. MODEL CALIBRATION AND DISCUSSION OF MODELING RESULTS

Model parameters were found while assuming that atoms of all alloying elements are completely dissolved in austenite. All the parameters are fitted to wide experimental data on austenite recrystallization in a wide range (12 steels) of chemical composition listed in **Table 1**. The table involves both the authors' results (steels S8-S10) and literature data [1-4,6].

Table 1 Chemical composition (wt%) of steels employed in model calibration

Steel	C	Mn	Si	Cr	Ni	Mo	Nb	V	Ti	Ref.
S0	0.17	0.74	0.01	–	–	–	–	–	–	[3]
S00	0.05	1.88	0.04	–	–	0.49	0.048	–	–	[6]
S1	0.11	0.55	0.26	–	–	–	–	–	–	[1,2,4]
S2	0.53	0.71	0.21	–	–	–	–	–	–	
S3	0.42	0.79	0.27	–	–	0.18	–	–	–	
S4	0.44	0.79	0.23	–	–	0.38	–	–	–	
S5	0.11	1.32	0.24	–	–	–	0.070	–	–	
S6	0.12	1.10	0.24	–	–	–	–	0.07	–	
S7	0.15	1.25	0.27	–	–	–	–	–	0.017	
S8	0.08	1.47	0.20	–	–	0.19	0.042	0.06	0.010	Own results
S9	0.04	1.90	0.25	0.11	0.45	0.31	0.051	0.02	0.020	
S10	0.11	0.36	0.23	0.39	1.91	0.31	0.011	0.01	–	

To determine an important parameter α_{rex}^*, equation (9) for the recrystallized grain size has been fitted to experimental data on steels S0 [3] and S00 [6]. The resulting $\alpha_{rex}^* = 8.6$ x 10^{-4} m^2 N^{-2} satisfactorily complies with these data covering practically significant ranges of temperature and strain degree of austenite. Other parameters have been fitted to wide data on austenite recrystallization kinetics in steels S1-S10 at relatively high temperatures where atoms of all alloying elements are in solid solution. Parameters of equation (10) for the boundary mobility are $\alpha_{GG}^{rex} = 0.64$, $\beta_{GG}^{rex} = 4.33$ x 10^{-4} K^{-1} and $M_0 = 5.4$ x 10^{-11} m^3 s^{-1} N^{-1}. Besides, $U_{rec} = 248000$ J/mol and $V_{rec} = 35b^3$ are used for the recovery activation energy and activation volume, respectively.

Kinetics of austenite recrystallization in steels S1-S10, as well as corresponding experimental data are represented in **Figure 1a-h** evidencing that derived parameters provide good prediction power of the model in a wide range of temperature (900÷1150 °C), chemical composition (**Table 1**), initial grain size (30÷190 μm) and deformation conditions (ε = 0.20÷0.35; dε/dt = 0.5÷3.6 s^{-1}).

Note that obtained $\alpha_{GG}^{rex} = 0.64$ confirms, as expected, that effective activation energy $Q_{GG}^{rex}(Y_{AE})$ for migration of recrystallized grain boundaries is comparable to that for the grain boundary self-diffusion. The range of chemical composition where the model displays good performance corresponds to a significant variation of $Q_{GG}^{rex}(Y_{AE})$ between 146.1 kJ/mol (S2) and 308.1 kJ/mol (S9). It is remarkable as well that the considered activation energy suggests a novel approach to the grain boundary mobility depending on the chemical composition of austenite, provided alloying elements are completely dissolved. Specifically, unlike the classical model of «solute drag effect» [10] or the later «statistical solute-pinning theory» [11], the present model enables reasonable predictions with no explicit allowance for any pinning by solute atoms. This is rather surprising insofar as the considered steels contain high amounts of Mn, Mo and Nb to which the solute drag is commonly ascribed [6].
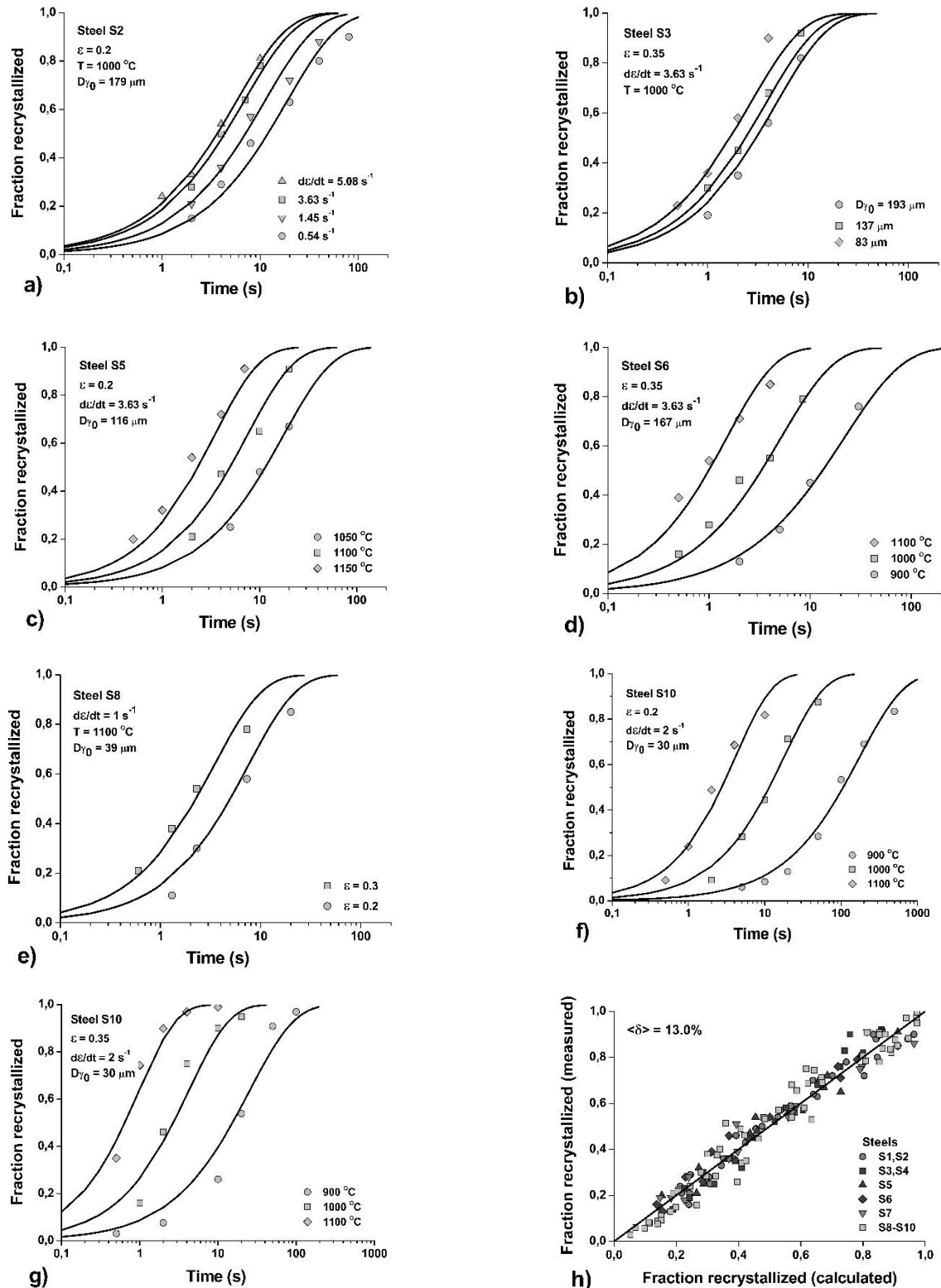
Figure 1 Comparison of simulated recrystallization kinetic curves (a-g) for steels S1-S10 at different temperatures, sizes of the initial austenite grain ($D_{\gamma 0}$) and deformation parameters (ε, dε/dt) to experimental data (symbols), and comparison of model predictions to actual recrystallized fractions (h) ($<\delta>$ is a magnitude of the average relative error)

4. CONCLUSIONS

A physically motivated model is formulated to predict the static recrystallization kinetics of austenite and the resulting grain size in complexly alloyed steels. The model simultaneously treats the interrelated phenomena of recrystallization and recovery. It is presumed that activation energy of the process is proportional to the activation energy of bulk self-diffusion, the latter being dependent on chemical composition of solid solution according to the previously established empirical expression.

Empirical parameters of the model were fitted to an extensive database on the kinetics of austenite recrystallization for 12 steels with a wide range of chemical composition in the case of complete dissolution of alloying elements including microalloying ones.

As shown in this work, the proposed model of austenite recrystallization complies well with experiments on numerous steels in a wide range of temperature, chemical composition, initial grain size and deformation conditions. The process activation energy in the considered range of chemical compositions vary by more than two times (146.1 to 308.1 kJ/mol). An interesting property of the model is that good correspondence to experimental data is achieved with no explicit allowance for the boundary pinning by dissolved atoms although the treated steels contain Mn, Mo and Nb to which the pronounced solute drag effect is commonly ascribed.

REFERENCES

[1] MEDINA, S.F., MANCILLA, J.E. Influence of alloying elements in solution on static recrystallization kinetics of hot deformed steels. *Iron and Steel Institute of Japan International*. 1996, vol. 36, no. 8, pp. 1063-1069.

[2] MEDINA, S.F., MANCILLA, J.E. Static recrystallization modelling of hot deformed steels containing several alloying elements. *Iron and Steel Institute of Japan International*. 1996, vol. 36, no. 8, pp. 1070-1076.

[3] SUN, W.P., MILITZER, M., HAWBOLT, E.B., MEADOWCROFT, T.R. Austenite grain refinement and growth during the thermomechanical processing of steels. In: Chandra T. et al. (ed.) *Thermec'97*. Warrendale: TMS. 1997, pp. 685-691.

[4] MEDINA, H.S., QUISPE, A. Improved model for static recrystallization kinetics of hot deformed austenite in low alloy and Nb/V micro-alloyed steels. *Iron and Steel Institute of Japan International*. 2001, vol. 41, no. 7, pp. 774-781.

[5] ZUROB, H.S., HUTCHISON, C.R., BRECHET, Y., PURDY, G. Modelling recrystallization of microalloyed austenite: effect of coupling recovery, precipitation and recrystallization. *Acta Materialia*. 2002, vol. 50, pp. 3075-3092.

[6] SARKAR, S., MOREAU, A., MILITZER, M., POOLE, W.J. Evolution of austenite recrystallization and grain growth using laser ultrasonics. *Metallurgical and Materials Transactions A*. 2008, vol. 39, pp. 897-907.

[7] VASILYEV, A.A., SOKOLOV, S.F., KOLBASNIKOV, N., SOKOLOV, D.F. Effect of alloying on the self-diffusion activation energy in γ-iron. *Physics of the solid state*. 2011, vol. 53, no. 11, pp. 2194-2200.

[8] VASILYEV, A.A., SOKOLOV, S.F., SOKOLOV, D.F., KOLBASNIKOV, N. Modeling of grain growth kinetics in complexly alloyed austenite. *Letters on Materials*. 2019, vol. 9, no. 4, pp. 419-423.

[9] VERDIER, M., BRECHET, Y., GUYOT, P. Recovery of AlMg alloys: flow stress and strain-hardening properties. *Acta Materialia*. 1999, vol. 47, no. 1, pp. 127-134.

[10] CAHN, J.W. The impurity-drag effect in grain boundary motion. *Acta Metall*. 1962, vol. 10, no. 9, pp. 789-798.

[11] HERSENT, E., MARTHINSEN, K., NES, E. A solute pinning approach to solute drag in multi-component solid solution alloys. *Modeling and Numerical Simulation of Material Science.* 2014, vol. 4, no. 1, pp. 8-14.