Multiscale Elasto-plastic Finite Element Analysis of Dual-phase Steel Based on Homogenization Method

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Abstract

High tensile steel, such as dual-phase steel consisting of ferrite and martensite, is still widely used in several industries. From a research and development point of view, it is important to clarify the relationship between microstructure and macroscopic mechanical properties. In this study, samples of dual- or single-phase steel consisting of similar constituent phases were experimentally produced, and their tensile properties were obtained by material testing. These data were introduced into the microstructure model generated by an image-based modeling method using SEM observation imaging. Using this model, multiscale FE simulation based on homogenization elasto-plasticity theory was conducted, and validation was investigated by comparison with experimental results.

Introduction

The development of high-strength steel materials is being actively promoted to, for example, meet the needs for the weight reduction of transport equipment such as automobiles. A typical material is dual-phase steel (hereinafter referred to as "DP steel"), which comprises ferrite and martensite phases. The material properties of such high-strength steel have been improved by controlling its internal structure. Many studies have been conducted to elucidate the effect of microstructure on macroscopic material properties such as mechanical properties, formability, and ductile fracture behavior.[1)-3)] In recent years, evaluation by multiscale simulation has been attracting attention as an effective means. However, there still are only a few analysis examples for steel[4), 5)] and, at present, the correlation between material properties and structural morphology has not been organized systematically.

This study focuses on DP steel, in which mechanical property data for each constituent phase has been obtained by material testing. An attempt has been made to create a mesh model for analysis to reproduce the structural observation results faithfully. In addition, a large deformation finite element (FE) simulation code based on homogenized elasto-plastic theory[6), 7)] has been developed to perform multiscale strength analysis using the above data.[8)] This paper examines the validity and effectiveness of the developed method by comparing the analysis results with the experimental results.

1. Material testing

1.1 Testing materials

The prepared samples included DP steel, as well as single-phase materials each having properties comparable to respective phase constituting the DP steel. First, a 20 kg vacuum induction melting furnace was used to melt three types of ingots that had been adjusted to meet the target compositions. **Table 1** shows the compositions of the ingots at this stage. The smelted ingots were heated at 1,150℃ for more than 30 minutes. Subsequently, they were forged at 800℃ to a round-bar shape of approximately ϕ10 × L150 mm. After that, they were heat-treated in a salt-bath furnace under the conditions shown in Table 1 to provide three types of samples for the benchmark testing. **Fig. 1** shows the SEM observation images of the internal structure of each sample.

Also, the amount of solid-solution carbon in the martensite phase was analyzed by EPMA. As a result, the average was 0.40 wt% in the DP steel sample (Fig. 1 (a)), while it was 0.49 wt% in the martensite single-phase sample (Fig. 1 (c)). This suggests that the obtained materials have characteristics almost comparable to those of martensite phase.

Furthermore, the structural image in Fig. 1 (a) was analyzed to calculate the surface fraction of the martensite phase in the DP steel sample, and the fraction turned out to be 10 to 15%.

1.2 Tensile testing

Multiple sheet specimens with a gauge length of 12.5 mm, a width of 3 mm, and a thickness of

Table 1 Compositions and heat treatment condition of each steel sample

Sample	Composition (wt%)			Heat treatment condition
	C	Si	Mn	
(a) Dual-phase	0.063	0.50	1.46	800℃-30min 650℃-10min WQ
(b) Ferrite	0.032	0.43	1.37	880℃-30min AC
(c) Martensite	0.49	0.59	1.59	880℃-30min WQ

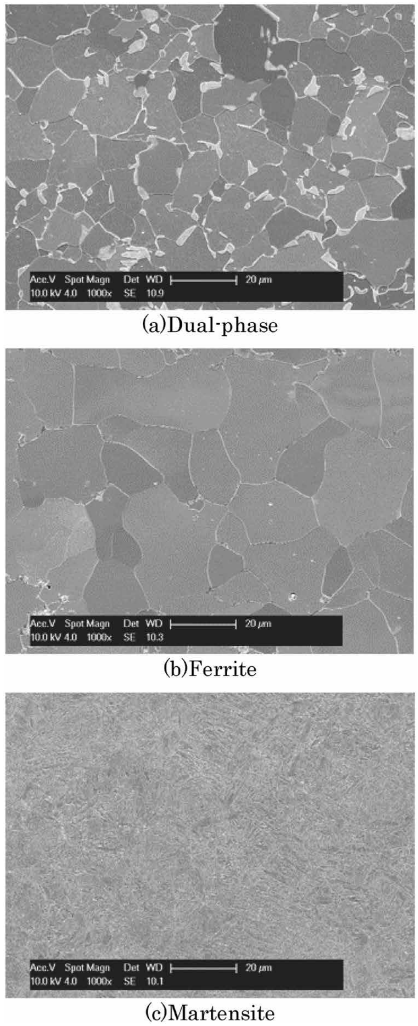

Fig. 1 SEM image of each steel sample

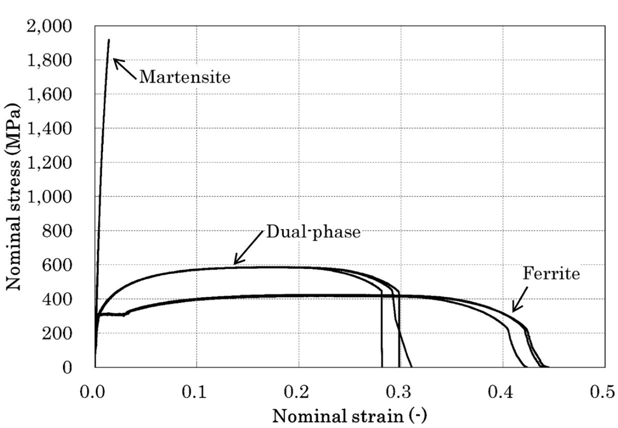

Fig. 2 Nominal stress vs. nominal strain curves of each steel sample

1.2 mm were cut out from each of the above samples. These specimens were subject to tensile testing using a universal testing machine under a crosshead displacement rate of 1 mm/min and room temperature environment.

Fig. 2 shows each sample's nominal stress–nominal strain diagram. Reproducible data were obtained for the DP steel and ferrite single-phase material. The tensile strength of the DP steel prepared this time was slightly less than 600 MPa. On the other hand, the martensite single-phase material exhibited extremely brittle behavior and resulted in fracture at an extremely low strain region (nominal strain 1.4% at the maximum).

2. Formulation based on homogenized elasto-plastic theory

Homogenization method[6), 7)] is one of the numerical analysis methods for coupling and analyzing mechanical behaviors of different scales. In the homogenization method, the governing equations of micro- and macro-scales satisfy physical and mathematical consistency and are versatile enough to handle any geometry in micro-construction.[6)] Therefore, in this study, an attempt has been made to formulate a FE simulation on the basis of the homogenization theory extended to the large deformation elasto-plastic problems.[6), 7)]

The displacement velocity vector $\dot{\boldsymbol{u}}$ at any material point is assumed to be additively decomposable as in the following equation:

$$\dot{\boldsymbol{u}} = \dot{\boldsymbol{u}}^0 + \dot{\boldsymbol{u}}^* \quad (1)$$

wherein the right superscript 0 and * represent the uniform macroscopic component and the perturbed component therefrom, respectively. The macroscopic component acts uniformly on the micro-scale structure, and the perturbed component is the quantity due to the heterogeneity of the micro-scale structure.

The homogenization method assumes that the perturbed component is distributed in the unit cell Y corresponding to the unit structure of the micro-scale, and this Y is placed periodically. This periodicity is referred to as Y-periodicity, and it is generally known that the obtained macroscopic response satisfies various mechanical consistency if the perturbed component $\dot{\boldsymbol{u}}^*$ is a function that changes periodically.[6)]

The following equation was adopted as the material constitutive law for micro-scale structure based on large deformation theory.

$$\check{\boldsymbol{\sigma}} = \boldsymbol{C}^{\mathrm{ep}} : \boldsymbol{D} \quad (2)$$

$$\check{\boldsymbol{\sigma}} \equiv \dot{\boldsymbol{\sigma}} - \boldsymbol{L}\boldsymbol{\sigma} - \boldsymbol{\sigma}\boldsymbol{L}^{\mathrm{T}} \quad (3)$$

wherein

- $\boldsymbol{\sigma}$: microscopic Cauchy stress tensor
- $\check{\boldsymbol{\sigma}}$: upper-convective derivative for microscopic Cauchy stress tensor
- $\boldsymbol{C}^{\mathrm{ep}}$: micro isotropic elasto-plastic coefficient tensor

$\boldsymbol{D}$: deformation rate tensor

$\boldsymbol{L}$: gradient tensor for displacement rate.

It should be noted that the plastic constitutive equation incorporates the related flow rule, and the Mises yield condition has been used for each phase that constitutes the micro-scale structure. According to the homogenization theory in the framework of large deformation by Ohno et al.,[7] the governing equations of micro-scale are derived as equation (4), and the homogenized elasto-plastic constitutive law of macro-scale is derived as equation (5) ;

$$\int_Y \left\{ \frac{1}{2} C^{ep}_{ijmn} \left(\dot{\chi}^{<kl>}_{m,n} + \dot{\chi}^{<kl>}_{n,m} \right) \delta \dot{u}^*_{i,j} + \dot{\chi}^{<kl>}_{i,m} \sigma_{m,j} \delta \dot{u}^*_{i,j} \right\} dY = \int_Y C^{ep}_{ijkl} \delta \dot{u}^*_{i,j} dY \quad \cdots\cdots (4)$$

$$\check{\boldsymbol{\Sigma}} = \boldsymbol{C}^{\mathrm{epH}} : \boldsymbol{D}^0 \quad \cdots\cdots (5)$$

$$C^{\mathrm{epH}}_{ijkl} \equiv \frac{1}{|Y|} \int_Y \left(C^{ep}_{ijkl} - C^{ep}_{ijmn} \dot{\chi}^{<kl>}_{m,n} \right) dY \quad \cdots\cdots (6)$$

$$\dot{u}^*_i = \dot{\chi}^{<kl>}_i D^0_{kl} \quad \cdots\cdots (7)$$

wherein

$\dot{\chi}^{<kl>}_i$: characteristic displacement rate vector

$\delta \dot{u}^*_i$: perturbed component of virtual displacement rate

$\check{\boldsymbol{\Sigma}}$: upper-convective derivative for macroscopic Cauchy stress tensor

$\boldsymbol{C}^{\mathrm{epH}}$: homogenized macroscopic elasto-plastic coefficient tensor

$\boldsymbol{D}^0$: macroscopic deformation rate tensor

$|Y|$: unit cell volume of micro-scale structure.

Discretizing equation (4) gives an element stiffness equation for determining the characteristic displacement rate in the micro-scale structure. The characteristic displacement rate obtained from the equation corresponds to the perturbed response when uniform macroscopic deformation information is given to the boundary value problem on the micro-scale side. On the other hand, the heterogeneity in the micro-scale is reflected in the macroscopic response from Eq. (6) via the spatial differentiation of the characteristic displacement rate, allowing response solutions on both scales while satisfying consistency on different microscopic/macroscopic scales.

3. Multiscale strength analysis of DP steel

A homogenized elasto-plastic FE simulation code has been developed on the basis of the formulation described in Section 2, and multiscale strength analysis has been performed on DP steel. This section compares the results of the strength analysis with the material testing results in Section 1 and describes the content of the examination of the validity and effectiveness of the development method.

3.1 Analysis model for DP steel microstructure

A mesh model for the unit cell of micro-scale has been created by image-based modeling using the microstructure image in Fig. 1 (a). As shown in **Fig. 3**, the martensite phase has been extracted by binarizing the SEM image. After removing noise, the geometry data of the phase has been created by a peripheral display. After performing mesh division with a quadrilateral bilinear element, one layer has been provided in the depth direction to create a 3D mesh model that has been divided using a hexahedron bilinear element (8-node isoparametric element). This mesh division has resulted in a unit cell FE model with 40,279 elements and 81,014 nodes, both in total.

Assuming that the above unit micro-scale structure is placed periodically, as shown in **Fig. 4**, the unit cell has been given periodic boundary conditions for the perturbed displacement component. The tensile testing results in Fig. 2 have been converted to the true stress–plastic strain relationship, which has been subjected to multipoint

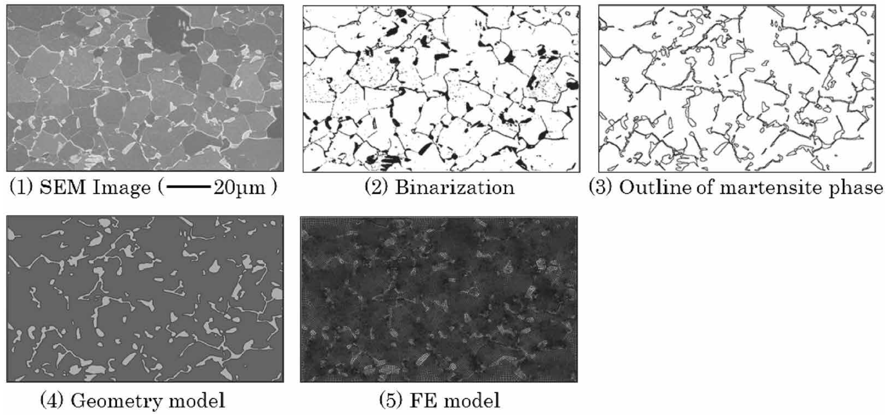

Fig. 3 Generation process of FE model for unit cell

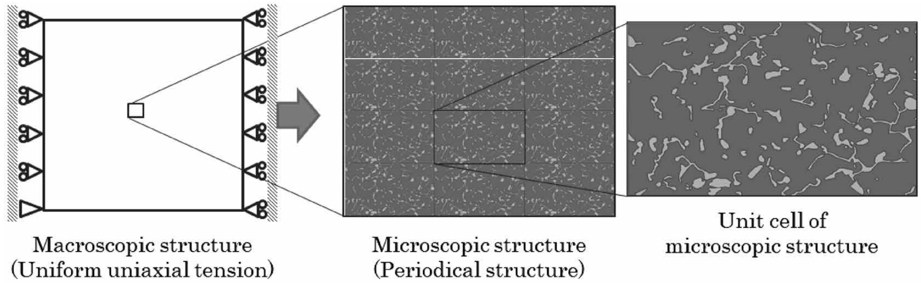

Fig. 4 Analytical model

approximation to yield the data for the stress–strain relationship of each phase constituting a unit cell. It should be noted that the damage of each phase has not been considered. In other words, the data obtained by applying the curve fitting with the power-law of the tensile testing result has been used for the stress value after the fracture limit strain of the martensite single-phase material.

On the other hand, the deformation of macro-scale structure was assumed to be uniform. Then, as input data to the boundary value problem of micro-scale structure, macroscopic strain increments equivalent to the uniaxial tension corresponding to the tensile testing have been given to all integration points in the unit cell for each increment calculation step (Fig. 4).

3.2 Results of multiscale simulation

Fig. 5 compares the simulation and experimental results of the true stress–plastic strain curves of the macro-scale structure obtained by the analysis model described in the previous subsection. The solid lines with the plot represent the input data given to each phase. The solid line without plot and the dashed line indicate the experimental result and the simulation result for DP steel, respectively. The tendency for the DP steel to have a stress value and apparent work hardening rate higher than those of ferrite single-phase has been reproduced, providing prediction results for stress-strain relations that are quantitatively close to the actual ones.

As examples of the evaluation of the mechanical behavior in the micro-construction by this simulation, the deformation of the unit cell at the elongation of 20% is depicted in **Fig. 6**, and the distribution of equivalent plastic strain is shown in **Fig. 7**. The distribution of Mises equivalent stress is shown in **Fig. 8**. The martensite phase surrounded by ferrite is elongated in the tensile direction, and the plastic deformation localizes in the ferrite phase near the region where the martensite phase is dense. The internal stress shows a high value in the hard martensite phase (Fig. 8 (a)), and focusing on the

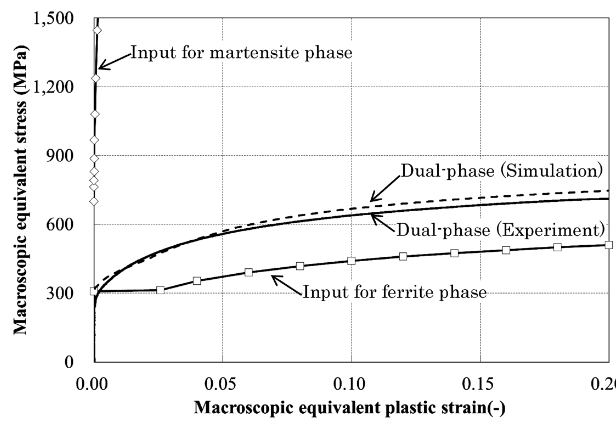

Fig. 5 Macroscopic stress-strain curves obtained by multiscale simulation

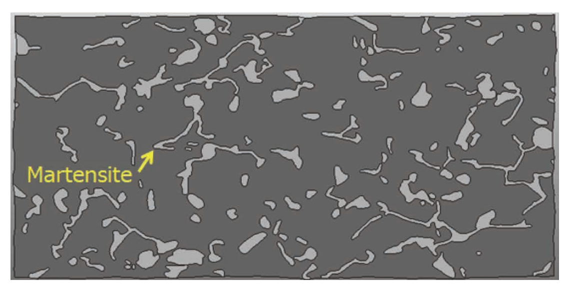

Fig. 6 Deformation of unit cell (at 20% elongation)

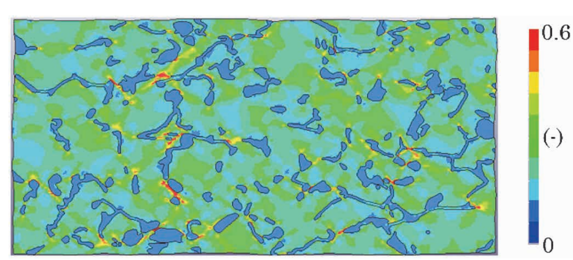

Fig. 7 Distribution of equivalent plastic strain (at 20% elongation)

ferrite phase, the internal stress is confirmed to be high in the region where plastic deformation is relatively large (Fig. 8 (b)). On the other hand, as shown in Fig. 7, plastic strain in the order of several percent occurs even in the martensite phase. In other words, the simulation result suggests that the deformability of the martensite phase is significantly higher in the case of DP steel than in the single-

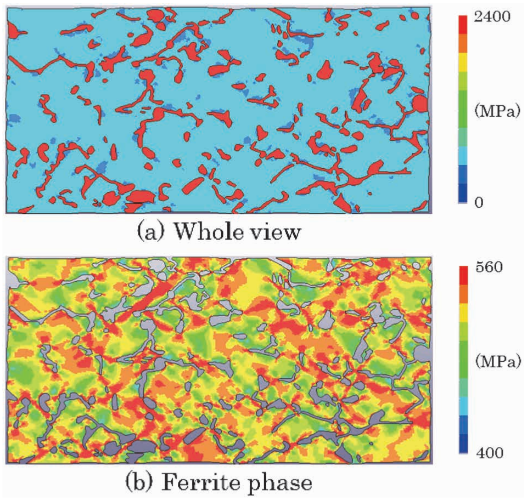

Fig. 8 Distribution of equivalent stress (at 20% elongation)

phase material that fractures in the extremely low strain region.

3.3 SEM observation of specimen after tensile testing

For comparison with the simulation results of the previous subsection, the structure near the fracture surface after the tensile testing (necking part) has been observed for the DP steel specimen to investigate the shape and characteristics of each phase of ferrite and martensite after deformation. As shown in **Fig. 9**, the martensite phase is greatly affected by the plastic deformation effect of the surrounding ferrite phase and is elongated in the tensile direction. This is the same tendency as found in the simulation results. In other words, the results suggest the occurrence of plastic deformation exceeding the fracture limit strain during the tensile testing of the single-phase sample. Macroscopically, the single-phase and DP steel samples have been subjected to the same uniaxial tension. In the martensite phase of DP steel, however, there is a microscopic change to a multiaxial stress field depending on the presence or absence of the surrounding ferrite phase and its deformed state. Therefore, it is presumed that a significant plastic deformation occurred before the fracture compared to the single-phase sample case. The elucidation of the mechanism by which the multiaxial stress field is configured is an issue for the future. A detailed comparative evaluation will be carried out with the help of the newly developed multiscale simulation.

In addition, many microscopic voids have been observed in the ferrite phase near each interface between the phases, mainly in the region where the martensite phase is densely concentrated. It is presumed that these voids have linked to each

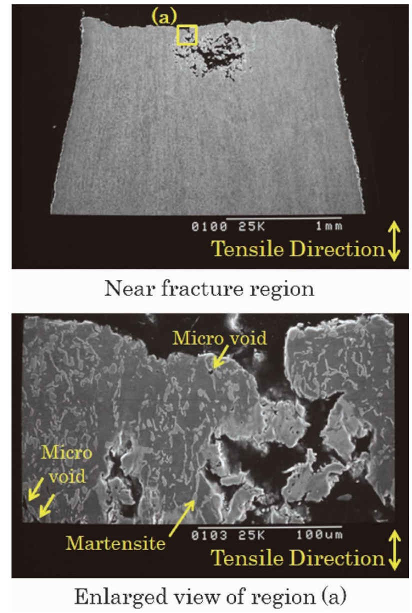

Fig. 9 SEM image near fracture region in specimen

other and led to the fracture. In other words, the microscopic plastic deformation behavior on the ferrite phase before fracture shows the same tendency as the simulation results of the previous subsection.

From the above, the multiscale simulation method developed in this study is concluded to be an effective method that allows simultaneous analysis of the microscopic heterogeneous deformation behavior caused by the internal structure in addition to the prediction of macroscopic mechanical properties.

Conclusions

In this study, multiscale strength analysis has been performed by FE simulation of large deformation based on the homogenized elasto-plastic theory for DP steel consisting of ferrite and martensite phases.

For the analysis, material testing data has been obtained for the single-phase sample with characteristics comparable to each phase constituting the DP steel of the benchmark target. Furthermore, the microstructural morphology information inside the material has been reflected in the analysis model by image-based modeling based on the SEM image. The effort has enabled simultaneous analysis of macro stress-strain relationship prediction and microstructural level mechanical behavior, a step toward elucidating the correlation between material properties and internal structure morphology.

Kobe Steel will strive to upgrade this multiscale analysis method so as to evaluate the effect of microstructural morphology on the strength properties and ductile fracture behavior in practical material.

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