Micromechanical Modeling of Ferrite–Pearlite Steels Using Finite Element Unit Cell Models

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An axisymmetric unit cell model based on a regular array of second-phase particles arranged on a BCC lattice is used to study deformation mechanisms of ferrite–pearlite structural steels. Microstructural characteristics of the steels were parameterized by the pearlite volume fraction, the aspect ratio of the pearlite particles, and the neighboring factor, which represents the ratio of interparticle spacing in the longitudinal direction to that in the transverse direction. FE analyses were carried out to investigate the macroscopic and microscopic response of unit cells with morphological features based on idealizations of the microstructures of the actual steels. Tensile properties of each constituent phase were obtained experimentally and used in the analyses. As compared to traditional axisymmetric models, the BCC cell model appears to be able to capture more realistically the behavior of the materials, and it accurately estimates the tensile behavior of the ferrite–pearlite steels even with a relatively large volume fraction of the pearlite phase. The effects of volume fraction and morphology of the second-phase particles on deformation behavior were also investigated.

KEY WORDS: structural steel; ferrite–pearlite steel; plastic deformation; unit cell model; FEM analysis.

1. Introduction

Controlling the microstructure is a key aspect to obtain optimum mechanical properties for many structural materials. Recently, high performance structural steels, such as high strength steels with low yield ratio for building use,1,2) and high strength line pipes with high hardening exponent,3) have been developed by using microstructure-control techniques. A number of models to predict microstructural properties from chemical compositions and process conditions have been developed and used in practice with reasonable accuracy. However, the relations between mechanical properties and microstructure are not yet clear enough to make precise predictions, especially for high strength structural steels having complex microstructures. In many cases, much experimentation is still necessary to optimize the mechanical properties of newly-developed materials.

Tomota et al. proposed a continuum model for predicting tensile behavior of two-ductile-phase alloys.4,5) This model can predict stress–strain curves of dual-phase materials from the tensile properties of each constituent phase, and it can be applied to three-phase materials.6) Hueper et al.7) examined the hardening behavior of two-phase high strength steels by using Tomota’s continuum model. Although this continuum model successfully predicts the stress–strain behavior of the multi-phase material, it does not provide the local stress–strain state inside each phase. As this continuum model is based on Eshelby’s inclusion theory8) and Mori–Tanaka’s mean field concept,9) stress and strain distributions are averaged inside each phase; while the actual stress–strain distribution in each phase of the material can display a substantial degree of localization. Furthermore, Tomota’s model has been mainly applied for materials containing spherical inclusions or second-phase particles, while many high strength structural steels are produced by controlled rolling processes, resulting in a microstructure elongated along the rolling direction, for which large effects of the shape and distribution of the second-phase on the mechanical properties can be expected.

In order to determine the local stress–strain state and the effect of the morphology of the second-phase particles, preliminary investigations have been conducted by finite element analysis.10,11) However, these two-dimensional FE analyses gave only qualitative information on the local stress–strain state, or the macroscopic behaviors of multi-phase materials because of the difficulty in constructing an adequate model which captures the real mechanical behavior of the microstructure, especially the interactions of heterogeneous representative volume elements.

Following its introduction by Tvergaard,12) the stacked-hexagonal-array axisymmetric cell model (SHA model) has been commonly used for FE-analysis of porous materials
and two-phase materials with spheroidal inhomogeneities. The distribution of voids or second-phase particles is idealized by an array of hexagonal cylinders, each containing a spherical void or second-phase particle. This model is quite accurate if the volume fraction of voids or second-phase particles is small, or when there is relatively small contrast in deformation resistance between the matrix and particle phases, however, it does not provide an adequate prediction for the macroscopic material behavior when the interaction between adjacent voids or second-phase particles is not negligible. Recently, Socrate and Boyce proposed a simplified axisymmetric finite element unit cell model to investigate macroscopic and microscopic stress–strain behavior of toughened polycarbonate. This axisymmetric unit cell model (V-BCC model) is based on a Voronoi tessellation of the BCC lattice, which better represents the spatial distribution of voids or second-phase particles, and can accommodate a local deformation mode consisting of shear localization of matrix materials between voids. Socrate and Boyce investigated porous materials, but this new micromechanical model can be valuable to investigate many cases of two-phase materials.

In this study, the axisymmetric Voronoi cell model was used to estimate the deformation behavior of two-phase structural steels, and to investigate the effects of volume fraction and the morphology of the second phase on macroscopic and microscopic response. The applicability of this new micromechanical model was verified by comparisons with experimental results.

2. Characterization of Microstructure

2.1. Tensile Properties of Two-phase Structural Steels

Figure 1 shows microphotographs of the steels used for the test. Ferrite–pearlite structural steels were selected for an investigation of the ability of the micromechanical models to estimate macroscopic properties. All steels have a ferrite–pearlite microstructure, but volume fractions and/or morphologies of the pearlite phase are different. Although pearlite itself consists of finely interspersed layered ferrite and cementite phases, the pearlite phase was treated as a single phase in this study, in order to simplify the model. Chemical composition and mechanical properties of the steels are shown in Table 1. Steels D1 and D2 have the same chemical composition and almost the same pearlite volume fraction, though Steel D2 was produced by controlled rolling, and it has an elongated microstructure along the rolling direction. Steel F1 has low carbon content, and the pearlite volume fraction is also low. Tensile tests of these two-phase steels were conducted using smooth round bar specimens with the tensile direction parallel to the rolling direction. The tensile properties of the steels are also listed in Table 1. All of those steels exhibit a Luders elongation of up to about 3% strain. The power law strain hardening exponents, n, as defined in Eq. (6), are also listed in Table 1.

2.2. Morphological Characteristics of the Pearlite Phase

As can be seen in Fig. 1, the second-phase particles (pearlite nodules) are not always spherical, and the spacings of adjacent pearlite nodules in the rolling direction differ from those in the transverse direction, because the microstructure is generally elongated in the rolling direction. These morphological characteristics can be represented by three geometrical parameters: the volume fraction of the second phase, \( f_p \), the particle aspect ratio, \( R_a \); and the neighboring factor, \( N_f \). A schematic idealization of the microstructure, used to illustrate the morphological parameters, is shown in Fig. 2. The aspect ratio is given by \( R_a = b/a \), where \( b \) and \( a \) are averaged nodule sizes in the rolling direction and in the transverse direction, respectively. The neighboring factor is defined as,

\[
N_f = \frac{\lambda_t}{\lambda_L}, \quad \text{.................................(1)}
\]

where \( \lambda_L \) and \( \lambda_T \) are average center-to-center spacings of

![Fig. 1. Microphotographs of the ferrite–pearlite steels.](image)

Table 1. Chemical composition and mechanical properties of the steels.

| Steel | Chemical composition (mass. %) | Manufacturing process | YS (MPa) | TS (MPa) | EL (%) | RA (%) | n  |
|-------|--------------------------------|-----------------------|----------|----------|--------|--------|----|
| D1    | 0.153 0.39 1.35 0.016 0.004 0.010 others | Conv. | 557      | 529      | 38     | 77     | 0.213 |
| D2    | CR    | 412 536 39 79 0.184 |          |          |        |        |     |
| F1    | 0.033 0.31 1.14 0.016 0.001 0.034 0.040 Cu, Ni | Conv. | 390 495 37 80 0.155 |        |        |     |

* Conv.: Conventional rolling, CR: Controlled rolling
with increasing the degree of undercooling. Chemical composition temperature, and the lamellar spacing decreases degree of undercooling from the equilibrium pearlite transformation. The driving force for pearlite transformation increases with the strong pearlite lamellar spacing. The tensile behavior of pearlite is essentially the same cooling rate imposed for the ferrite–pearlite steel, a fully pearlitic steel with eutectoid composition of 0.68%C–0.24%Si–0.87%Mn (in mass%) was prepared by a conventional hot rolling process mainly. However, those empirical expressions were obtained from experiments over limited ranges of chemical compositions and manufacturing processes, and their accuracy and availability are limited. In this section, stress/strain curves for each constituent phase are estimated from experimental data and numerical expressions proposed in the literature.

2.3. Estimation of Stress/Strain Curves for each Constituent Phase

The definition of a stress/strain relation for each constituent phase is essential for the development of the micro-mechanical models to investigate macroscopic and microscopic behavior of multi-phase materials. There have been a number of numerical expressions proposed for estimating the tensile properties of single phase in multi-phase steels. However, those empirical expressions were obtained from experiments over limited ranges of chemical compositions and manufacturing processes, and their accuracy and availability are limited. In this section, stress/strain curves for the ferrite and pearlite phases are estimated from experimental data and numerical expressions proposed in the literature.

To obtain the tensile behavior of the pearlite phase in a ferrite–pearlite steel, a fully pearlitic steel with eutectoid composition of 0.68%C–0.24%Si–0.87%Mn (in mass%) was prepared by a conventional hot rolling process maintaining essentially the same cooling rate imposed for the ferrite–pearlite steels. The tensile behavior of pearlite is strongly affected by the pearlite lamellar spacing. The driving force for pearlite transformation increases with the degree of undercooling from the equilibrium pearlite transformation temperature, and the lamellar spacing decreases with increasing the degree of undercooling. Chemical composition can also affect the pearlite structure; manganese is thought to be an alloying element which decreases the lamellar spacing under isothermal transformation. Although there may be slight differences in the chemical composition between the pearlite phase in the ferrite–pearlite steels and that of the fully pearlitic steel, the degree of undercooling for both steels are similar under continuous cooling with the same cooling rate. The stress/strain curve of this fully pearlite steel is shown in Fig. 3. Luders elongation was not observed in the pearlite phase. The pearlite volume fraction of the ferrite–pearlite steels is under 20% in this study, so the effects of differences in the pearlite tensile properties on the macroscopic behavior of the ferrite–pearlite steel are relatively small compared with those of the ferrite properties.

The mechanical properties of the ferrite phase have a major effect on the macroscopic response of the ferrite–pearlite steels used in this study. An extensive investigation on tensile behavior of single phase steels was carried out, and empirically-based numerical expressions which predict the tensile properties from chemical compositions and microstructural characteristics were proposed. However, it is difficult to accurately estimate the stress/strain relation of the ferrite phase in the ferrite–pearlite steels, because the contributions of microalloying elements, such as Nb and V, depend on the thermo-mechanical condition during hot rolling, and only a small difference in precipitation conditions may dramatically change the resulting mechanical behavior of the ferrite phase. The mechanical properties of the ferrite phase in microalloyed ferrite–pearlite steel is to measure the hardness of the ferrite phase. Suehiro et al. proposed a simple relation between tensile strength and hardness of carbon-manganese steels as follows,

\[ TS = 3.04HV \]  

where \( TS \) and \( HV \) are the tensile strength (MPa) and the Vickers hardness, respectively. Hardnesses of the ferrite phase of the three steels were measured using a micro Vickers hardness test machine with a test load of 0.49 N (50 gf). Figure 4 shows a Weibull distribution of the ferrite hardness for the three steels. Hardness data show a large scattering for all steels. This scattering is probably caused by microscopic inhomogeneities of chemical composition.

Table 2. Microstructural characteristic of the steels.

| Steel | Pearlite volume fraction, \( f_p(\%) \) | Ferrite grain size, \( d (\mu m) \) | Aspect ratio, \( R_a \) | Neighboring factor, \( N_f \) |
|-------|-----------------------------------|-------------------------------|------------------|-------------------|
| D1    | 18.8                              | 13.4                         | 1.60             | 1.12              |
| D2    | 18.3                              | 7.5                          | 2.69             | 1.95              |
| F1    | 2.6                               | 17.0                         | 1.19             | 0.96              |

![Fig. 2. Schematic view of measurement of the pearlite shape and distribution.](image)

![Fig. 3. Nominal stress/nominal strain curves for each phase.](image)
An increase brought about by addition of Nb (\textsuperscript{21}), therefore, the coefficient for V was taken to be one third of that of Nb in Eq. (5).

The tensile properties of the ferrite phase in the ferrite–pearlite steels are estimated based on Eqs. (2), (3) and (5). Stress/strain curves can be constructed using these parameters (TS, YS and n) as discussed in the following. The stress/strain curves of the ferrite–pearlite steels exhibit a Luders elongation, while the pearlite phase shows continuous hardening after yielding. This means that the ferrite phase should show a Luders elongation, and this discontinuous behavior in the stress/strain relation should be taken into account in the micromechanical models. The plastic part of stress/strain curve which has a Luders elongation is expressed as:

\[ \sigma = \sigma_y(1 + \varepsilon) \quad \text{if} \quad \varepsilon \leq \varepsilon_k \quad \text{................(6)} \]

\[ \sigma = F\varepsilon^n \quad \text{if} \quad \varepsilon > \varepsilon_k \quad \text{................(7)} \]

where \( \sigma \), \( \sigma_y \), \( \varepsilon \), \( \varepsilon_k \) and n are true stress, true yield stress, true strain, strain at the onset of hardening and hardening exponent, respectively. F is called the strength coefficient, and is given by:

\[ F = YS(1 + \varepsilon_k)/\varepsilon_k^n \quad \text{................(8)} \]

where YS is the yield strength, which is identical to \( \sigma_y \). The hardening exponent is approximately equal to the true strain corresponding to the ultimate tensile stress, \( \sigma_u \). This relation can be expressed by:

\[ \sigma_u = TS(1 + n) = Fn^n \quad \text{................(9)} \]

where TS is the tensile strength. The strain at the onset of hardening can be obtained by combining Eqs. (8) and (9).

Tensile properties evaluated for ferrite and pearlite phases are listed in Table 3. The stress/strain curves calculated for ferrite phase by using Eqs. (6) and (7) are also plotted in Fig. 3 together with the experimental stress/strain curve of the pearlite phase.

Table 3. Tensile properties of the ferrite and pearlite phases.

| Steel | YS (MPa) | TS (MPa) | n  | e_k (%) | YS (MPa) | TS (MPa) | n  |
|-------|----------|----------|----|---------|----------|----------|----|
| D1    | 347      | 498      | 0.20 | 1.3     | 490      | 837      | 0.26 |
| D2    | 407      | 468      | 0.17 | 2.6     |          |          |     |
| F1    | 389      | 501      | 0.13 | 0.7     |          |          |     |

3. Micromechanical Modeling for Two-phase Materials by Axisymmetric Unit Cell

3.1. Stacked Hexagonal Array (SHA) Model

In general, second-phase particles are not uniform in size and are distributed randomly throughout the matrix. In order to simulate the deformation behavior of porous materials, Tvergaard\textsuperscript{(22)} proposed a stacked hexagonal array (SHA) model, a three-dimensional periodic array of hexagonal cylinders of matrix material each containing a void, as shown in Fig. 5(a). The hexagonal cylinders can be replaced with equivalent circular cylinders, and only half of the cylinder is needed for analysis because of assumed periodicity and symmetry, which is illustrated in Fig. 5(b).

Accordingly, a two-dimensional axisymmetric unit cell containing ferrite and pearlite steels was estimated as one third of the corresponding micromechanical model, a three-dimensional periodic array of hexagonal cylinders of matrix material each containing a void, as shown in Fig. 5(a). The hexagonal cylinders can be replaced with equivalent circular cylinders, and only half of the cylinder is needed for analysis because of assumed periodicity and symmetry, which is illustrated in Fig. 5(b).
contain a second-phase particle can represent the entire two-phase material under proper boundary conditions which ensure macroscopic compatibility of the deformation field (i.e., no separation or overlapping of material at the boundary of two adjacent cells). This model was extensively applied for investigating the macroscopic and microscopic behavior of polymers and metal-matrix composites.

The initial geometry of the SHA cell can be characterized by the parameters \( H_0 \) and \( R_0 \) as indicated in Fig. 5(b). If the microstructure is elongated in the \( z \)-direction and the initial height of the unit cell is chosen as \( H_0 = 1.0 \), the initial radius of the cell is defined as \( R_0 = 1/N_f \). The geometry of the second-phase particle is defined according to the specific volume fraction of the second-phase, \( f_p \), and the average aspect ratio, \( R_a \). The boundary conditions for this SHA model are prescribed as: (i) points on the \( z \)-axis and points on the \( r \)-axis are constrained in the radial and axial direction, respectively; (ii) points on the top plane \( (z = H_0) \) are required to have equal axial displacement; (iii) points at the outer radius of the cell \( (r = R_0) \) are required to have equal radial displacement.

Although the SHA model has been widely used in many studies on deformation mechanisms of voided or two-phase materials, we found that this model was unable to capture the deformation behavior of matrix materials between particles or voids precisely, especially, when the volume fraction of the voids or particles is relatively large and there is large contrast in the deformation resistance of the two phases, as shown in Fig. 3.

### 3.2. Voronoi Tessellation of BCC Lattice (V-BCC) Model

In order to solve the inherent limitations of the SHA model, an alternative model based on a staggered array of particles was introduced by Socrate and Boyce. In this model, a truncated octahedron, i.e., the Voronoi cell of the BCC lattice is used as a space-filling polyhedron as shown in Fig. 6(a). The second-phase particles are arranged on a regular body centered cubic lattice (Fig. 6(b)). The Voronoi cell is produced by following procedure. First, the center of a reference cube is connected by straight lines to its eight vertices and to the centers of the six adjacent cubes. Second, each segment is perpendicularly bisected by a plane. As a result, the truncated octahedron is formed as a 14 sided body with six square faces bisecting the ‘center–center’ segments and eight hexagonal faces bisecting the ‘center–vertex’ segments. Because of the periodic symmetry, only half of this Voronoi cell is used to define the unit cell. Under axisymmetric loading conditions, the cell geometry can be approximated as axisymmetric. Fig. 7(a) shows two adjacent axisymmetric cells, \( C_0 \) and \( C_1 \). Areas of the cross section of the \( C_0 \) and \( C_1 \) cells with the plane \( z = \xi \) are denoted as \( A_d(\xi) \) and \( A_l(\xi) \), respectively. Considering the space-filling properties of the unit cells in the BCC lattice, the following constraints are dictated by symmetry conditions if the initial height of the unit cell was chosen as \( H_0 = 1.0 \).

\[
A_d(\xi) + A_l(\xi) = \text{constant}, \quad \text{.................(10)}
\]

\[
A_d(\xi) = A_l(1 - \xi), \quad \text{.................(11)}
\]

Substituting Eq. (9) and (10) gives,
The constraint condition for outer boundary of the reference cell, Eq. (12), can then be expressed in terms of \( R_0(z) \) as,

\[
(R_0(\xi))^2 + (R_0(1-\xi))^2 = 2(R_0|_{0.5})^2, \quad \cdots \cdots \cdots \cdots (14)
\]

where \( R_0|_{0.5} \) is the radius of the cell at the midplane, \( \xi = 0.5 \). For the cells which have the neighboring factor of \( N_f \),

\[
R_0|_{0.5} = \frac{1}{N_f} \sqrt{\frac{2}{\pi}} \cdot \cdots \cdots \cdots \cdots (15)
\]

When axisymmetric loading is applied, the deformed outer radius of the cell, \( R(z) = R_0(z) + U_z(z) \), must satisfy following condition, analogous to Eq. (14),

\[
[R(z)(\xi) + U_z(\xi)]^2 + [R(z)(1-\xi) + U_z(1-\xi)]^2 = 2[R_0|_{0.5} + U_z|_{0.5}]^2, \quad \cdots \cdots \cdots \cdots (16)
\]

where \( U_z(\xi) \) is the radial displacement for a point on the outer boundary of the cell which is at \( z = \xi \) in the undeformed configuration, and \( U_z|_{0.5} \) is the radial displacement of the point at the outer radius with initial coordinate of \( (r=R_0|_{0.5}, z=0.5) \). Axial displacements of points on the outer boundary are also introduced by symmetry conditions for the two adjacent cells, as expressed by:

\[
U_z(\xi) + U_z(1-\xi) = 2U_z|_{0.5}, \quad \cdots \cdots \cdots \cdots (17)
\]

where \( U_z(\xi) \) is the axial displacement for a point on the outer boundary of the cell which is at \( z = \xi \) in the undeformed configuration, and \( U_z|_{0.5} \) is the axial displacement of the point at the outer radius with initial coordinate of \( (r=R_0|_{0.5}, z=0.5) \).

Equations (16) and (17) define the constraint condition for the outer boundary which must be imposed on the V-BCC cell to account for the antisymmetric adjacent cells which form the BCC lattice. Other boundary conditions are identical to those of the SHA cell: (i) points on the \( z \)-axis and points on the \( r \)-axis are constrained in the radial and axial direction, respectively, (ii) points on the top plane \( (z = 1.0) \) are required to have equal axial displacement. Note that, from these conditions plus Eq. (17), \( U_z \) on the top plane is required to be \( 2U_z|_{0.5} \).

It should be noted that the idea of this anti-symmetric boundary conditions, Equations (16) and (17), for an axisymmetric unit cell model was first proposed by Tvergaard, in order to investigate the tensile behavior of metal-matrix composite.\(^{25}\) Tvergaard also applied the anti-symmetric boundary conditions to study void interaction mechanisms in porous materials.\(^{25}\) However, the distinctive features of this kind of models were not fully explored.

### 3.3. Finite Element Implementation

FE analyses were carried out to investigate the macroscopic and microscopic response of ferrite–pearlite steels and the effects of morphology and pearlite volume fraction under monotonic tensile loading condition. The FE program ABAQUS ver. 5.8 (Hibbitt, Karlsson and Sorensen, Inc.) was used for this analysis. The V-BCC and SHA cells were modeled using axisymmetric second-order elements. Figure 8 shows examples of the finite element meshes for two-phase materials used in this analyses. Configurations of these meshes were defined in accordance with the actual microstructure of the ferrite–pearlite steels in which shape and distribution of the pearlite phase is parameterized by the volume fraction, \( f_p \), the aspect ratio, \( R_a \), and the neighboring factor, \( N_f \). However, the aspect ratio of the pearlite phase and the neighboring factor of steel F1 were taken as

**Fig. 7.** The axisymmetric V-BCC model: (a) an axisymmetric V-BCC cell with a neighboring antisymmetric cell, (b) deformation of the unit cell under the axial stress.

**Fig. 8.** Finite element meshes for ferrite–pearlite steels.
For cases where the aspect ratio of the second phase is greater than 1.0, the pearlite particle was modeled as a cylinder capped with a hemispherical end. The Poisson’s ratio was taken as 0.3 and the Young’s modulus as 206,000 MPa for all phases. The stress/strain relations evaluated in the previous section (Fig. 4) were used as material data characterizing the ferrite matrix and the pearlite phase. As described above, the most distinctive characteristics of the V-BCC model are the boundary conditions expressed by Eqs. (16) and (17), and these displacement boundary conditions were imposed via a “Multi Point Constraint (MPC)” user subroutine in the ABAQUS program.

4. Results of FE Analysis

4.1. Macroscopic Response of the Cells

Figure 9 compares the predictions of the V-BCC and SHA models to the experimental nominal stress/nominal strain curves for Steel D1. The stress–strain curves of each constitutive phase are also shown in Fig. 9. The V-BCC model for Steel D1 shows quite good agreement with experimental results, while the SHA model overestimates the level of nominal stress. Figures 10 and 11 show the comparison between the experimental nominal stress/nominal strain curves and model predictions for Steels D2 and F1, respectively. The V-BCC model gives good estimates for both Steels D2 and F1. In Fig. 10, the SHA model estimates nominal stress higher than experimental values for Steel D2 which has almost the same pearlite volume fraction as Steel D1, but elongated pearlite nodules. On the other hand, results of the SHA model for Steel F1, which has a very small pearlite volume fraction, are almost identical to the experimental nominal stress/nominal strain curve.

The hardening exponent of the estimated stress/strain curves by the V-BCC model for Steel D1, D2 and F1 are 0.219, 0.187 and 0.137, respectively. These values are also very close to the corresponding experimental values listed in Table 1.

By comparing the results for Steel D1 and Steel D2, it should be noted that the ferrite strength is smaller for Steel D2, but these two steels have almost the same pearlite volume fractions tensile strengths. This implies that the elongated microstructure affects the macroscopic response of the ferrite–pearlite steels, and this topic will be discussed in detail later.

4.2. Microscopic Stress–Strain Behavior in the Cells

As mentioned before, when the volume fraction of the second phase is relatively large and there is large contrast in the deformation resistance of the two phases, interaction between adjacent second-phase particles affects the microscopic behavior of two-phase materials. Figure 12 shows contour plots of Mises stress and equivalent plastic strain for Steel D1 at a nominal strain level of 20%. It is shown that the SHA model predicts higher levels of Mises stress and larger levels of deformation in the pearlite phase as compared to the V-BCC model. The outer boundary of the SHA model cannot change its cylindrical shape, and this boundary condition constrains plastic flow of the matrix material. As a result, equivalent deformation of the second phase is needed to keep the outer boundary shape, and this causes higher stress in the pearlite phase. On the other hand, the V-BCC cell has a less constraining boundary condition, which permits material on the outer boundary to shear and rotate, and this readily allows large plastic flow in the matrix materials without imposing deformation in the pearlite phase.

Stress–strain state of the entire material can be illustrated by periodic arrangements of the unit cells. Figure 13 shows the equivalent plastic strain distribution for Steel D1 at the nominal strain level of 20% in a wider view that contains
several pearlite particles. Plastic flow of the interparticle matrix can be seen easily in this figure. It is obvious that the region of matrix material at higher levels of plastic strain is larger for V-BCC model. The SHA model shows high equivalent plastic strain in the matrix material localized in the polar regions between pearlite particles. However, the equatorial regions between adjacent particles show a quite limited plastic strains because of the overly-constraining boundary condition.

Figure 14 shows the equivalent plastic strain distribution at the nominal strain level of 20% for Steel D2 and Steel F1 obtained by the V-BCC model. In Steel D2, large plastic strain regions are observed only near the poles of the pearlite particles, while the strain level in the equatorial regions is small. The mean spacing of adjacent particles in the loading direction is larger than the spacing in the transverse direction for Steel D2. This geometrical condition does not allow the matrix material to undergo substantial plastic deformation in the equatorial regions between the particles because of the constraints introduced by the elongated pearlite particles. Plastic deformation of the pearlite particles is needed to accommodate the global deformation, so that Steel D2 shows higher flow stress in spite of the relatively low strength of the ferrite phase. On the other hand, relatively homogeneous distribution of equivalent plastic strain in the ferrite matrix is observed in Steel F1. Because the interparticle distance is large compared to the diameter of pearlite particles, the pearlite phase in Steel F1 can be treated as an isolated particle with very small effects due to particle interactions, and a stress/strain behavior dominated by the material properties of the ferrite phase, as shown in Fig. 11. In this case, the behavior at the outer boundary of the cell is not largely affected by the pearlite particles, resulting in the same nominal stress/nominal strain curves of the V-BCC and SHA models.

Figure 15 shows the radial distribution of axial stress on the r-axis for Steels D1 and F1 at the nominal strain of 20% (undeformed coordinates).
models show almost same stress in the pearlite phase for Steel F1. This microscopic stress behavior reflects macroscopic response of the ferrite-pearlite steels; accordingly, the SHA model overestimates the level of nominal stress for Steel D1 while the estimated nominal stress/nominal strain curve is identical to that of the V-BCC model for Steel F1. As indicated in this section, macroscopic mechanical behavior of the material can be explained by microscopic stress/strain conditions of each constitutive phase. It can be stated that constructing a micromechanical model that captures the actual material behavior is quite important in order to make accurate predictions of the mechanical behavior of materials.

5. Discussion

It was shown that the V-BCC model can precisely estimate macroscopic material response even with relatively large volume fraction of the strong second phase, while the ordinary unit cell model (SHA model) generally overestimates the stress level. The V-BCC model is considered to be a useful tool to investigate the effect of microstructure on mechanical behavior of two-phase materials for the purpose of microstructural designing. In this section, the independent effects of the volume fraction and morphology of the pearlite phase on the tensile behavior are investigated numerically using the V-BCC model.

Figure 16 shows the effect of the pearlite volume fraction on the nominal stress/nominal strain curves estimated by the V-BCC model.

Figure 17 shows the estimated flow strength at a nominal strain of 10% as a function of the pearlite volume fraction. In order to clarify the difference in the macroscopic behavior of the cells, the estimations by SHA cells having the same microstructural configurations are also plotted in the figure. It is clearly shown that the flow strength of the V-BCC cell increases as the pearlite volume fraction increases, and the elongated cells give a higher strength increase. The strength increase by the elongated morphology increases with the pearlite volume fraction for the V-BCC model; the flow strength of the elongated cell ($R_a=2.0$, $N_f=2.0$) with the pearlite volume fraction of 40% is 6.5% higher than that of the non-elongated cell, while the flow strengths are almost same in the case of $f_p=5\%$. As suggested before by comparing Figs. 14(a) and 15(a), the plastic deformation of the interparticle matrix is constrained by the elongated pearlite particles because of the small distance between adjacent pearlites and its elongated shapes. The constraint effect by the elongated pearlite particles becomes more significant when the pearlite volume fraction is higher because the width of the interparticle matrix decreases with increasing perlite volume fraction. On the other hand, the SHA model with larger pearlite volume fraction estimates higher strength than the V-BCC model. The increase of the flow strength by the elongated microstructure is smaller than that of the V-BCC model, and the results from the cells with $R_a=N_f=2.0$ and $R_a=N_f=4.0$ are the almost same. Plastic flow of the matrix material is already suppressed by the outer boundary in the SHA model, and the effect of the elongated pearlite particles is hidden by this overly-constrained boundary condition. This illustrates the inherent limitation of the SHA model in describing the microscopic behavior of two-phase materials.

Figure 18 shows the effects of the morphology of pearlite phase on the stress/strain curve. Aspect ratio, $R_a$, and neighboring factor, $N_f$, were changed simultaneously from 1.0 to 4.0 while keeping the pearlite volume fraction constant as $f_p=20\%$. Effect of the elongated morphology becomes saturated as $R_a$ and $N_f$ increase under the constant pearlite volume fraction. It is suggested that increasing pearlite volume fraction is the most effective measure to increase the strength of the ferrite-pearlite steels if the materials properties of the ferrite and pearlite phases do not
change.

A few examples of the investigation of the microstructural effects on the tensile properties of ferrite–pearlite steels, by using the axisymmetric unit cell models, were presented in this section. Accurate definitions for the material properties of each phase and microstructural characteristics are needed for more precise estimation of the macroscopic and microscopic behavior of the two-phase materials. These results illustrate how the mechanical properties of structural materials can be imposed by controlling microstructural features, and demonstrate the potential of this kind of finite element analysis to become a useful tool in the development of new materials.

6. Conclusions

A finite-element unit cell model based on a regular array of second-phase particles, which is equivalent to the Voronoi tessellation of the BCC lattice (V-BCC model), was used to study deformation mechanisms of ferrite–pearlite structural steels. The effect of the microstructural characteristics on tensile properties under monotonic loading was investigated using the V-BCC model. Applicability of this new micromechanical model was verified by comparisons with experimental results for steels having different microstructures.

The estimated nominal stress/nominal strain curves obtained from the V-BCC model show quite good agreement with experimental results for all steels considered, while the ordinary stacked hexagonal type cell model (SHA model) overestimates the stress level for steel with higher pearlite volume fractions. The V-BCC cell model appears to be able to capture the realistic behavior of the materials because of the less constrained boundary condition which permits material on the outer boundary to rotate. This results in more reliable predictions of macroscopic and microscopic response of the materials, compared with the SHA model which has inherent limitations in predicting the mechanical behavior of two-phase materials with a relatively large volume fraction of the second phase, and high contrast in deformation resistance between the two phases.

The V-BCC model can quantitatively assess the effects of microstructural parameters on tensile properties of the ferrite–pearlite steels. Furthermore, this kind of finite element analysis can be a useful tool for the purpose of microstructural designing of structural materials.

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