A Constitutive Model for Transformation Superplasticity under External Stress during Phase Transformation of Steels

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(Received on July 16, 2001; accepted in final form on October 4, 2001)

Most models of superplastic deformation behavior under external stress during phase transformation have been derived under the assumption of plastic deformation in the weaker phase. In the present paper, we suggested a constitutive model for the transformation induced superplastic deformation of steels based on a concept of Migration of Transformation Interface induced Plasticity (MITIP) including the phase transformation kinetics. The concept is that the migration of atoms in the transformation interface is a principal mechanism of superplastic deformation under stresses during phase transformation. The model could well describe the effect of the cooling rate, the transformed phase and the transformation temperature on the amount of the transformation induced superplastic strain. In order to calculate the deformation behavior under stresses during phase transformation of steels, the elastic strain, the volumetric strain due to thermal and phase transformation, the viscoplastic strain, and the transformation induced superplastic strain were taken into account. The calculated results were found to be in good agreement with the experimental data obtained from literature.

KEY WORDS: transformation superplasticity; migration of transformation interface; constitutive model; phase transformation.

1. Introduction

It has been reported that when phase transformation takes place under an applied stress, even for the stress lower than the yield stress of material, a permanent strain occurs.\(^1\)\(-\)\(^7\) These experiments were carried out with steels by the method of temperature cycling through \(\gamma\)\(-\)\(\alpha\) transformation, and the large elongated specimens like superplastically deformed ones were obtained. Therefore, this phenomenon has been called as the transformation superplasticity: it takes place only when transformation progresses.

Several interpretations have been given for the transformation superplasticity. Assuming an ideally plastic material undergoing a phase transformation, Greenwood and Johnson\(^2\) derived an approximate analytical solution for the transformation superplastic strain. They regarded the mechanism of the transformation superplasticity as each element of the weaker phase in serration of the transformation front plastically deforms to accommodate the applied stress and the internal stress caused by the volume change of a neighbouring element during phase transformation. To describe the permanent strain under an applied stress lower than the yield stress of the material, the internal stress as a form of the volume mismatch, \(\Delta V/V\), was introduced to the model:

\[
\Delta e^{ts} = \frac{5}{6} \frac{\Delta V}{V} \frac{\sigma}{\sigma_Y} \quad \text{......................}(1)
\]

where \(\Delta e^{ts}\), \(\sigma\) and \(\sigma_Y\) are the transformation superplastic strain increment, the applied stress and the yield stress of the weaker phase, respectively.

Based on the internal stress model of Greenwood and Johnson, several modified models have been proposed.\(^8\)\(-\)\(^10\) Most models predict a linear relationship between the applied stress and the transformation superplastic strain and are only valid under low applied stresses. Recently, Zwigl and Dunand\(^10\) extended the linear model by Greenwood and Johnson and derived a nonlinear closed form solution valid over the whole range of stresses from the low-stress regime to the high-stress regime, where the strain increases nonlinearly as the applied stress approaches the yield stress of the weaker phase:

\[
\delta = \frac{1}{4} + \frac{1}{6\alpha} + \frac{1}{2\sqrt{2\alpha}} \left( \frac{3\alpha}{4} - \frac{1}{6} - \frac{1}{9\alpha} \right) \ln \left( \frac{(3\alpha + 3\sqrt{2\alpha} + 2)^2}{9\alpha^2 - 6\alpha + 4} \right) \quad \text{......................}(2)
\]

where the dimensionless parameters \(\delta = \sigma/\sigma_Y\) and \(\alpha = (\Delta e^{ts}/2)/(\Delta V/V)\) were introduced.

To apply the internal stress models to the calculation of stress field in material during phase transformation, the yield stress value of weaker phase in Eqs. (1) and (2)
should be determined. Fundamentally the plastic deformation of the weaker phase in transformation front, which is the basic mechanism of the internal stress models, has not been experimentally observed yet.

Poirier\textsuperscript{11} derived a dislocation based model, and showed the result can be reduced to Eq. (1). This model was extended by Gautier \textit{et al.} to include the kinetics of the phase transformation.\textsuperscript{6} Denis \textit{et al.}\textsuperscript{12,13} modified the model to calculate the residual stresses of a steel specimen during heat treatment:

\[
\Delta e^s = K(1 - X)\Delta X\sigma \hspace{1cm} \text{(3)}
\]

where $X$ is the volume fraction of the transformed phase and $K$ is a constant which could be obtained from the experiments under uniaxial stress states. The equation also shows a linear relationship between the applied stress and the transformation superplastic strain, and is only valid at low applied stresses. Recently, Tsutsumi \textit{et al.} suggested an empirical model from the results of beam deflection tests of a TMCP steel under constant cooling rates\textsuperscript{14}:

\[
\Delta e^s = D\sigma^m\Delta T \hspace{1cm} \text{(4)}
\]

where $\Delta T$ is temperature drop for a time step at a given cooling rate, and $D$ and $b$ are constants which could be experimentally determined. The exponent, $b$, was introduced to describe the nonlinear behavior of the transformation superplastic strain at high applied stresses.

On the other hand, \textit{in-situ} observations of the microstructural changes associated with the transformation superplasticity in iron were carried out with a high temperature optical microscope and a dark field reflection microscope by Saotome and Iguchi.\textsuperscript{15} The investigation confirmed that the sliding of the migrating transformation interface is a principal mechanism of the transformation superplasticity. Recently, Suh \textit{et al.}\textsuperscript{16} observed that the misorientation from Kurdjumov-Sachs relationship increased during the austenite to ferrite transformation of steel under the uniaxially stressed condition using EBSD technique. This phenomenon can be understood with the sliding of the migrating transformation interface.

In the present paper, we suggested a constitutive model for the transformation superplasticity of steels based on the concept of the Migration of Transformation Interface induced Plasticity (MITIP). Using the model, the effect of the cooling rate, the transformed phase and the transformation temperature on the amount of the transformation superplastic strain was investigated. In order to calculate the deformation behavior under stresses during phase transformation of steels, the elastic strain, the density change due to thermal and phase transformation, the viscoplastic strain, and the transformation superplastic strain were taken into account. The calculated results were compared with the experimental data.

2. Model Development

2.1. Constitutive Equation for the MITIP

Through an \textit{in-situ} microstructural observation and a micro-grid analysis of the transformation superplasticity in iron by Saotome and Iguchi,\textsuperscript{15} it was confirmed that the sliding of the migrating transformation interface mainly contributes to the transformation superplasticity. According to the observation, it is a reasonable assumption that during transformation the migration of transformation interface occurs through the movement of atoms across the transformation interface where the atomic interaction is relatively weak. Without stress field, the migrating atoms will rearrange to the possible nearest atomic site in the transformed phase. However, when a stress is applied, the migrating atoms will move to the direction where they can release the stress field. This phenomenon may be similar to the mechanism of Coble creep. At a given time interval, the amount of migrating atoms in the transformation interface are in proportion to the volume swept by moving transformation interface, which is the increment of transformed phase. As a result, the increment of the transformation superplastic strain at an instance is controlled by the increment of transformed phase and the migration rate of atoms in the transformation interface, which strongly depends on the applied stress and the temperature as the creep deformation. Based on the hypothesis, the increment of the transformation superplastic strain at a given time step can be described by the equation:

\[
\Delta e^s = \Delta X\sigma^m\exp(-Q_s/RT) \hspace{1cm} \text{(5)}
\]

where $\Delta X$ is the transformed phase fraction for a given time step and the activation energy for the migration of atoms in the transformation interface, respectively. $A$, $m$, and $R$ are a proportional constant, a constant for the nonlinear relationship between the stress and the Migration of Transformation Interface induced Plastic (MITIP) strain, and the gas constant, respectively.

To calculate $\Delta X$ during cooling of C–Mn steels, a thermodynamic calculation and a phase transformation kinetics model based on a sublattice model and the Avrami equation, respectively, were used. The constants, $A$, $m$, and $Q_s$, are determined from the austenite to ferrite and pearlite transformations were determined by using an optimization method with the experimental data.

2.2. Calculation of Phase Transformation Kinetics

The phase diagram were obtained from the thermodynamic analysis of the Fe–C–Mn system using a two-sublattice model, (Fe,Mn)(C,V\text{a})c/a, where V\text{a} denotes the vacancy, and the subscript, c/a, is the site ratio of the substitutional sublattice to the interstitial one.\textsuperscript{17} The phases considered in this study are austenite, ferrite, and cementite. Thermodynamic data used were obtained from the studies by Lee \textit{et al.}\textsuperscript{18}. The calculated equilibrium temperatures and compositions were used in the modeling of phase transformation kinetics of C–Mn steels.

The isothermal kinetics of the decomposition of austenite has been characterized by the Avrami type equation:

\[
X = 1 - \exp(-kt^n) \hspace{1cm} \text{(6)}
\]

where $X$ is the transformed fraction and $t$ is the time. $X^*$ is the thermodynamic equilibrium fraction, which can be determined from the equilibrium phase diagram at a given temperature and a chemical composition. The rate constant $k$ depends on the temperature and the transformation mechanism, and the time exponent $n$ is a constant over the temperature range when a unique transformation mechanism
operates.

An extension of Eq. (6) to non-isothermal transformation behavior leads to the additivity concept which is based on the theory advanced by Scheil.\(^{19}\) He proposed that the non-isothermal transformation kinetics can be described as sum of a series of the small isothermal steps on the assumption that the phase transformation is the isokinetic reaction. The transformed phase fraction until the \(i\)-th step, \(X_i\), is expressed as follows:

\[
X_i / X_0 = 1 - \exp[-k_i(t' + \Delta t_i)^n], \quad t' = \left[-1/k_i \ln(1 - X_{i-1}/X_i)\right]^{1/n}
\] ...........................(7)

where \(t'\) is equivalent transformation time needed to transform into the fraction of \(X_{i-1}\) at the temperature of the \(i\)-th step, and \(\Delta t_i\) is the time step corresponding to the \(i\)-th step. The constants of Eq. (7), \(k\) and \(n\), were determined from the dilatation data obtained by the continuous cooling tests using an inverse additivity technique.\(^{20,21}\) The \(k\) and \(n\) values of the austenite to ferrite and pearlite transformations are listed on Table 1, respectively. Here \(C_r\) is the carbon content in untransformed austenite, and AGS (\(\mu m\)) means the prior austenite grain size.

2.3. Modeling of Deformation-phase Transformation under Uniaxial Tensile State

For calculating deformation behavior of a steel specimen under uniaxial tensile state undergoing a phase transformation, the total strain increment, \(\Delta \varepsilon\), can be expressed as follows:

\[
\Delta \varepsilon = \Delta \varepsilon^e + \Delta \varepsilon^{th} + \Delta \varepsilon^p + \Delta \varepsilon^{vp} + \Delta \varepsilon^{ab} \quad .................(8)
\]

where \(\Delta \varepsilon^e\), \(\Delta \varepsilon^{th}\), \(\Delta \varepsilon^p\), \(\Delta \varepsilon^{vp}\) and \(\Delta \varepsilon^{ab}\) are the elastic strain increment, the thermal strain increment which is related to the thermal expansion coefficients of each phase of the steel, the volumetric strain increment due to volume change associated with the phase transformation, the conventional viscoplastic strain increment, and the transformation superplastic strain increment, respectively.

The elastic strain increment, \(\Delta \varepsilon^e\), is linearly related to the applied stress by Hooke’s law. Here, temperature dependent Young’s modulus\(^{22}\) was used as shown in Table 2. Both the thermal strain increment \(\Delta \varepsilon^{th}\), and the volumetric strain increment \(\Delta \varepsilon^{th}\) are caused by the density change of the material. Therefore, the sum of \(\Delta \varepsilon^{th}\) and \(\Delta \varepsilon^e\) can be expressed by:

\[
\Delta \varepsilon^{th} + \Delta \varepsilon^e = \frac{1}{\rho} \sum \frac{\rho_j}{\rho_f} \quad .................(9)
\]

Table 1. \(k\) and \(n\) values of Eq. (7) for phase transformation.\(^{21}\)

| Transformation          | \(k\)                          | \(n\) |
|------------------------|--------------------------------|-------|
| Austenite to Ferrite   | \(-25.049+0.071\) \(\%\C\)     | 0.8674+1.7506 \(\%\C\)   |
|                        | +(-2.013+1.873\(\%\C\)) \(1+0.867\) \(\%\(\text{Mn}\) \ln(T_{tr}-T) + (30193.0-192.8\(\%\C\)-13342.8\(\%\C\)) \(1-6387.4\%\(\text{Mn}\)) / T + 1.854 \(\text{ln(AS)}\)
| Austenite to Pearlite   | \(-17.359+0.021+2.977\(\%\C\) \(0.716\%\(\text{Mn}\)) \ln(T_{tr}-T) + (-34165.1+11133.1\(\%\C\)) +597.8\(\%\(\text{Mn}\)) / T + 0.759 \(\text{ln(AS)}\) |
|                        | 1.5                             |       |

Table 2. Young’s modulus of steel at various temperatures.\(^{22}\)

| Temperature (°C) | 500 | 700 | 800 | 900 | 1000 | 1100 |
|------------------|-----|-----|-----|-----|------|------|
| Young’s Modulus (GPa) | 154 | 131 | 107 | 93  | 99   | 93   |

\[
\rho_f = \left(7875.96 - 0.2977 T - 5.62 \times 10^{-5} T^2 \right) \left(1 - 2.62 \times 10^{-2} C_g \right)\rho_f = \left(8099.79 - 0.5067 T - 1.146 \times 10^{-2} C_g \right)\rho_f = \left(8508.87 - 0.6339 T - 1.265 \times 10^{-2} C_g \right)
\]

where \(C_g\) is the carbon content in untransformed austenite, and \(C_g\) is the carbon content of austenite and ferrite, respectively. The units of temperature (°C) and solute carbon content (wt.%), respectively. \(C_g\) is the carbon content in untransformed austenite, which can be calculated from the mass balance of carbon in austenite and transformed phases.\(^{22,23}\) The solute carbon content in ferrite, \(C_{\alpha}\), was assumed as an equilibrium value calculated by the thermodynamic model. In this study, the pearlite density was assumed as that of ferrite, because the difference between the pearlite and cementite densities is negligible\(^{23}\) and pearlite mainly consists of ferrite. Density of phase mixture can be expressed as:

\[
\frac{1}{\rho} = \sum \frac{f_i}{\rho_f} \quad .................(11)
\]

where \(\rho\) is the temperature and phase dependent density of steel. It has been well known that the density of carbon steel is a strong function of the solute carbon content in steel. In this study, the densities of austenite and ferrite were used as functions of temperature and the solute carbon content.\(^{23}\)

\[
\Delta \varepsilon^p = C \exp(-Q_{vp} / RT) \sinh(\beta l / \varepsilon) \varepsilon^{vp} \quad .................(12)
\]

where \(C\), \(\beta\), \(l\) and \(m\) are constants, and \(Q_{vp}\) is an activation energy for the viscoplastic deformation of the steel. These constants for each phase of the steel are listed on Table 3. For the small stress level with which this study dealt, the viscoplastic strain calculated from Eq. (12) is expected to be very little.

Using Eq. (8) together with Hooke’s law and Eqs. (5), (9) and (12), the deformation behavior of a steel specimen under uniaxial tensile state undergoing a phase transformation.


3. Results and Discussion

Figure 1 shows maximum volume fractions of ferrite calculated from the thermodynamic analysis of various carbon steels. The maximum fraction of ferrite was determined by the lever rule with the phase boundaries of $\alpha/(\alpha+\gamma)$ and $(\alpha+\gamma)/\gamma$ in the temperature range above $\text{Ae}_1$. Where as, in the temperature range below $\text{Ae}_1$, the phase boundaries of $\alpha/(\alpha+\gamma)$ and $\gamma/(\text{cementite}+\gamma)$ were used. Therefore the maximum fraction of ferrite increases in the temperature range above $\text{Ae}_1$ and decreases in the temperature range below $\text{Ae}_1$ as temperature decreases. The maximum ferrite fraction were used as the value of $X_e$ in equation (7) in the modeling of phase transformation kinetics of the carbon steels. It can be seen that the maximum fraction of ferrite decreases with increasing carbon content. This indicates that the transformed phase of high carbon steels is mainly pearlite.

The constants of Eq. (7), $k$ and $n$, were determined from the dilatation data obtained by continuous cooling tests using an inverse additivity technique. The $k$ and $n$ values of austenite to ferrite, pearlite and bainite are listed in Table 1, respectively. Here $C_\gamma$ is carbon content in untransformed austenite which was calculated from the mass balance of carbon in austenite and transformed phases. Figure 2 shows examples of comparison between the measured phase transformation behavior and the calculated one under various continuous cooling conditions. The calculated results based on the kinetic constants in Table 1 are in good agreement with the experimental data.

Figure 3(a) shows a strain-temperature curve for 0.16wt%C–0.52wt%Mn steel during cooling under the uniaxial stress of 39.2 MPa. The cooling rate of the experiment was 2.5°C/sec. In austenite region, very small strain can be observed. The small strain at this region seems to be the contribution of the viscoplastic strain of austenite. After phase transformation begins a large strain occurs, and when pearlite evolution is finished the total strain increment become close to zero. It can be seen that the strain behavior at the phase transformation region resembles the shape of the transformed phase fraction predicted from the phase transformation model as shown in Fig. 3(b). Moreover, it is noted that the ferrite and pearlite evolution can be distinguished from Fig. 3(a) like typical phase transformation curve. The transformed fractions of the steel were calculated under the assumption of the prior austenite grain size of $32\mu$m. From these figures, it can be confirmed that the variation of the transformed phase fraction is closely connected with the transformation superplastic behavior of the steel.

Based on Eq. (8) together with Hooke’s law and Eqs. (5), (9) and (12), a strain–temperature curve for the 0.16wt%C–0.52wt%Mn steel during cooling under the uniaxial stress
of 39.2 MPa was calculated. The comparison between the experimental data and the predicted results is shown in Fig. 4. An optimization was done while changing the constants in Eq. (5) systematically until the sum of the squared differences between the experimental and calculated strains was minimum:

\[ \sum_{i=1}^{N} (\varepsilon_{\text{exp}} - \varepsilon_{\text{cal}})^2 = \min \]  \hfill (13)

where \( N \) is the number of points measured, and the subscripts, exp and cal, mean the experimental data and the calculated results, respectively. As shown in Fig. 4, there is a very good agreement between the experiment and the model. Table 4 summarizes the constants in Eq. (5) for each phase transformation determined from the optimization of the experimental data. The MITIP activation energy for the austenite to ferrite transformation is very similar to one for pearlite transformation, and is slightly smaller than the value, 159 kJ/mol, known as the activation energy \(^{27}\) of the boundary diffusion in austenite. Figure 4 shows also each strain component calculated with the temperature variation. At the initial stage of cooling, the volumetric strain decreases because of the thermal contraction of austenite. As the phase transformation proceeds, the volumetric strain increases, and as the phase transformation vanishes, the volume contraction takes place again. The viscoplastic strain of austenite and transformed phase slowly increases with the progress of time.

Figure 5(a) shows the comparison between the predicted strain–temperature curves and the total strains \(^{19}\) measured at 600°C during cooling of 2.5°C/sec for 0.16wt% C–0.52wt% Mn and 0.83wt% C–0.42wt% Mn steels under 39.2 and 29.4 MPa. As shown in this figure, the predicted results very well agree with the experimental data. As for the 0.83wt% C–0.42wt% Mn steel in which only pearlite transformation takes place, the strain is smaller because of the lower transformation temperature as shown in Fig. 5(b). The activation energy term in Eq. (5) well describes the temperature dependency of MITIP strain.

Figure 6(a) shows the calculated relationship between the MITIP strain at 600°C and the applied stress during cooling of 10, 2.5 and 0.1°C/sec for the 0.16wt% C–0.52wt% Mn steel. A nonlinear relationship of the MITIP strain for the applied stress is shown, and the nonlinearity increases as the applied stress increases. The MITIP strain decreases with increasing the cooling rate as was experimentally observed by Nozaki \( \text{et al.}^{28} \). This phenomenon can also be described by using Eq. (5) and the lowered transformation temperature with increasing the cooling rate as shown in Fig. 6(b).

### Table 4. Constants in Eq. (5) of steel specimen.

|                 | \( A \) | \( m \) | \( Q_e (kJ/mol) \) |
|-----------------|---------|---------|---------------------|
| Austenite to Ferrite | 9.12    | 2.093   | 120.8               |
| Austenite to Pearlite | 31.91   | 2.179   | 121.8               |
In order to calculate the deformation behavior under stresses during phase transformation of steels, the elastic strain, the volumetric strain due to thermal and phase transformation, the viscoplastic strain, and the transformation superplastic strain were taken into account. The calculated results were in good agreement with the experimental data. The constitutive model based on the MITIP could well describe the effect of the cooling rate, the transformed phase and the transformation temperature on the amount of the transformation superplastic strain.

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