Analysing mobility from austenite grain growth data

Winfried Kranendonk
Tata Steel, P.O. Box 10.000, 1970 CA IJmuiden, the Netherlands

Winfried.Kranendonk@tatasteeleurope.com

Abstract. To obtain information on mobility of grain boundaries in austenite grain growth data has been collected from the open literature, to fit a physics-based grain growth model, which relates the mean grain size to the annealing time. The suitability of this model for predicting the grain size as a function of time is discussed and some preliminary results on the reduced mobility are presented. For the compositions in the database it has been found that the activation energy ranges from 100 to 600 kJ/mol. Such high activation energies cannot be explained well with many solute drag models.

1. Introduction
Metallurgical models have an increasingly important role in product development and process control in modern steel production. Both performance and reduction of CO₂ emissions from cars nowadays drives the development of steels with higher strength, combined with a good formability. To meet these requirements, new steel grades, like Advanced High Strength Steels and modern HSLA steels lead to an increasing variety in chemical compositions and process conditions. Because of this large variety the preference is more for physics-based models rather than empirical models, because properly constructed physics-based models are in general more valid over a wide range of compositions and process parameters (temperatures, rolling reductions etc.) and are more reliable in extrapolation outside the validation range.

In the production of these new steel grades recrystallisation and grain growth are two metallurgical phenomena, which also determine the final microstructure and, hence, the mechanical properties of these steels. For modelling the grain growth and recrystallisation in metals, the mobility of grain boundaries is essential, because it relates the migration rate of the grain boundaries directly to the driving force. Thus, knowledge of the mobility is of great value for developing models, especially the relation between the mobility and the temperature and the chemical composition of alloys.

2. Aim of the project
Despite the importance of modelling the mobility, its research on even single-phase grain boundary migration for steel is quite limited. Most models on grain growth and recrystallisation are empirical [1-3]. Although several models for the role of solutes on mobility have been formulated [4-8] these models have hardly been tested for steel. The only known study is by Yogo et al [9, 10], who presented an analysis of Hillert’s model but tested it on a very small database.

This project aims to test and validate the solute drag theories, and mobility models in general, using data from the open literature. Here, a brief introduction will be given on the database, the methodology,
and some preliminary results. A more detailed analysis of the database and discussion of the results will appear in a later publication.

3. The database

Data on grain growth in austenite have been collected from the open literature, i.e. scientific journals and monographs. For the analysis of the mobility and testing the models only data are used where grain sizes were measured for several holding times under isothermal conditions. By far the most experimental data are only available in the form of plots. These figures were digitized and the time-grain size data points were extracted from the images.

Data have been taken from 23 sources. An impression of the database, which was used for the preliminary analysis as presented in these proceedings, is given in table 1. Because grain growth kinetics can be influenced by Zener pinning from precipitates, the information of the database has been split up with respect to the presence of precipitate forming elements.

Table 1. The statistics of the database, used for the analysis. Row 2 gives the overall information and rows 3 to 8 give more detailed information with respect to the presence of precipitate-forming elements.

| Composition                        | Number of compositions | Number of isotherms | Number of data points |
|------------------------------------|------------------------|---------------------|-----------------------|
| All compositions                   | 72                     | 309                 | 1815                  |
| Without Al, Nb, V, Ti              | 23                     | 83                  | 469                   |
| With only Al                       | 30                     | 141                 | 832                   |
| With Al + Nb                       | 4                      | 15                  | 109                   |
| With Al + V                        | 10                     | 48                  | 294                   |
| With Al + Ti                       | 2                      | 10                  | 50                    |
| With Nb, V and/or Ti, without Al   | 3                      | 12                  | 61                    |

4. The model

The model as proposed by Grey and Higgins was chosen to model the grain growth data [11]. The Grey-Higgins model is a mean value model, where the rate of the mean grain radius \( \bar{R}_g \) is related to a driving force, based on the mean radius and the mean grain boundary energy \( \gamma \). The mobility \( M \) is the proportional factor between the migration rate and the driving force. The time \( t \) is the isothermal annealing time. The model assumes that for very long times the mean grain size goes to a limit value \( R_{\text{limit}} \). Grey and Higgins formulated their model based on grain growth experiments in zone refined metals and diluted alloys, where all the experimental time-grain size curves tended to have a limit to a finite grain size.

\[
\frac{d\bar{R}_g}{dt} = 2 \cdot \gamma \cdot M \left( \frac{1}{\bar{R}_g} - \frac{1}{R_{\text{limit}}} \right)
\]  

This model is one of the simplest models, which still has a physical basis and the reduction of the evolution of the grain size distribution to one of a mean value guarantees a limited computing time. The reduced mobility \( (\gamma M) \), the limit grain size \( (R_{\text{limit}}) \) and the initial grain size were fitted for each isotherm (with a minimum number of 4 data points) using a least squares fit program, in which equation (1) was approximated numerically using a 4th order Runge-Kutta algorithm.
5. Preliminary results
Here, two preliminary results of the analysis are briefly discussed: the suitability of the Grey-Higgins model to describe the (literature) data and some examples of the reduced mobility as a function of the temperature.

5.1. Suitability of the model
The goodness-of-fit of the model is illustrated in figures 1 and 2 as representative examples. In most of the isotherms the Grey-Higgins model gives a good representation of the experimental data, especially for short times. For long times, however, the Grey-Higgins model predicts an asymptote for the grain size evolution. Data for long holding time are very rare: the only available data have been measured by Miller [13]; up to 5000 hours for some isotherms. One example of these data (steel 1) is replotted in figure 3 with the original double-logarithmic axes. Even after soaking for 300 hours no sign of an asymptotic behaviour is observed, so the Grey-Higgins model represents these experimental data less accurately, as is shown in figure 4, where the same data for steel 1 were used as in figure 3. The absence of an asymptotic value limits the use of the Grey-Higgins model to short times.

Figure 1. Isothermal grain growth data and model fit for a Mn-Ni-Cr-Mo steel (steel G) [3].

Figure 2. Isothermal grain growth data and model fit for a C-Mn steel (steel 1) [12].

Figure 3. The isothermal grain growth data for steel 1 with the double logarithmic axes as presented in [13].

Figure 4. The isothermal grain growth data and model fit for steel 1 from [13].
Short times are quantified here using the characteristic time, as defined by Grey and Higgins:

\[ t_{\text{char}} = \frac{\mu_{\text{limit}}}{2\gamma M} \]  

(2)

When \( t_{\text{max}} \) is the longest soaking time in an isotherm, the ratio \( \frac{t_{\text{max}}}{t_{\text{char}}} \) is a reasonable indicator for the applicability of the Grey-Higgins model: for values smaller than 10 a satisfactory goodness-of-fit for the Grey-Higgins model is found. Deviations between the experimental data and the model were found for ratios larger than 10, which only occur for the data of Miller [13].

5.2. The reduced mobility

The reduced mobility (equation (1)) has been estimated for each isotherm with more than 3 data points using a least squares fit. The reduced mobilities have been plotted as a function of the reciprocal of the temperature 1000/T for each composition; three examples are shown in figures 5 to 7. The compositions for these figures correspond to those in figures 1 to 4.

The reduced mobility versus 1/T plots can be well represented by an Arrhenius function for most compositions. Taking into account the estimated errors in the reduced mobility the logarithm of the reduced mobility is a linear function of 1/T:

\[ \gamma M = \gamma M_0 \exp \left( \frac{-Q}{RT} \right) \]  

(3)

However, some compositions deviate from a linear \( \ln(M) \) versus 1/T relation, and a further analysis of these cases has yet to be done.

The Arrhenius function (3) has been applied to all compositions with two or more isotherms and the pre-factor \( \gamma M_0 \) and the activation energy have been estimated from a (second) least squares fit. An overview of the \( \gamma M \) versus the activation energy of all compositions is given in figure 8.

Figure 5. The reduced mobility versus 1/T for steel 1 from ref. [13].

Figure 6. The reduced mobility versus 1/T for a Mn-Ni-Cr-Mo steel (steel G) [3].
6. Discussion and conclusions

This paper presents the preliminary results of an analysis on a collection of grain growth data in austenite. Most of the isotherms can be accurately represented by a model, which was proposed by Grey and Higgins, although data from one source indicates that this model fails for very long soaking times. A more severe test of the Grey-Higgins model for short times, namely a study of the distributions of the residuals as a function of time, has to be done yet.

For most of the compositions the reduced mobility can be described as an Arrhenius function of the temperature. However, the most remarkable finding is the large variety in the values for the activation energy of the mobility; they range from 100 kJ/mol to more than 600 kJ/mol (figure 8). Especially the very high values should be compared with the activation energies of the diffusivities of solutes (in the order of 250 kJ/mol), which enter the classical solute drag models of Cahn and Hillert [4, 5]. These models cannot, therefore, explain the highest activation energies for the reduced mobility, unless rather unrealistic values are used for the physical properties in these solute drag models. Alternative explanations are not available yet.

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References

[1] Lee S-J and Lee Y-K 2008 Prediction of austenite grain growth during austenitization of low alloy steels Materials and Design 29 1840-4
[2] Lee S-J 2013 Predictive model for austenite grain growth during reheating of alloy steels ISIJ International 53 (10) 1902-4
[3] Uhm S, Moon J, Lee C, Yoon J and Lee B 2004 Prediction model for the austenite grain size in the coarse grained heat affected zone of Fe-C-Mn steels: considering the effect of initial grain size on isothermal growth behavior ISIJ International 44 1230-7
[4] Cahn J W 1962 The impurity-drag effect in grain boundary motion Acta Metallurgica 10 789-98
[5] Hillert M and Sundman B 1976 A treatment of the solute drag on moving grain boundaries and phase interfaces in binary alloys Acta Metallurgica 24 731-43
[6] Machlin E S 1962 Theory of solute atom limited grain boundary migration *Transactions of the Metallurgical Society of AIME* 224 1153-67
[7] Hersent E, Marthinsen K and Nes E 2013 The effect of solute atoms on grain boundary migration: A solute pinning approach *Metallurgical and Materials Transactions A* 44 3364-75
[8] Westengen H and Ryum N 1978 On the effect of solute atoms on grain-boundary migration *Philosophical Magazine A* 38(3) 279-95
[9] Yogo Y, Tanaka K, Ikehata H, Iwata N, Nakanishi K and Ishikawa T 2011 Calculation for grain growth rate of carbon steels by solute drag model considering segregation effect of each substitutional element *Materials Science and Technology* 27 1593-8
[10] Yogo Y, Tanaka K, Ikehata H, Iwata N, Nakanishi K and Ishikawa T 2012 The solute drag model to calculate grain growth rate at high temperatures in carbon steels *Materials Science Forum* 706-709 1574-9
[11] Grey E A and Higgins G T 1973 Solute limited grain boundary migration: A rationalisation of grain growth *Acta Metallurgica* 21 309-21
[12] Kobayashi H 1977 Effect of vanadium and niobium on austenite grain growth kinetics in low carbon high strength steel *Tetsu-to-Hagane* 63 73-9
[13] Miller O O 1951 Influence of austenitizing time and temperature on austenite grain size of steel *Transactions of the American Society for Metals* 43 260-89