Microstructure-based multiscale approach to obtain mechanical property of duplex stainless steel according to ICME concept

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Abstract. We have proposed a microstructure-based multiscale simulation framework based on Integrated Computational Material Engineering (ICME) concept and applied it to the simulation of hot rolling process of a duplex stainless steel. In the study, the finite element simulation of the hot rolling process is performed. The mechanical property of a slab is calculated on the basis of its underlying solidified microstructures, which are simulated by the multi-phase field method coupled with CALPHAD thermodynamic database. The properties of constituent phases in the solidified microstructure is obtained by the first-principles calculation, the molecular dynamics simulation and nano-indentation tests. The mathematical homogenization method is used to calculate the property of slab based on the microstructure. This paper reviews the application of the multiscale simulation framework to a SUS304 duplex stainless steel.

1. Introduction

Although the exact origin of Finite Element Method (FEM) cannot be identified [1], it leaves no doubt that more than 60 years have passed since FEM was first applied to engineering problems [2]. Any complex geometries could be modeled with FEM only if the geometries were divided into simple shapes like tetrahedrons and hexahedrons. Materials also have complexities, for example, most metals have to be treated as polycrystalline aggregate in microscale, composites consist of two or more materials, dislocations in nanoscale affect stress-strain relationship in macroscale. However, the complexities were simplified to material properties, or the relationship between a gradient of field and its conjugate flux, for example, strain and stress in the mechanical properties. The material properties could be obtained by experiments without considering microstructures in materials, most of engineers have used the material properties identified by the experiments for the phenomenological material models [3-8].

On the other hand, homogenization methods which enables us to estimate macroscopic material properties based on microstructures, have been studied [9]. After the first analytical mean-field homogenization method was studied [10-12], mathematical homogenization methods were also developed [13-15]. As the mathematical homogenization methods require the geometrical dataset of microstructures and material properties of constituent phases to make a representative volume element (RVE), the methods were mainly applied to composite materials which contain simple periodic microstructures [16, 17] and metallic materials with idealized microstructures [18]. The application of
the mathematical homogenization methods to real metallic materials, however, were much less because the geometrical data of the microstructures were difficult to obtain.

Recent improvement of the multi-phase field (MPF) method [19] enabled us to simulate microstructure evolutions in metallic materials in various processes, e.g. solidification, recrystallization, grain growth and phase transformations [20-22]. Using the MPF method and the mathematical homogenization method, the estimations of material properties based on microstructures have been reported [23-26].

In this study, we propose a multiscale simulation framework [25] to estimate the material properties based on the microstructure data simulated by the MPF method and applied the framework to hot rolling processes along with solidification during a continuous casting of a SUS304 duplex stainless steel. Figure 1 shows the proposed framework based on Integrated Computational Material Engineering (ICME). The framework bridges various simulation software over multiscale. At Step 1, continuous casting is simulated using MPF simulation software MICRESS [27] coupled with the CALPHAD software Thermo-Calc [28]. Temperature profile in the slab is calculated by FEM software FINAS/STAR TPS Edition [29]. Microstructures of a slab are obtained as a result of Step 1. Mechanical properties of its constituent phases in the microstructures are obtained at Step 2. Elastic properties are obtained by the molecular dynamics software, LAMMPS [30], and the first principle calculation software, VASP [31]. Plastic stress-strain curves are obtained by a nano-indentation test. At Step 3, macroscopic homogenized mechanical properties are obtained by homogenization calculation software HOMAT [32] and FEM software Abaqus [33]. By using the macroscopic homogenized properties, macroscopic hot rolling simulation is performed by Abaqus as Step 4. As a result of the step, plastic strain energy density distribution is obtained.

![Multiscale simulation framework proposed in this study](image)

**Figure 1** Multiscale simulation framework proposed in this study and software used in this procedure [27-33]

2. Methodology
In our study, a hot rolling experiment of a SUS304 duplex steel slab in laboratory is assumed. Its chemical composition is Fe-18wt%Cr-8wt%Ni-0.08wt%C. Figure 2 shows the dimension of slab. The finite element model of the slab is divided into two types of sections. At the region near the surface of slab, columnar solidification is assumed to be occurred due to a large temperature gradient along a normal direction to the surface when the slab is being cooled in a continuous casting process. At the region inside the slab, however, temperature gradient is small enough that equiaxed solidification is generated. Temperature distribution in the slab is obtained by FEM calculation. The initial temperature and cooling rate at the slab surface are set to 1733 K and 25 K/s, respectively. The resultant temperature
profile at the surface and at the center of the slab is used for MPF simulation of columnar and equiaxed solidifications, respectively.

![Figure 2. Dimension of a slab for hot rolling experiment in laboratory.](image)

At Step 1, solidification processes in the slab are simulated using the MPF method coupled with CALPHAD database. The columnar and equiaxed solidifications are simulated separately. $128 \times 128 \times 256$ finite difference grids are used for the MPF simulation of the columnar solidification. As the spacing of the finite difference grids is 0.5 $\mu$m, the size of total computational domain is $64 \times 64 \times 128$ $\mu$m$^3$. As the initial condition, the initial nucleus of body-centered cubic (bcc) $\delta$-ferrite are placed on the surface of the slab. In the MPF simulation of the equiaxed solidification, $128 \times 128 \times 128$ finite difference grids are used. The size of total computational domain is $64 \times 64 \times 64$ $\mu$m$^3$. The initial $\delta$-ferrite nucleus are randomly placed at the bottom of the computational domain so that the mean distance between the nucleus is $30 \mu$m.

At Step 2, the mechanical properties of constituent phases in the solidified microstructures ($\delta$-ferrite and $\gamma$-austenite phases) are calculated. The calculated material properties are used to simulate hot rolling process using FEM. Assuming the elastic modulus tensors of $\delta$-ferrite and $\gamma$-austenite phases can be expressed as a cubic symmetry, the components of the elastic modulus tensors at 0 K are identified by the nanoscale simulations using the first principal calculation and molecular dynamics. The components of the elastic modulus tensors at 900 °C are identified by using the temperature dependency [34-36]. The stress-strain curve of each phase is obtained by a nano-indentation test. Using the reverse algorithm by Dao et al.[37], parameters, yield stress and strain-hardening exponent of $\delta$-ferrite phase at room temperature are identified from single indentation test with a Berkovich triangular pyramid indenter. The stress-strain curves of $\delta$-ferrite and $\gamma$-austenite at 900 °C are estimated from the experimental data of stress–strain curve of SUS304 stainless steel at both room temperature and 900 °C [38].

At Step 3, macroscopic homogenized material properties are calculated. With the microstructures obtained by Step 1 and microscopic material properties of the constituent phases obtained by Step 2,

| Phase          | $C_{11}$ [GPa] | $C_{12}$ [GPa] | $C_{44}$ [GPa] |
|----------------|----------------|----------------|----------------|
| $\gamma$-austenite | 171.4          | 107.4          | 95.1           |
| $\delta$-ferrite  | 180.3          | 104.3          | 94.3           |

![Figure 3. True stress-true strain curves of the constituent phases at 900 °C.](image)
macroscopic elastic properties are calculated by the homogenization method. Furthermore, macroscopic strain-stress relationship is obtained by virtual tensile tests performed by non-linear FEM under the assumption of isotropic hardening. The macroscopic homogenized properties are calculated for the both columnar and equiaxed microstructures.

At Step 4, a single-pass hot rolling process is simulated. The finite element mesh shown in figure 2 and the homogenized material properties obtained in Step 3 are used. The thickness reduction during the single pass rolling process is assumed to be 40%. The diameter of a roller is assumed to be 160 mm and the surface velocity of the roller is set to be 18 m/min.

In our paper [25], the static recrystallization after the hot rolling was also simulated using the MPF method. The detail of the MPF simulation of static recrystallization can be found elsewhere [25].

3. Results and discussions

Figure 3 shows the evolutions of columnar and equiaxed solidification microstructures. The δ phase grows at first and, then, δ→γ transformation occurs at the δ–liquid interface. The phase distributions of the columnar microstructure at 1173 K and the equiaxed microstructure at 1352 K were used to construct the RVEs. The volume fraction of residual δ phase in the columnar and equiaxed microstructures are 12.5% and 17.1%, respectively. Table 1 shows the elastic constants of each phase at 900 °C. Figure 4 shows the stress-strain curves of each single phase at 900 °C.

![Figure 4](image_url)

**Figure 4.** Evolutions of columnar and equiaxed solidifications microstructures simulated by the MPF simulation coupled with CALPHAD database.

Using the RVEs of the solidified microstructures shown in figure 4, the elastic modulus tensors are calculated based on the mathematical homogenization method. The calculated elastic modulus tensor of the columnar solidified microstructure is given as

\[
C_{col} = \begin{bmatrix}
186.8 & 102.0 & 97.7 & 5.3 & -0.9 & 0.0 \\
102.0 & 187.6 & 96.9 & -5.2 & -0.2 & 3.4 \\
97.7 & 96.9 & 192.0 & 0.0 & 1.0 & -3.4 \\
5.3 & -5.2 & 0.0 & 85.6 & 0.0 & -0.2 \\
-0.9 & -0.2 & 1.0 & 0.0 & 79.8 & -0.2 \\
0.0 & 3.4 & -3.4 & -0.2 & -0.2 & 77.6
\end{bmatrix}
\]

and that of the equiaxed solidified microstructure is given as
The elastic tensor of the equiaxed microstructure is obtained in Step 2 of the multiscale simulation framework. The elastic modulus tensor of equiaxed microstructure is given by Eq. (2), which is used for the elastic modulus tensor of equiaxed microstructure.

\[
\mathbf{C}_{\text{equ}} = \begin{bmatrix}
222.3 & 83.4 & 81.0 & 0.9 & 6.8 & -3.1 \\
83.4 & 212.7 & 90.6 & 6.1 & -4.7 & 16.4 \\
81.0 & 90.6 & 215.1 & -7.0 & -2.2 & -13.2 \\
0.9 & 6.1 & -7.0 & 67.8 & -1.3 & -2.4 \\
6.8 & -4.7 & -2.2 & 62.5 & -6.1 & -6.1 \\
-3.1 & 16.4 & -13.2 & -2.4 & -6.1 & 75.2
\end{bmatrix}.
\]  

(2)

Note that these matrices are shown in the Voigt notation and the index order is the same as Abaqus documentation [33]. Although the elastic tensor of the equiaxed microstructure is predicted to be isotropic, Eq. (2) indicates strong anisotropy of the elastic tensor. For example, the difference between 11, 22 and 33 components of the elastic tensor given by Eq. (2) is about 5%. We assumed that the RVEs are distributed in random orientations in a macroscopic scale. The homogenization scheme based on the Voigt’s concept to take the average of rotated elastic tensor for all orientations is applied to obtain the equiaxed elastic tensor as;

\[
\bar{\mathbf{C}} = \left( \sum_{\mathbf{R} \in \mathbf{R}^{(\text{all})}} \mathbf{C}(\mathbf{R}) \right) / \sum_{\mathbf{R} \in \mathbf{R}^{(\text{all})}} 1
\]  

(3)

where \( \mathbf{R}^{(\text{all})} \) is a set of all three-dimensional rotation tensors, \( \mathbf{C}(\mathbf{R}) \) is a rotated elastic modulus tensor calculated by rotating the tensor given Eq.(2) with a rotation tensor \( \mathbf{R} \). By applying Eq.(3) to Eq.(2), the following tensor is obtained:

\[
\bar{\mathbf{C}} = \begin{bmatrix}
218.8 & 83.9 & 83.9 & 0.0 & 0.0 & 0.0 \\
83.9 & 218.8 & 83.9 & 0.0 & 0.0 & 0.0 \\
83.9 & 83.9 & 218.8 & 0.0 & 0.0 & 0.0 \\
0.0 & 0.0 & 0.0 & 67.5 & 0.0 & 0.0 \\
0.0 & 0.0 & 0.0 & 0.0 & 67.5 & 0.0 \\
0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 67.5
\end{bmatrix}.
\]  

(4)

Eq.(4) is used for the elastic modulus tensor of equiaxed microstructure.

Using the elastic modulus tensors, the stress-strain curves of the solidified microstructures are computed. The stress-strain curves of the columnar and equiaxed microstructure are shown in figure 5 and figure 6, respectively.

Using the stress-strain relationship obtained by the homogenization method, the FEM simulation of the hot rolling process of SUS304 duplex stainless steel. The plastic strain energy density distributions in the columnar and equiaxed solidification zone of the slab are shown in figure 7 and figure 8.

The proposed multiscale simulation framework successfully estimates macroscopic material property on the basis of the microstructure. Once the microscopic property of the constituent phases are obtained in Step 2, the simulation for continuous casting process and the hot rolling process is bridged.

**Figure 5.** Macroscopic stress-strain relationship for columnar microstructure at 900 °C.

**Figure 6.** Macroscopic stress-strain relationship for equiaxed microstructure at 900 °C.
without any experiments. This can reduce the cost and time for both material development and material process optimization, which is an objective of ICME.

The validation of our multiscale simulation framework, however, is difficult because it involves not only the macroscopic slab property but also its microscopic structure and properties of constituent phases. The validation itself and the method for validating the framework are future issues.

4. Summary
The application of the multiscale simulation framework to the hot rolling process of a SUS304 stainless steel was reviewed. The framework successfully bridges the nano-, micro- and macroscale simulation software. The results showed that the framework can predict the microstructure evolutions during the continuous casting and estimate the macroscopic mechanical properties of the steel used for the finite element simulation of the hot rolling process. The future works are validation of the framework with experimental results.

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