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Determination of static recrystallization and recovery parameters for steel by fitting model to stress relaxation data

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Abstract. A model for static recrystallization by Zurob et al. [1] has been fitted to experimental stress relaxation [2] data obtained on a low-alloyed steel using a Gleeble thermomechanical simulator. The model has been implemented as an algorithm that calculates the stress relaxation as a function of time, including physical descriptions of the recovery and recrystallization processes. The activation energy and volume were used as fitting parameters for recovery, and the activation energy of diffusion and nucleation site density were used as the fitting parameters for recrystallization. The four fitting parameters were determined from the experimental data by applying the Nelder-Mead algorithm within Matlab software. It can be concluded from the preliminary results that Zurob’s model can be successfully fitted to the stress relaxation data in order to illustrate the static restoration characteristics and kinetics in carbon steels using these fitting parameters.

1. Introduction

In order to control the microstructural evolution during thermomechanical processing, computational models are needed to accurately capture the microstructural phenomena that occur during processing. In the hot rolling of steel, during the interpass time between the rolling passes, both static recovery and static recrystallization take place. Since the resulting austenite microstructure affects the phase transformation occurring during the subsequent cooling and the resultant mechanical properties, computational models provide a way to simulate and optimize the processing conditions that lead to the desired outcome.

Although recovery dominates stress relaxation immediately after deformation and recrystallization mainly dictates stress relaxation at longer times, there is a noticeable overlap of the two phenomena in the intermediate time scales. One of the methods of determining the time dependence of recrystallization is stress relaxation testing, where the time region of recrystallization is interpreted from the shape of a stress relaxation curve. The fraction of recrystallization is determined by separating the recovery and recrystallization and fitting the corresponding part of the curve with an Avrami type function [2]. On the other hand Zurob et al. presented a coupled model to describe simultaneously occurrence of recovery, recrystallization and precipitation [1]. In the current study, we focus our attention on an implementation of the Zurob’s model of recrystallization and recovery by fitting the model parameters to stress relaxation data.
2. Experiments
A Gleeble 3800 thermomechanical simulator coupled with a Hydrawedge module was used to carry out the stress relaxation experiments on a low-alloy steel of the following composition (in wt.%): 0.16 C, 0.97 Mn, 0.33 Si, 0.22 Mo, 0.009 V, 0.001 Nb. Cylindrical test specimens of the dimensions φ 10 x 12 mm were first reheated at 10 °C/s to 1200 °C, held for 5 minutes, followed by cooling at 2 °C/s to the temperature at which the samples were deformed and relaxed for 200 s before subsequently quenching to room temperature. The deformation temperatures were 950, 1000 and 1050 °C and the strain rates were 1 and 10/s and strains were 0.2, 0.3 and 0.4.

3. Modelling and simulation
In order to concisely describe the model and the constructed algorithm, the nomenclature, constants and function definitions of the model are given in tables 1 and 2, while the initial conditions and the algorithm are presented with the flow charts shown in figures 1 and 2.

Table 1: Nomenclature and constant values used in the model [1,3–6]

| Symbol | Description                                                                 |
|--------|-----------------------------------------------------------------------------|
| $\sigma_{\text{rec}}(t)$ | The recovery stress, i.e. the stress as function of time due to recovery only |
| $\sigma_{\text{gg}}(t)$ | The stress as function of time due to grain growth only                      |
| $\sigma_{\text{rel}}(t)$ | The relaxation stress, i.e. the stress as function of time due to recovery, recrystallization and grain growth processes |
| $\nu_d$ | Debye frequency                                                             |
| $M_T$ | 3.1 Taylor factor                                                           |
| $\alpha_r$ | 0.15 Constant                                                               |
| $U_B$ | Activation enthalpy of recovery (fitting parameter)                         |
| $V_d$ | Activation volume of recovery (fitting parameter)                           |
| $\rho$ | Dislocation density                                                         |
| $\sigma_y$ | Yield stress of fully recrystallized material                              |
| $b$ | 2.5 Å Length of the Burgers' vector                                         |
| $G$ | Driving force of recrystallization                                          |
| $A_c$ | Area of single nucleus on the grain boundary                                 |
| $\gamma_{\text{gb}}$ | Grain boundary energy                                                       |
| $N_{\text{rec}}$ | Number of recrystallization nuclei per unit volume                          |
| $k$ | Geometrical factor (fitting parameter)                                       |
| $S_s$ | Surface to volume ratio (fitting parameter)                                 |
| $M_{\text{pure}}$ | Grain boundary mobility for pure iron                                       |
| $\delta$ | 0.5 nm grain boundary width                                                 |
| $D_{\text{gb}}$ | 6.35×10^{-15} Self diffusion constant for iron grain boundary [3]          |
| $D_{\text{gb}}$ | Self diffusion coefficient for austenite grain boundary                     |
| $Q_F$ | 55.7 kJ/mol Activation energy of self diffusion [3]                         |
| $V_{mFe}$ | 55.845×10^{-3} / $\rho_V$ Molar volume of iron, $\rho_V$ is the temperature dependent density of austenite calculated according to [4] |
| $E$ | Modulus of elasticity (temperature dependent, calculated according to [6]) |
| $\mu$ | $\frac{3}{2}E$ Shear modulus                                               |
| $R$ | 8.3145 J/mol Universal gas constant                                         |
| $k_B$ | 1.3807×10^{-23} Boltzmann constant                                          |
| $Q_d$ | Grain boundary mobility                                                     |
| $Q_F$ | Activation energy for the diffusion of alloying elements (fitting parameter) |
| $f(t) = \int_0^t M_{\text{gb}}(t')G(t')dt'$ | Integral                                                                     |
| $X_{\text{rec}}$ | Fraction of recrystallized volume                                           |
Table 2: The equations applied in the calculation of recovery, recrystallization and relaxation [1,3,5]

\[
\frac{d\sigma_{rec}}{dt}(t, T, \sigma_{rec}) = \frac{6p(\sigma_{rec}-\sigma_{y})^3}{9M_c\sigma_{y}^2E} \exp \left( -\frac{U_{y}}{k_B T} \right) \sinh \left( \frac{(\sigma_{rec}-\sigma_{y})R_{y}}{k_B T} \right)
\]

\[
\rho(t, \sigma_{rec}) = \left( \frac{\sigma_{rec}-\sigma_{y}}{M_c\sigma_{y}} \right)^3
\]

\[
G(t, \rho) = \frac{\rho}{\rho_{y}^2}
\]

\[
A_c(G) = 4\pi \left( \frac{\nu_{gb}}{G(t)} \right)^2
\]

\[
\gamma_{gb} = 1.3115 - 0.0057T
\]

\[
N_{\text{rel}}(k, S, \nu, \rho) = \frac{\rho S}{A_c}
\]

\[
M_{\text{pure}}(t, T) = \frac{10^6 D_{gb} \nu_{max}}{10^8 R_g T} \quad [1], \text{where} \quad D_{gb} = D_{gb0} \exp \left( -\frac{Q_{gb}}{k_B T} \right) \quad [3]
\]

\[
M_{gb}(t, T, M_{\text{pure}}) = M_{\text{pure}} \exp \left( -\frac{Q_{gb}}{k_B T} \right)
\]

\[
l(t, M_{gb}, G) = \int M_{gb}(t') G(t') dt'
\]

\[
X_{\text{rec}}(t, I) = 1 - \exp \left( -N_{\text{rel}} I^2 \right)
\]

\[
\sigma_{\text{rel}}(t, X_{\text{rec}}, \sigma_{gb}) = (1 - X_{\text{rec}}(t)) \sigma_{\text{rec}}(t) + X_{\text{rec}}(t) \sigma_{gb}(t)
\]

\[
\sigma_{gb}(t) = \sigma_{y} + b \log_{10}(t) \quad \text{(function fitted to relaxation (t > 10 s) data, } \sigma_{y} \and b \text{ are fitting parameters)}
\]

Slightly differently to Zurob’s model, the temperature dependent Debye frequency \( \nu = \left( \frac{6\pi \nu N}{V} \right)^{1/3} \) [7] was calculated using values for unit cell volume \( V \) [8] (number of atoms / unit cell \( N = 4 \)) and the speed of sound \( v = \sqrt{E/\rho_{y}} \), which is in turn calculated using the elastic modulus \( E \) [6] and austenite density \( \rho_{y} \) [4], providing temperature dependent quantities instead of constant values. Also, the grain boundary mobility is calculated using \( M_{gb} = M_{\text{pure}} \exp \left( -\frac{Q_{gb}}{R_{y} T} \right) \), since Nb precipitation is not relevant for the current steel composition.

The initial definitions and the algorithm used for calculating the stress, recovery and relaxation as a function of time are presented as flow charts in figures 1 and 2, respectively.

![Flow chart of initial definitions](https://via.placeholder.com/150)

![Flow chart of algorithm](https://via.placeholder.com/150)

Figure 1: Initial definitions of the algorithm, which are calculated before the time loop described in figure 2.
Figure 2: Flowchart describing the algorithm used for calculating the relaxation stress as a function of time corresponding to the recovery, recrystallization and grain growth.

The fitting parameters used in the model were the activation enthalpy $U_a$ and activation volume $V_a$ of recovery, the activation energy for the diffusion of the alloying elements $Q_d$ and the product of $k$ and $S_Y$, which is proportional to the number of recrystallization nucleation sites. In order to obtain an evenly distributed amount of fitting points in the stress vs. $\ln t$ diagram, additional fitting points were created for $t < 1$ s by linearly interpolating the data between the measurement points. This ensured that for the fitting, the data in the stress vs. $t$ curve, when $t < 1$ s were equally emphasized as the data when $t > 1$ s. The lower bound of $5 \times 10^{-5}$ was set for parameter $k$ in the fitting, as proposed in [1].

4. Results and discussion

We implemented the model described in section 3 to simulate the recovery and recrystallization processes after deformation. The model was numerically fitted to the experimental data by applying
the Nelder-Mead algorithm [9], using the Matlab software *fminsearch* function [10]. The initial fitting parameters were \( U_a \) and \( V_a \) for the recovery and \( Q_d \) and \( kS_V \) for the recrystallization. The representative comparison of calculated vs. experimental data for some of the tests is shown in figure 3 a). The comparison of all the simulation results against the experimental data is shown in figure 3 b).

The fitted parameter values are given in table 3 for all the cases where fitting was successful. The results show that the implemented Žurob’s model describing the recovery and recrystallization can be adequately fitted to the experimental data using the chosen fitting parameters. It can be seen from the obtained parameter values that the parameter \( kS_V \) is significantly affected by the experimental conditions, while the variation of the other parameters is relatively small. Though small, a noticeable increase of activation volume can be seen with the decrease of strain.

The obtained values for the activation enthalpy \( U_a \) and activation energy \( V_a \) are close to the values used in [1]: \( U_a = 286 \times 10^3 \) J/mol and \( V_a = 45 \times 7.03 \times 10^{-28} \) m\(^3\). In [11], the effect of solute alloying elements on the apparent activation energy of recrystallization is described by \( Q_{\text{ ally}} = Q_0 + Q_{\text{ alloy}} \), where \( Q_0 = 148636.8 \) J/mol would be the activation energy in the absence of alloying and \( Q_{\text{ alloy}} = -71981.3(\%C) + 21180(\%Mn) + 56537.6(\%Si) + 121243.3(\%Mo) + 64469(\%V) + 109731.9(\%Nb)^{0.15} \). The calculated value according to [11] is then \( Q_{\text{ alloy}} = 93760 \) J/mol, which is very close to the values obtained for \( Q_d \) from our fitting shown in table 3. In [1] it is estimated that, the parameter \( k \) can vary between \( 5 \times 10^{-5} \) and \( 5 \times 10^{-2} \), where the former was used as a lower bound in the fitting in the current study. Assuming a reasonable value of \( S_V = 80 \times 10^3 \) 1/m implies that the product \( kS_V \) would vary between 4 and 4000, which is consistent with the fitted parameter values shown in table 3.
Table 3: Model parameter values obtained from fitting.

| 10/s, Temp 950 °C | Strain | U_a (J/mol) | V_a (m^3) | Q_d (J/mol) | kS_V (1/m) |
|-------------------|--------|-------------|-----------|-------------|------------|
| 0.2               | 3.05×10^5 | 9.17×10^{-28} | 1.18×10^5 | 4179.41     |
| 0.3               | 3.09×10^5 | 8.11×10^{-28} | 0.96×10^5 | 4.04        |
| 0.4               | 3.12×10^5 | 7.91×10^{-28} | 1.20×10^5 | 4769.55     |

| 1/s, Temp 950 °C | Strain | U_a (J/mol) | V_a (m^3) | Q_d (J/mol) | kS_V (1/m) |
|------------------|--------|-------------|-----------|-------------|------------|
| 0.2              | 3.09×10^5 | 8.99×10^{-28} | 1.17×10^5 | 3185.09     |
| 0.3              | 3.13×10^5 | 7.99×10^{-28} | 1.12×10^5 | 355.69      |
| 0.4              | 3.10×10^5 | 7.76×10^{-28} | 1.15×10^5 | 2093.75     |

| 10/s, Temp 1000 °C | Strain | U_a (J/mol) | V_a (m^3) | Q_d (J/mol) | kS_V (1/m) |
|-------------------|--------|-------------|-----------|-------------|------------|
| 0.2               | 3.07×10^5 | 9.14×10^{-28} | 0.893×10^5 | 4.04        |
| 0.3               | 3.01×10^5 | 7.01×10^{-28} | 0.903×10^5 | 4.04        |
| 0.4               | 2.95×10^5 | 5.72×10^{-28} | 1.06×10^5  | 565.88      |

| 1/s, Temp 1000 °C | Strain | U_a (J/mol) | V_a (m^3) | Q_d (J/mol) | kS_V (1/m) |
|------------------|--------|-------------|-----------|-------------|------------|
| 0.2              | 3.09×10^5 | 9.44×10^{-28} | 0.878×10^5 | 4.04        |
| 0.3              | 3.11×10^5 | 7.57×10^{-28} | 1.16×10^5  | 4882.72     |
| 0.4              | 2.95×10^5 | 4.73×10^{-28} | 1.07×10^5  | 1317.69     |

| 10/s, Temp 1050 °C | Strain | U_a (J/mol) | V_a (m^3) | Q_d (J/mol) | kS_V (1/m) |
|-------------------|--------|-------------|-----------|-------------|------------|
| 0.2               | 2.97×10^5 | 6.74×10^{-28} | 1.13×10^5 | 3088.08     |

| 1/s, Temp 1050 °C | Strain | U_a (J/mol) | V_a (m^3) | Q_d (J/mol) | kS_V (1/m) |
|------------------|--------|-------------|-----------|-------------|------------|
| 0.2              | 3.15×10^5 | 9.30×10^{-28} | 1.18×10^5 | 5998.31     |
| 0.3              | 3.01×10^5 | 5.01×10^{-28} | 1.13×10^5 | 3371.02     |

5. Conclusions
A model based on Zurob’s model was successfully fitted to data obtained from stress relaxation tests for different temperatures, strains and strain rates. The obtained model parameter values were in reasonable agreement with those found in literature. In future, the model will be fitted to larger set of experimental data in order to see the parameter dependence on different conditions, and we are planning to couple the model with finite element modelling in order to predict the recovery and recrystallization in different locations of deformed material.

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