ANALYSIS OF THEORETICAL METHODS OF EVALUATION OF BAINITIC HARDENABILITY
OF STEELS

Maciej PIETRZYK, Roman KUZIAK

AGH University of Science and Technology, Krakow, Poland, EU, maciej.pietrzyk@agh.edu.pl
Institute for Ferrous Metallurgy, Gliwice, Poland, EU, rkuziak@imz.pl

Abstract

The phase transformation model was developed and applied to evaluate the hardenability of bainitic steels. The objective was to provide a tool, which will help designing the chemical composition of these steels with enhanced hardenability. Two general indexes, which are based on the relation between bainite volume fraction and cooling rate and which characterize the hardenability, were proposed. Calculations of these hardenability factors were performed for selected steels with different chemical compositions. Correlation between the chemistry and the hardenability factor was evaluated.

Keywords: bainitic steels, hardenability, phase transformation model

1. INTRODUCTION

Hardenability describes the capability of a steel to transform to a given microstructure in a heat treatment process. This has been most successfully applied to martensitic steels. On the contrary, bainitic hardenability remains difficult to define. During recent years, a new generation of bainitic steels with extensive perspective applications have been developed and there is a need for fast evaluation of hardenability of these steels [1]. The objective of the current work was to propose numerical methods of defining and assessing bainitic hardenability that could be easily applied in industrial practice. Development of the phase transformation model was the first step of the procedure. Modified Avrami equation was used as a model and coefficients of this model were identified on the basis of dilatometric tests and inverse analysis [2]. A series of low carbon low alloy steels have been subject to this procedure and hardenability of these steels was compared.

2. MODEL

The complete phase transformation model for steels describes kinetics of four transformations: ferritic, pearlitic, bainitic and martensitic. In the present paper the first three transformations, which are controlled by diffusion, are described by the Avrami type equation:

\[ X = 1 - \exp\left(-kt^n\right) \]  

where: \( X \) - volume fraction of a new phase, \( t \) - time

One of the coefficients \((k)\) is described as a function of temperature. The modified Gaussian function was suggested in [3] for the ferritic transformation:

\[ k = \frac{a_8}{D_\gamma} \exp\left(-\left(\frac{T - T_{nose}}{a_8}\right)^{a_9}\right) \quad T_{nose} = Aa_3 + \frac{400}{D_\gamma} - a_6 \]  

Coefficient \( k \) in equation (1) for pearlitic \( k_p \) and bainitic \( k_b \) transformations is:

\[ k_p = \frac{a_{14}}{D_\gamma a_{15}} \exp\left(a_{13} - \frac{a_{12}T}{100}\right) \]

\[ k_b = \frac{a_{14}}{D_\gamma a_{15}} \exp\left(a_{13} - \frac{a_{12}T}{100}\right) \]
\[ k_b = a_{23} \exp \left( a_{22} - \frac{a_{21}T}{100} \right) \]  

(4)

Incubation time was introduced for pearlitic \( \tau_p \) and bainitic \( \tau_b \) transformations:

\[ \tau_p = \frac{a_b}{(A\varepsilon_1-T)^{a_1}} \exp \left[ \frac{a_{10} \times 10^3}{R(T+273)} \right] \]  

(5)

\[ \tau_b = \frac{a_{18}k_b}{(B_\gamma-T)^{a_{18}}} \exp \left[ \frac{a_{18} \times 10^3}{R(T+273)} \right] \]  

(6)

Additional relationships in the model and equilibrium carbon concentrations are presented in table 1, where:

- \( c_\gamma \) – average carbon content in the austenite,
- \( c_\alpha \) – carbon content in the ferrite,
- \( c_0 \) – carbon content in the steel,
- \( c_{\gamma\alpha} \) and \( c_{\gamma\beta} \) – carbon concentration in the austenite at the \( \gamma-\alpha \) and \( \gamma-cementite \) boundary, respectively,
- \( X_{f0} \) – equilibrium ferrite volume fraction in steel.

Equilibrium concentrations \( c_{\gamma\alpha} \) and \( c_{\gamma\beta} \) as well as carbon content in the ferrite \( c_\alpha \), are introduced as temperature functions determined using ThermoCalc software.

Table 1. Additional equations in the phase transformation model.

<table>
<thead>
<tr>
<th>Equation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>( c_\gamma = \frac{(c_0 - X_f c_\alpha)}{1 - X_f} )</td>
<td>( X_{f0} = \frac{c_{\gamma\alpha} - c_0}{c_{\gamma\alpha} - c_\alpha} )</td>
</tr>
<tr>
<td>( c_{\gamma\alpha} = c_{\gamma\alpha0} + c_{\gamma\alpha1}T )</td>
<td>( c_{\gamma\beta} = c_{\gamma\beta0} + c_{\gamma\beta1}T )</td>
</tr>
<tr>
<td>( c_\alpha = f(T) )</td>
<td></td>
</tr>
</tbody>
</table>

The start temperatures for the bainitic (Bs) and martensitic (Ms) transformations are calculated as:

\[ B_s = a_{26} - 42.5[C] - 42.5[Mn] - 31.5[Ni] - 70[Cr] \]  

(7)

\[ M_s = a_{26} - a_{22}c_\gamma \]  

(8)

Fraction of austenite, which transforms into martensite is calculated using equation proposed in [4]:

\[ X_m = 1 - \exp \left[ 0.011(M_s - T) \right] \]  

(9)

Equation (9) represents volume fraction of martensite with respect to the whole volume of the austenite, which remained at the temperature \( M_s \). The volume fraction of martensite with respect to the whole volume of the material is:

\[ F_m = \left( 1 - F_f - F_p - F_b \right) \left[ 1 - \exp \left[ 0.011(M_s - T) \right] \right] \]  

(10)

where: \( F_f, F_p, F_b \) – fraction of ferrite, pearlite and bainite with respect to the whole volume of material.

In the ferritic transformation, the transformed volume fraction \( X_f \) is calculated with respect to the maximum volume fraction of ferrite \( X_{f0} \) in the current temperature. Thus, this volume fraction of ferrite with respect to the whole volume is \( F_f = X_f \times X_0 \). During simulations at the varying temperature the current value of \( X_f \) has to be corrected to account for the change of the equilibrium (maximum) volume of ferrite \( X_0 \). Simulation of the progress of transformation continues until the transformed volume achieves 1. However, when carbon content in austenite reaches the limiting value \( c_{\gamma\beta} \) (Table 1), the austenite-pearlite transformation begins in the remaining volume of austenite. Calculations of the transformed volume fraction \( X_f \) was performed using Avrami equation (1) and the additivity rule [4] was applied to account for the changes of temperature.
3. EXPERIMENT

The materials were bainitic steels with the chemical composition given in Table 2. The two steels in the last rows of the table (1037 and 1038) are with higher content of alloying elements. Dilatometric tests were performed for various cooling rates. The procedure included preheating at 1200°C for 600 s, cooling to 1050°C, plastic deformation at this temperature and further slow cooling to 850°C followed by controlled cooling with various cooling rates. It gave grain size of 30 μm at the beginning of transformations. The microstructure of samples before and after cooling was investigated. All the test data were used as an input for the inverse analysis, which was performed to identify the parameters in the phase transformation models.

Table 2. Chemical composition of the investigated bainitic steels, wght%.

<table>
<thead>
<tr>
<th>Steel</th>
<th>C</th>
<th>Mn</th>
<th>Si</th>
<th>Cr</th>
<th>Ni</th>
<th>Al</th>
<th>Cu</th>
<th>Nb</th>
<th>V</th>
<th>Ti</th>
<th>P</th>
<th>S</th>
<th>N</th>
</tr>
</thead>
<tbody>
<tr>
<td>1109</td>
<td>0.08</td>
<td>1.85</td>
<td>0.21</td>
<td>0.54</td>
<td>0.16</td>
<td>0.034</td>
<td>0.16</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>0.012</td>
<td>0.012</td>
<td>-</td>
</tr>
<tr>
<td>1210</td>
<td>0.074</td>
<td>2.0</td>
<td>0.1</td>
<td>0.1</td>
<td>0.034</td>
<td>0.1</td>
<td>0.038</td>
<td>-</td>
<td>0.13</td>
<td>0.012</td>
<td>0.012</td>
<td>0.0038</td>
<td></td>
</tr>
<tr>
<td>1218</td>
<td>0.046</td>
<td>1.46</td>
<td>0.3</td>
<td>-</td>
<td>0.53</td>
<td>0.02</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>0.014</td>
<td>0.009</td>
<td>0.0027</td>
</tr>
<tr>
<td>1260</td>
<td>0.045</td>
<td>1.46</td>
<td>0.31</td>
<td>-</td>
<td>0.3</td>
<td>0.022</td>
<td>0.4</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>0.01</td>
<td>0.01</td>
<td>0.003</td>
</tr>
<tr>
<td>1261</td>
<td>0.046</td>
<td>1.48</td>
<td>0.3</td>
<td>-</td>
<td>0.5</td>
<td>0.022</td>
<td>0.4</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>0.012</td>
<td>0.01</td>
<td>0.003</td>
</tr>
<tr>
<td>1037</td>
<td>0.1</td>
<td>2.05</td>
<td>0.24</td>
<td>2.07</td>
<td>-</td>
<td>0.006</td>
<td>-</td>
<td>-</td>
<td>0.19</td>
<td>-</td>
<td>0.011</td>
<td>0.013</td>
<td>0.0171</td>
</tr>
<tr>
<td>1038</td>
<td>0.09</td>
<td>2.02</td>
<td>0.2</td>
<td>1.89</td>
<td>1.93</td>
<td>0.005</td>
<td>-</td>
<td>-</td>
<td>0.19</td>
<td>-</td>
<td>0.011</td>
<td>0.013</td>
<td>0.0177</td>
</tr>
</tbody>
</table>

Thermodynamic parameters were determined using ThermoCalc program on the basis of the chemical composition of steel. Coefficients in equations (table 1) describing equilibrium carbon content at the γ-α and γ-cementite boundaries obtained by approximation of data from ThermoCalc are given in Table 3.

Table 3. Parameters of equations describing equilibrium content of carbon for the investigated steels.

<table>
<thead>
<tr>
<th>Steel</th>
<th>C_γα0</th>
<th>C_γα1</th>
<th>C_γβ0</th>
<th>C_γβ1</th>
</tr>
</thead>
<tbody>
<tr>
<td>1109</td>
<td>4.5726</td>
<td>-0.005476</td>
<td>-1.0825</td>
<td>0.0025</td>
</tr>
<tr>
<td>1210</td>
<td>4.8365</td>
<td>-0.005818</td>
<td>-1.09</td>
<td>0.00259</td>
</tr>
<tr>
<td>1218</td>
<td>4.7337</td>
<td>-0.005634</td>
<td>-1.24</td>
<td>0.00267</td>
</tr>
<tr>
<td>1260</td>
<td>4.571</td>
<td>-0.005435</td>
<td>-0.992</td>
<td>0.0024</td>
</tr>
<tr>
<td>1261</td>
<td>4.4529</td>
<td>-0.00532</td>
<td>-0.85633</td>
<td>0.002167</td>
</tr>
<tr>
<td>1037</td>
<td>4.18</td>
<td>-0.005067</td>
<td>-1.12</td>
<td>0.002</td>
</tr>
<tr>
<td>1038</td>
<td>4.805</td>
<td>-0.0062</td>
<td>-2.01</td>
<td>0.0032</td>
</tr>
</tbody>
</table>

4. IDENTIFICATION OF THE COEFFICIENTS IN THE MODEL

The model contains several coefficients, which are grouped in the vector a. The values of these coefficients are different for different steels and they depend on microstructure at the beginning of transformation and on the deformation of austenite. Difficulties connected with determination of these coefficients are the main factor, which limits wide application of the model to simulation and control of processes of cooling of products. The method, which allows fast and easy determination of vector a components is described in [1]. It is composed of two parts. The first is solution of the direct problem, based on the model. The second part is solution of the inverse problem, in which optimization techniques are used. The objective function is defined as a square root error between measured and calculated output parameters:
\[ \Phi = \sqrt{\frac{1}{n} \sum_{i=1}^{n} \left( \frac{T_{im} - T_{c}}{T_{c}} \right)^2 + \frac{1}{k} \sum_{i=1}^{k} \left( \frac{X_{im} - X_{c}}{X_{c}} \right)^2} \]  

where: \( T_{im}, T_{c} \) – measured and calculated start and end temperatures of phase transformations, \( n \) – number of temperature measurements, \( X_{im}, X_{c} \) – measured and calculated volume fractions of phases, \( k \) – number of measurements of volume fractions of phases.

The model was identified using inverse calculations with the objective function (11). Values of coefficients \( a \) for the investigated steels are given in table 4. The whole model for all transformations contains all together 27 coefficients. However, not all of them are active in the present model.

Table 4. Parameters of equations describing equilibrium content of carbon for the investigated steels.

<table>
<thead>
<tr>
<th>steel</th>
<th>(a_1)</th>
<th>(a_2)</th>
<th>(a_3)</th>
<th>(a_4)</th>
<th>(a_5)</th>
<th>(a_6)</th>
<th>(a_7)</th>
<th>(a_8)</th>
<th>(a_9)</th>
<th>(a_{10})</th>
<th>(a_{11})</th>
<th>(a_{12})</th>
<th>(a_{13})</th>
<th>(a_{14})</th>
</tr>
</thead>
<tbody>
<tr>
<td>1210</td>
<td>1.685</td>
<td>0.016</td>
<td>224.1</td>
<td>45.08</td>
<td>1.174</td>
<td>7.35</td>
<td>0.0001</td>
<td>0.0000</td>
<td>1.87</td>
<td>0.088</td>
<td>6.29</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1218</td>
<td>2.47</td>
<td>7.35</td>
<td>204.5</td>
<td>22.82</td>
<td>1.384</td>
<td>3.73</td>
<td>4.0</td>
<td>0.0019</td>
<td>0.565</td>
<td>0.679</td>
<td>33.74</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1260</td>
<td>1.56</td>
<td>0.929</td>
<td>226.7</td>
<td>85.94</td>
<td>3.0</td>
<td>1/25</td>
<td>0.088</td>
<td>0.6394</td>
<td>0.078</td>
<td>3.17</td>
<td>0.0037</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1261</td>
<td>1.85</td>
<td>0.988</td>
<td>232.6</td>
<td>79.33</td>
<td>3.0</td>
<td>13.81</td>
<td>0.086</td>
<td>0.2816</td>
<td>0.075</td>
<td>3.02</td>
<td>0.0036</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1037</td>
<td>0.814</td>
<td>0.0175</td>
<td>202.6</td>
<td>109</td>
<td>2.827</td>
<td>3461.7</td>
<td>0.095</td>
<td>0.059</td>
<td>0.075</td>
<td>3.024</td>
<td>0.0036</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1038</td>
<td>0.414</td>
<td>0.0914</td>
<td>67.08</td>
<td>381.7</td>
<td>2.815</td>
<td>6304.2</td>
<td>0.00036</td>
<td>0.015</td>
<td>0.075</td>
<td>3.024</td>
<td>0.0036</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Comparison of results obtained from measurements and predicted by the models with optimized coefficients was performed next. Analysis of the results showed that reasonably good agreement between experiments and predictions was obtained for all investigated steels, see for example figure 1 for steels 1210 and 1038.
5. BAINITIC HARDENABILITY

The developed model was applied to evaluate the hardenability of steels. The objective was to design the composition of bainitic steel, which will give the best hardenability. In order to enable comparison of hardenability of various steels, search for certain general factors which characterize this hardenability, was made. The analysis has shown that evaluation of the hardenability cannot be based on the absolute values of parameters. Thus, the following features, all based on the plot $F_b = F_b(C_i)$, were considered:

- The area under the curve – the largest is this area the better is the hardenability of steel.
- Maximum volume fraction of bainite and the cooling rate, at which this maximum occurs – the larger this maximum is and at lower cooling rate it occurs, the better is the hardenability.

Thus, having the mentioned features in mind the following two hardenability factors were proposed:

- ratio between maximum volume fraction of bainite $F_{b\text{max}}$ and the cooling rate $C_{\text{max}}$, at which this volume fraction was obtained:

$$\psi_1 = \frac{F_{b\text{max}}}{C_{\text{max}}}$$

(12)

- the area under the plot $F_b = F_b(C_i)$ in the range, in which volume fraction of bainite exceeds 0.3:

$$\psi_2 = \frac{1}{C_{\text{max}} C_{\text{UL}}} \int X_b dC_i$$

(13)

where: $C_{\text{UL}}$, $C_{\text{UL}}$ - lower and upper cooling rate, at which volume fraction of bainite $F_b = 0.3$.

Comparison of the factors $\psi_1$ and $\psi_2$ calculated for the investigated steels is shown in Figure 2. Factor $\psi_2$ for the steel 1037 is about ten times larger (946) and for the steel 1038 even about 50 times larger (6170) than for the remaining steels. Therefore, the plots for these steels were cut at the value of 14. Analysis of this plot shows that the steels 1037 and 1038 show the highest hardenability. Medium hardenability factors were obtained for the 1260 and 1261 steels and 1210 and 1218 steels are characterized by the lowest hardenability. This result can be directly connected to the chemical composition of experimental steels. Steels 1037 and 1038 are characterized by the highest carbon content, as well as alloying elements content.
6. CONCLUSIONS

The phase transformation model was developed and its capability to describe process of cooling of bainitic steels was analyzed. The model was identified using inverse analysis of the dilatometric tests. Predictive capabilities of the optimized model were evaluated and good accuracy was obtained as far as the start temperatures for all transformations are considered. The accuracy for the end temperatures for the pearlitic and bainitic transformation was slightly worse.

Hardenability of all investigated steels was evaluated and the following conclusions can be drawn:

- Hardenability factors based on the absolute values of parameters are difficult in interpretation. Differences between this factors for various steels are very large.
- On the basis of the two proposed factors the steels can be classified as follows: 1037 and 1038 with the highest hardenability, 1260 and 1261 with medium hardenability followed by 1218 with lower and 1210 with the lowest hardenability.
- Ferritic transformation has very small influence on the area of bainite for the alloyed steels 1037 and 1038. This effect is much stronger for the remaining steels.
- Martensitic transformation has noticeable influence on the area of bainite for all investigated steels. This effect is the smallest for the steels S, 1260 and 1261.

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LITERATURE