Prediction of Prior Austenite Grain Size of High-phosphorous Steels through Phase Transformation Simulation

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The effects of phosphorous content and cooling rate on the phase evolution of low carbon steels were analyzed by DICTRA simulation focusing on the micro-segregation behavior of phosphorous during solidification and subsequent cooling process. Through the phase transformation simulation, the effects of metallurgical parameters such as P content, cooling rate, and primary dendrite arm spacing on the starting temperature of austenite grain growth were clarified. Using the values of austenite grain growth starting temperature calculated by the phase transformation simulation, prior austenite grain size of low carbon steels were estimated based on a classical grain growth modeling in a P content range from 0.01 to 0.20 mass% and in a wide cooling rate range from 1.7 to 800 K s$^{-1}$. The prior austenite grain size predicted with the present approach showed good agreement with a group of selected experimental data of 100 mm thick slabs and 2 mm thick strips.

KEY WORDS: phase transformation simulation; cooling rate; high P steel; dendrite arm spacing; prior austenite grain size; grain refinement; grain growth modeling.

1. Introduction

There is an increasing interest in the creation of high quality steels from low quality iron resources such as used scrap and low grade ores due to the environmental reasons and increasing difficulties in securing high quality ores. The authors have investigated the various metallurgical aspects of impurity elements in steels1–6) in order to design a new conceptual metallurgical process in which it is aimed to utilize impurity elements in a positive way. In our previous report,2,3,5,6) we experimentally confirmed the beneficial effect of phosphorous addition on prior austenite grain refinement of as-cast low carbon steels and proposed an analytic model2,3) to explain the decrease of prior austenite grain size (hereafter PAGS) with phosphorous addition.

In the literature,7–11) the mechanism of the austenite grain growth in the as-cast steels is summarized as follows; (1) Austenite grain growth is very sluggish in the multi-phase region due to the pinning of $γ$ grain boundary movement by residual phases. (2) Rapid growth of austenite grain starts after the completion of peritectic transition into austenite single phase region. (3) Thus, $T_{rg}$ which is defined as the temperature at which the austenite phase fraction becomes unity during cooling process becomes the starting temperature of austenite grain growth. From (1) to (3), it can be easily deduced that PAGS can be refined by reducing $T_{rg}$.

In our previous report, the austenite grain refinement with P addition was explained as a result of the $T_{rg}$ decrease due to the bcc stabilizing effect of phosphorous. And, in the grain growth modeling, $T_{rg}$ was determined by Calphad method12) using a collection of the local composition measured by EPMA (electron probe micro-analyzer) at room temperature. However, our previous model had its theoretical drawbacks in determining $T_{rg}$, since (1) the composition measured at room temperature cannot reflect the phase relation during continuous cooling at elevated temperatures and (2) the phase evolution during continuous cooling cannot be calculated properly only by thermodynamics without considering the diffusion of solute elements.

In the present study, the effects of phosphorous content and cooling rate on the phase evolution of low carbon steels were analyzed by DICTRA simulation focusing on the micro-segregation behavior of phosphorous during solidification and subsequent cooling process. Through the phase transformation simulation, the effects of metallurgical parameters such as P content, cooling rate, and primary dendrite arm spacing on the starting temperature of austenite grain growth were clarified. Using the values of austenite grain growth starting temperature calculated by the phase transformation simulation, prior austenite grain size of low carbon steels were estimated based on a classical grain growth modeling in a P content range from 0.01 to 0.20 mass% and in a wide cooling rate range from 1.7 to 800 K s$^{-1}$. The prior austenite grain size predicted with the present approach showed good agreement with a group of selected experimental data of 100 mm thick slabs and 2 mm thick strips.

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cooling rate and the unit-segregation zone size (which is a half of primary dendrite arm spacing) on the starting temperature of rapid grain growth of austenite, \( T_{rg} \), were evaluated by the phase transformation simulation. Peritectic transformation was simulated using DICRA®. Fe-data ver. 313) and MOB214) were used as the thermodynamic and kinetic databases, respectively. The detailed description of the phase transformation model and the schematic illustration of it can be found elsewhere.15)

2.2. Austenite Grain Growth Modeling

In the austenite grain growth modeling, it was assumed (1) that the initial austenite grain size, \( d_0 \), before growth equals to primary dendrite arm spacing (hereafter PDAS) and (2) that austenite grains do not grow before the austenite phase fraction becomes unity during continuous cooling process.

The growth amount, \( \Delta d_g \), of austenite grains below \( T_{rg} \) was calculated based on the approach of Burke and Turnbull16–18) with an assumption that the growth kinetics is driven by the reduction of the austenite grain boundary energy. The detailed description of the grain growth modeling can be found elsewhere.2,3) By using the initial grain size \( d_0 \) and the calculated growth amount \( \Delta d_g \), the PAGS \( d_g \) was obtained as follows;

\[
d_g = \sqrt{(d_0)^2 + (\Delta d_g)^2}
\]

Then, the calculated PAGS under various conditions of P content and cooling rate was favorably compared with the measured data.

3. Results and Discussions

3.1. Parameters Controlling the \( T_{rg} \)

3.1.1. Effect of P Content

Figure 1 shows the change of the Fe(0.15Si–0.60Mn–P, in mass%)–C pseudo-binary phase diagrams with phosphorous addition (0.01, 0.1 and 0.2 mass% P). The addition of P resulted in the decrease of A4 temperature since it is one of the strongest bcc stabilizing elements. The open circles in Fig. 1 indicate the starting temperature of austenite single phase region of 0.1 mass% C steels under each P content condition during cooling. The shrinkage of austenite single phase region with P addition is well manifested in Fig. 1. The austenite single phase region may shrink more, with P addition, than what is depicted in Fig. 1 if the micro-segregation is taken into account.

Figure 2 shows the effect of P content on the starting temperature of \( \gamma \) grain growth, \( T_{rg} \), which was estimated by a phase transformation simulation. The chemical compositions of the steels used in the present study are listed in Table 1. The unit segregation zone size, \( L_0 \), and the cooling rate during solidification, \( R_c,LS \), were assumed to be constant as 1.5 \( \times \) 10\(^{-4}\) m and 1.7 K s\(^{-1}\), respectively. With P addition, the completion of austenite formation is suppressed and \( T_{rg} \) is greatly decreased. The dashed line shows the \( T_{rg} \) which was estimated by thermodynamic equilibrium calculation using a Calphad method. The temperature difference between dashed and solid lines corresponds to the contribution of the micro-segregation which occurred during the solidification.

3.1.2. Effect of Cooling Rate

Figure 3 shows the effect of cooling rate on \( T_{rg} \). In the calculation, the chemical composition of 010P steel in
Table 1 was employed and unit-segregation-zone size was set to be constant as $1.24 \times 10^{-4}$ m. In reality, the unit-segregation-zone size is greatly influenced by the cooling rate. The constant unit-segregation-zone size is an imaginary condition to estimate the contribution of the mass transfer change with the cooling rate. The coupled effects of the cooling rate and the unit-segregation-zone size on $T_{rg}$ will be discussed in the following section. With increasing the cooling rate, the mass transfer in the segregation zone is suppressed in Fig. 3. As a result, liquid and solid phases are retained to lower temperature during peritectic transformation, which results in a depression of $T_{rg}$. The dashed line in Fig. 3 indicates the $T_{rg}$ determined by thermodynamic equilibrium calculation. The discrepancy between the two curves shows how greatly phase evolution can be changed by the constraint imposed upon the mass transfer. It can be seen from Fig. 3 that a higher cooling rate facilitates the austenite grain refinement not only by the decrease in the grain growth time but also by the suppression of the start of grain growth.

### 3.1.3. Effect of Unit-segregation-zone Size

Figure 4 shows the effect of unit-segregation-zone size, $L_0$, on $T_{rg}$. The chemical composition of 010P steel was employed and the cooling rate was set to be constant as $1 \text{ K s}^{-1}$. It is shown that $T_{rg}$ decreases greatly with increasing the unit-segregation-zone size, $L_0$. The decrease in $T_{rg}$ with the increase in $L_0$ can be attributed to the fact that the mass transfer through $T_{rg}$ becomes more difficult as $L_0$ becomes larger. The dashed line in Fig. 4 indicates the $T_{rg}$ determined by thermodynamic equilibrium calculation. The difference between the dashed and solid lines in Figs. 2 to 4 shows how dominant role the mass transfer plays in the phase evolution.

### 3.2. Effects of Composition and Cooling Rate on $L_0$ (PDAS/2)

In the present study, the unit-segregation-zone size was assumed to be the half of PDAS. Since PDAS is affected by the composition and the cooling rate, their effects on PDAS should be considered as well in the phase transformation simulation in order to estimate $T_{rg}$ with high accuracy.

Figure 5 shows the effects of phosphorous content on PDAS under different cooling rate conditions of $800 \text{ K s}^{-1}$ (2 mm thick strips, Fig. 5(a)) and $1.7 \text{ K s}^{-1}$ (100 mm thick slabs, Fig. 5(b)). The solid squares in Fig. 5(a) show the experimental PDAS which was measured in 2 mm thick strips. The dashed lines in Fig. 5 show the PDAS which was estimated by the following expression:

$$S_i = K(R_{LS})^l(C_C)^m(C_P)^n$$

where $S_i$ is PDAS, $K$ a constant that depends on materials’ characteristics and process conditions, $R_{LS}$ the cooling rate during solidification, $C_C$ and $C_P$ the nominal contents of carbon and phosphorous, and $l$, $m$, and $n$ the exponents. For the exponents $l$ and $m$, $-0.2063$ and $-0.3162 + 2.0325C_C$ were used respectively after the report of El-Bealy et al. The value of the exponent $n$ was determined as $0.0361 + 1.6865C_P$ in our previous report by the linear regression analysis of the experimental data. $K$ value for the dashed lines in Fig. 5(a) was determined as...
183.4992 by fitting the data using Eq. (2). It is evidently shown in Fig. 5(a) that the dashed lines estimated by Eq. (2) describes the P content dependence of experimental PDAS quite well. In Fig. 5(b), \( K \) value for the dashed lines was determined as 344.4529 by using the experimental PDAS data which was measured at a quarter thickness position of 100 mm thick slab of 001P steel (indicated by solid square in Fig. 5(b)). Then, the PDAS values for 010P and 020P steels were estimated by Eq. (2) with \( K = 344.4529 \). The PDAS values estimated with considering the effect of P addition in Fig. 5(b) are used for the phase transformation simulation to determine the \( T_{rg} \) values which are necessary to calculate PAGS in the following section.

### 3.3. Prediction of PAGS

Table 2 shows the conditions of the phase transformation simulation and the calculated results of \( T_{rg} \). \( R_{c,LS} \) implies the average cooling rate in the temperature range above \( T_{rg} \). In Table 2, S010P implies the 2 mm thick strip specimen which contains about 0.10 mass\% P. All other specimens were taken from a quarter thickness position of 100 mm thick slabs. \( R_{c,LS} \) of 100 mm thick slabs (001P, 010P and 020P) was reported in our previous report\(^5\) and that of S010P specimen was newly evaluated by taking the average of cooling rates from 1803 to 1550 K of 2 mm thick strip. For 001P and S010P specimens, experimentally reported \( L_0 \) values (solid squares in Fig. 5) were used, while the values estimated by Eq. (2) (open squares in Fig. 5(b)) were used for 010P and 020P specimens. Figure 6 compares the \( T_{rg} \) values which were calculated with and without considering the effect of P content on \( L_0 \). The difference between solid and open squares becomes larger in higher P content. It is clearly seen that the effect of P addition on austenite grain refinement is exaggerated substantially without considering the decrease of \( L_0 \) (PDAS/2) with P addition especially in a high P content range.

Figure 7 shows the relationship between \( T_{rg} \) and the calculated PAGS of 100 mm thick slabs. \( R_{c,T} \) means the average cooling rate in the austenite single phase region. It is quite evident that the decrease of \( T_{rg} \) caused by P addition results in the austenite grain refinement. Note the slope of the PAGS to \( T_{rg} \) is steeper in a higher temperature region since the grain growth rate becomes higher as temperature increases. The PAGS values calculated with the present approach is favorably compared with the measured data in Fig. 8. The results of calculation show good agreement with the experimental data under various P content and different cooling conditions. It should be noted that the present model predicts the PAGS with high accuracy in a large cooling rate range from 1.7 to 800 K s\(^{-1}\) (the average cooling rates between 1803 and 1753 K) and a P content range from 0.01 to 0.2 mass\% P.

### 4. Conclusions

The effects of P content and cooling rate on the phase evolution of low carbon steels were rigorously analyzed using a phase transformation simulation. The effects of such parameters as P content, cooling rate and PDAS, which are controlling phase evolution, on the starting temperature of austenite grain growth, \( T_{rg} \), were clarified using a DICTRA simulation. The clarified effect of each parameter on \( T_{rg} \) can be summarized as;

1. \( T_{rg} \) decreases with P addition (see Fig. 2).
2. Micro-segregation of P facilitates the effect of P on the decrease in \( T_{rg} \) (see Fig. 2).
3. \( T_{rg} \) decreases with the increase in cooling rate (see Fig. 3).
4. \( T_{rg} \) decreases with the increase in PDAS (see Fig. 4).

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**Table 2.** The conditions of the phase transformation simulation and the calculated results of \( T_{rg} \)

<table>
<thead>
<tr>
<th>Chemical composition, mass%</th>
<th>( L_0 )</th>
<th>( R_{c,LS} )</th>
<th>( T_{rg} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>Si</td>
<td>Mn</td>
<td>P</td>
</tr>
<tr>
<td>001P</td>
<td>0.108</td>
<td>0.160</td>
<td>0.576</td>
</tr>
<tr>
<td>010P</td>
<td>0.010</td>
<td>0.176</td>
<td>0.607</td>
</tr>
<tr>
<td>020P</td>
<td>0.104</td>
<td>0.169</td>
<td>0.592</td>
</tr>
<tr>
<td>S010P</td>
<td>0.09</td>
<td>0.17</td>
<td>0.62</td>
</tr>
</tbody>
</table>
From (1) to (4), it could be concluded that $T_{rg}$ decreases when the degree of inhomogeneity of P distribution in the unit-segregation-zone increases.

Using the $T_{rg}$ values calculated by phase transformation simulation, PAGS of low carbon steels was estimated based on the classical grain growth modeling with various P content under different cooling conditions. The estimated PAGS showed good agreement with the experimental data in a P content range from 0.01 to 0.20 mass% and in a large cooling rate range from 1.7 to 800 K s$^{-1}$.

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REFERENCES