A MULTI-PHASE-FIELD SIMULATION OF CARBON STEEL UNDER ACTUAL CONDITIONS OF A HOT ROLLING PROCESS

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1 INTRODUCTION

It is well known that mechanical properties such as yield stress (YS), tensile strength (TS) and elongation (EL) of hot rolled steels are related to microstructure. Therefore, mathematical models to predict representative microstructural characteristics of hot rolled steel have been investigated for many years. Generally, these models predict macroscopic metallurgical information such as average grain size and the volume fraction of each transformed phase considering metallurgical phenomena such as deformation, recrystallization and transformation. Then, mechanical properties are calculated by an empirical model which explains the effects of macroscopic metallurgical information on mechanical properties [1]. However, it has been found that the evolution of microstructure also affects mechanical properties, and this has been the subject of both theoretical and experimental study. Furthermore, due to the difficulty of observation of microstructural evolution during the process, theoretically based simulations have the potential to be useful in this area. In recent years, a phase-field method has attracted much attention as a mesoscopic scale simulation tool which calculates the morphological change during growth of precipitated structure. Many investigations with experimental conditions have been carried out and reported to show its capability.

Pariser [2], Mecozzi [3,4], Militzer [5] and Yamanaka [6] have simulated the transformation from austenite (γ) to ferrite (α) using a multi-phase-field (MPF) method [7]. We also employed a MPF method to calculate γ-α transformation [8]. This paper describes simulations of the γ-α transformation in low carbon steels performed using in-house MPF code for further studies on its application to actual hot rolling process conditions.

Aside from this mesoscopic scale analysis, we performed macroscopic scale analysis using our system named MPPS (Material Properties Prediction System) [9]. The key components of MPPS are the hot deformation and the transformation simulation based on physical-metallurgical modeling. MPPS predicts macroscopic metallurgical information such as changes in the average diameter, dislocation density and volume fraction of each phase during the rolling and cooling processes as representative values of microstructural information.
In this paper, a weak linkage between the macroscopic and the mesoscopic microstructure analysis has been established. The temperature paths of the head and the tail parts of a hot rolling strip were simulated. The \( \gamma \rightarrow \alpha \) transformation is calculated through the calculated temperature path during cooling using the MPPS and MPF method. The transformation rates calculated by macroscopic and mesoscopic analysis demonstrated the same tendencies.

2 MICROSTRUCTURE EVOLUTION IN THE ROLLING PROCESS

Figure 1 shows an example of a conventional hot rolling process and microstructural evolution. A slab is heated in the reheating furnace to around 1200 °C then discharged and rolled in the mill. The slab is rolled by several passes in the roughing mill (RM) to produce a transfer bar with a thickness of 30 to 50 mm. This transfer bar is then fed into the finishing mill (FM) where the thickness is reduced in each successive rolling stand to produce the desired target thickness (typically in the range 1.2 to 25.4 mm). The temperature at the exit of the finishing mill is around 900 °C and the strip is then cooled as it travels along the run out table to its target coiling temperature (around 550 to 700 °C in case of carbon steels) using laminar flow cooling. Some steels require cooling trajectory control schemes to achieve their metallurgical requirements.

During rolling, microstructural characteristics such as the austenite grain diameter and dislocation density change in accordance with the level of deformation and temperature. The steel transforms from austenite to ferrite-pearlite during cooling succeeding to the rolling. The volume fraction of ferrite is dominant if the carbon content is low, and the volume fraction of pearlite increases with increasing carbon content. The cooling rate influences on the ferrite grain size, with smaller ferrite grain sizes giving higher strength and toughness. In this way, the metallurgical information closely relates to the mechanical properties of the strip.
diffusion occurs. Therefore, a phase field variable $\phi_i(\vec{r}, t)$ which represents the existence probability of each grain and the carbon concentration $c(\vec{r}, t)$ are defined as functions of time $t$ and coordinates $\vec{r}$.

The phase field variable $c(\vec{r}, t)$ is a dependent variable which satisfies the following equation for all coordinates.

$$\sum_{i=1}^{N} \phi_i = 1$$

(1)

The time evolution equation of the phase field variable is defined as follows:

$$\frac{\partial \phi_i}{\partial t} = -\sum_{j=1}^{N} \frac{M_{\phi_{ij}}}{n} \left( \frac{\delta G_{sys}}{\delta \phi_i} - \frac{\delta G_{sys}}{\delta \phi_j} \right)$$

(2)

where, $\phi_i$ and $\phi_j$ are phase field variables for grain $i$ and for grain $j$ that is adjacent to grain $i$, respectively, $N$ is the number of grains consisting in the system, $M$ is phase field mobility, $n$ is a number of locally existing grains, $G_{sys}$ is the Gibbs free energy of the $N$-grain system. The phase field variable $\phi_i$ is increased or decreased by Gibbs free energy, which represents the growth of grains in the stable phase and the dissipation of grains in the unstable phase. Using the measurable physical quantities, equation (2) is rewritten as follows:

$$\frac{\partial \phi_i}{\partial t} = \sum_{j=1}^{n} \frac{\mu_{ij}}{n} \left[ \sum_{k=1}^{N} \left( \sigma_{jk} - \sigma_{ik} \right) N^2 \phi_k + \left( \sigma_{jk} - \sigma_{ik} \right) \frac{\pi^2}{\eta} \phi_k \right] + \frac{2\pi}{\eta} \sqrt{\phi_i} \phi_j \Delta G_{ij}$$

(3)

where $\mu_{ij}$ is the interface mobility between grain $i$ and $j$, $n$ is the number of locally existing grains, $\sigma_{jk}$ and $\sigma_{ik}$ are the interface energies between grain $j-k$ and $i-j$, respectively, $\eta$ is the interface thickness and energy $\Delta G_{ij}$ is the phenomenological thermodynamic driving force. The number of locally existing grains $n$ needs to be defined. It is known that $n = 7$ is big enough as the upper limit value. In the numerical calculation, equation (3) is calculated for a maximum of 7 adjacent grains (grains adjacent to grain $i$). The value of $n$ changes over time since grain $i$ bumps into different grains as it grows. As the carbon solubilities in the $\gamma$-phase and the $\alpha$-phase are different, there is a concentration gradient in the boundary due to carbon diffusion. To express the phenomena, the time evolution of the carbon concentration $c(\vec{r}, t)$ in grains is defined as follows:

$$\frac{\partial c}{\partial t} = \nabla \cdot \left( \sum_{i=1}^{N} \phi_i \nabla c_i \right)$$

(4)

$$c = \sum_{i=1}^{N} \phi_i c_i$$

(5)

where $D_i$ and $c_i$ denote the diffusion constant for carbon atoms and the carbon concentration in the grain $i$ belonging to $P$ phase, respectively. $D_i$ is calculated as

$$D_i = D_0 \exp \left( -\frac{Q}{RT} \right)$$

(6)
where, $Q$ is the activation energy of the carbon diffusion and $R$ is the gas constant. Using a phase diagram, the local concentration of carbon $c_i^p$ defined by the equation (5) is calculated as follows:

$$c_i^p = \frac{k_i c_i}{\sum_{j=1}^{N} \phi_j k_j}$$

where, $k_i$ and $k_j$ are proportionality coefficients for carbon concentration of grain $i$ and $j$, respectively. For the $\gamma$-$\alpha$ transformation, the interfacial mobility is given by the Arrhenius-type equation with a pre-exponential factor $\mu_0$ and the activation energy of the interfacial mobility $Q_m$ as follows:

$$\mu_{ij} = \mu_0 \exp\left(-\frac{Q_m}{RT}\right)$$

### 4 MATERIAL PROPERTIES PREDICTION SYSTEM

Figure 2 gives an outline of the mechanical properties prediction procedure. The key components of the system are the hot deformation model and the transformation model [3-5, 10]. First, the reheating furnace model calculates $\gamma$-grain growth in the reheating furnace. The hot deformation model [10] simulates the structural transitions during hot rolling and produces as its result a prediction of the final $\gamma$-grain diameters and dislocation densities at the exit of the finishing mill. Next, the transformation model, which employs thermodynamics, simulates transformation from deformed $\gamma$ during cooling on the run out table and calculates the transformed structure ($\alpha$ grain diameter and volume fraction of ferrite, pearlite and martensite phase) based on the chemical composition [11]. The mechanical properties such as YS, TS and EL are then calculated from this transformed structure using a model of the relationship between microstructure and mechanical properties [1].

Figure 3 shows the accuracy of MPPS. The calculated and measured tensile strength (Figure 3 left) and the ferrite diameter (Figure 3 right) agree with the actual data obtained from commercially hot rolled carbon steels. The temperature change pattern of the strip as it progresses through the hot rolling process influences on flow stress, microstructure and mechanical properties. Accordingly, the temperatures are calculated using the finite difference method (FDM). The cooling behavior of the strip is mainly influenced by the physical processes of radiation, conduction, convection, and so on. The physical model uses a non-stationary differential equation (Fourier’s heat equation) to calculate these influences, including consideration of the cooling effect of each spray.
5 RESULTS AND DISCUSSION

MPPS simulations and 2-dimensional MPF simulations were performed to analyze the transformation of low carbon steel. The carbon concentration of the simulated steel was 0.04 [wt %]. Firstly, the hot rolling process from a 230 mm thickness slab to a 3.5 mm thickness coil was simulated. The target temperatures at the exit of the finishing mill and at the entry of coiler were 900 [°C] and 700 [°C], respectively. These are the general target temperatures for the specific steel grade in commercial hot rolling of coil. The target points were the head and
tail of the strip. To achieve the target temperatures, temperature path during rolling and cooling were calculated. The calculated cooling rates along the run out table at head and tail were 14 [°C/s] and 10 [°C/s], respectively. The calculated TS of the tail part was about 40 [MPa] higher than that of the head part in MPPS simulation.

Secondly, The MPF simulations for γ-α transformation during cooling were performed with the cooling rates for the head and tail parts. The size of the MPF simulated structure was 50 x 50 [μm²]. The average γ-grain diameter of the matrix structure was 16 [μm].

Figure 4 and Figure 5 show results of MPF simulation for γ-α transformation and carbon diffusion during cooling with respective cooling rates of 14 [°C/s] and 10 [°C/s]. Regardless of the cooling rate, the average α-grain diameters after cooling were about 10 [μm] in both MPF and MPPS simulation. As the α-grain grows, the carbon concentration in the α-phase decreased due to carbon diffusion from the α-phase to the γ-phase. The growth rate of the α-grains was faster for a lower cooling rate. This tendency agreed with the experimental data [12] and MPPS results (Figure 6).

![Figure 4: Change in phase field variable (upper figures) and carbon concentration (lower figures) during cooling with cooling rate 14 [°C/s] (head point)](image-url)
6 CONCLUSIONS

Macroscopic-scale and mesoscopic-scale analyses of transformation in the hot rolling process for low carbon steels were performed using in-house simulators. The temperature path difference in the head and tail parts of the strip and their macroscopic metallurgy were accurately predicted by MPPS. For the mesoscopic-scale analysis, the MPF method was adopted and the transformation to the $\alpha$-grains during $\gamma$-$\alpha$ transformation was simulated. The simulation results allowed the following conclusions:
- MPF method gives a visual understanding of morphological characteristics and evolution of $\gamma$-$\alpha$ transformation.
- The weak linkage of macroscopic and mesoscopic analysis was established.
- The strengthening of the linkage between macroscopic and mesoscopic analysis, parameter tuning for a wider range of steel grades or temperature paths, and transformation to the phases other than the $\alpha$-phase such as pearlite will be future work.

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REFERENCES