Flow Stress Analysis using the Kocks–Mecking Model for Ferrite–Cementite Steels with Various Ferrite Grain Sizes

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True stress (σ)–true strain (ε) curves were calculated by using the Kocks–Mecking (KM) model for the ferrite–cementite steels with various ferrite grain sizes between 0.47 and 13.6 μm. In the KM model, the effect of ferrite grain size on flow stress is described by the athermal stress component that follows the Hall–Petch equation. The effects of temperature and strain rate on flow stress, which are correlated with the thermal stress component, are independent of the ferrite grain size. The calculated σ–ε curves by using the KM model agree with the measured ones at various temperatures and strain rates including high-speed tensile test with a strain rate of 10^3 s^{-1}. From the calculations based on a micromechanic model, it is found that the volume fraction of second phase affects the grain size dependence in multi-phase steels. The m-value showing strain rate sensitivity for the external stress was decreased with a decrease in grain size and that for the thermal stress was independent of grain size.

KEY WORDS: stress–strain curve; grain size; temperature; strain rate; Kocks–Mecking model.

1. Introduction

Recently, vigorous attention has been focused on grain refinement strengthening as one of the effective strengthening mechanisms to obtain high strength without using alloying elements.1,2) The effect of grain size on mechanical properties has been investigated for a number of fine-grained steels with grain sizes finer than 5 μm in recent papers.3,4)

In our previous studies,5–8) the ferrite grain size was varied between 0.47 and 46.2 μm for ferrite–cementite (FC) and ferrite–pearlite (FP) steels, and the effects of grain size on flow stress were investigated by low temperature tensile tests conducted at strain rates between 10^{-6} s^{-1} and 10^1 s^{-1}. Not only the high strength but also a high absorbed energy at high-speed deformation5–8) was confirmed for ultrafine-grained steels. Accordingly, the effect of grain size on flow stress should be described by taking count of temperature and/or strain rate dependence to comprehensively tell the performances of ultrafine-grained steels.

All the experimental evidence5–8) indicate that the effect of ferrite grain size on flow stress is almost independent of temperature and strain rate. This means the grain size dependence can be described simple by the athermal component of flow stress. In the next step, the thermal component has to be discussed by considering thermal activation process9) at various temperatures and strain rates. The Kocks–Mecking (KM) model10,11) based on the thermal activation process has been investigated to predict true stress (σ)–true strain (ε) curves at a wide range of temperatures and strain rates including high-speed deformation for various materials.13–17) It is another advantage of the KM model that the flow stress is composed of the athermal stress component and the thermal one. In this study, therefore, σ–ε curves of the FC steels with different ferrite grain sizes at a wide range of strain rates below room temperature were analyzed by using the KM model in order to make clear the overall effect of grain size on flow stress quantitatively.

2. Outline of the Kocks–Mecking Model

Flow stress (σ) has two components of the athermal one σ_a and the thermal one σ_T as follows9):

\[ \sigma = \sigma_a + \sigma_T(\dot{\varepsilon}, T) \] ..............................(1)

In the KM model10,11) σ_T(\dot{\varepsilon}, T) is described as superposition of several strengthening mechanisms associated with barriers for dislocation motion.18) The following equation is employed for simplicity in the KM model as a function of test temperature (T), strain rate (\dot{\varepsilon}), and ε,

\[ \frac{\sigma}{\mu} = \frac{\sigma_0}{\mu_0} + s_T(\dot{\varepsilon}, T) \frac{\dot{\varepsilon}}{\mu_0} + s_\varepsilon(\varepsilon, T) \frac{\dot{\varepsilon}}{\mu_0} \] ......................................(2)

where \( \mu \) is the temperature-dependent shear modulus and \( \mu_0 \) the shear modulus at 0 K. In this study, \( \mu \) was taken as 88.7 GPa (0 K), 86.3 GPa (77 K), 82.3 GPa (210 K), and 80.7 GPa (296 K).19) The first term of the right hand side is
\( \sigma_s \) that means the flow stress at a temperature above a critical temperature. The second and the third terms are two different kinds of obstacles for dislocation motion accompanying relevant thermal activation mechanisms. The second term refers to yielding and the third term to work-hardening. The thermal stress is specified by using the mechanical threshold stress (MTS)\(^{11} \) that means the flow stress at 0 K. In terms of two MTS in Eq. (2), \( \sigma_t \) is associated with the yield strength and \( \sigma_D \) work hardening, i.e. dislocation–dislocation interactions. \( s_a(T, \dot{e}) \) and \( s_b(T, \dot{e}) \) mean the temperature and strain rate dependencies, which are given by the ratios of yield strength and work-hardening at a certain \( T \) and a certain \( \dot{e} \) to those at 0 K,\(^{10,11} \) respectively.

\[
\begin{align*}
    s_a(T, \dot{e}) &= 1 - \left( \frac{kT}{g_0b^3} \ln \left( \frac{\dot{e}_0}{\dot{e}} \right) \right)^{1/\beta} \\
    s_b(T, \dot{e}) &= 1 - \left( \frac{kT}{g_0b^3} \ln \left( \frac{\dot{e}_0D}{\dot{e}} \right) \right)^{1/\beta}
\end{align*}
\]

where \( k \) is Boltzmann’s constant, \( b \) the Burgers vector, \( g_0 \), \( \dot{e}_0 \) and \( q \) are constants\(^{11,20,21} \) and their suffixes I and D refer to yielding and work-hardening, respectively. The combination of \( p \) and \( q \) is commonly accepted for various barriers.\(^{18,20,21} \) By combining Eq. (2) into Eq. (4), the following equation of the \( \sigma - \dot{e} \) curve is obtained,

\[
\frac{\sigma}{\mu} = \frac{\sigma_s}{\mu} + \left[ 1 - \left( \frac{kT}{g_0b^3} \ln \left( \frac{\dot{e}_0}{\dot{e}} \right) \right)^{1/\beta} \right] \frac{\sigma_D}{\mu_0} \\
+ \left[ 1 - \left( \frac{kT}{g_0b^3} \ln \left( \frac{\dot{e}_0D}{\dot{e}} \right) \right)^{1/\beta} \right] \frac{\sigma_D}{\mu_0}
\]

The MTS \( \sigma_D \) in Eq. (5), which means the dislocation structure evolution associated with work-hardening, is usually increased during deformation as a function of \( \dot{e} \). It is written by,

\[
\sigma_D = \sigma_{D_0} \left[ 1 - \exp \left( \frac{-\Theta_0}{\sigma_{D_0}} \right) \right]
\]

where \( \Theta_0 \) is the stage II work-hardening rate of approximately \( \mu/15 - \mu/20 \).\(^{15} \) The \( \sigma_{D_0} \) is the saturation stress of \( \sigma_D \) associated with the saturated dislocation substructure obtained by extremely heavy plastic deformation. Equation (6) is connected with the work-hardening law proposed by Kocks\(^{12} \) and is derived from the following Voce law,\(^{22} \)

\[
\Theta = \frac{d\sigma_D}{d\dot{e}} = \Theta_0 \left[ 1 - \frac{\sigma_D}{\sigma_{D_0}} \right]
\]

where \( \Theta \) refers to work-hardening rate that decreases linearly with an increase in stress during the stage III deformation.\(^{12} \)

3. Results and Discussions

3.1. Application of the Kocks–M Rebecca Model

The \( \sigma - \dot{e} \) relations of the FC steels under uniform deformation were focused to investigate in this study, although yield drop and Lüders elongation were observed at the early stage of deformation.\(^{6,8} \)

In the determination of the athermal stress (\( \sigma_{a} \)), the following Larson–Miller parameter (\( \xi \))\(^{23} \) was used,

\[
\xi = T(\ln \dot{e}_0 - \ln \dot{e})
\]

where \( \dot{e}_0 \) was assumed to be 20.\(^{15} \) The experimentally observed \( \sigma_{a} \) values at various \( \dot{e} \) are plotted as a function of \( \xi \) in Fig. 1. The \( \sigma_{a} \) was determined as flow stress at \( \xi = 20 \) 000 K and described by using the following Ludwik equation,

\[
\sigma_{a} = \sigma_{a_0} + K\dot{e}^n
\]

where \( \sigma_{a_0}, K \) and \( n \) were constants. By summarizing the determined \( \sigma_{a} \) for the FC steels, the following equation was obtained as a function of ferrite grain size (\( D \)) and \( \dot{e} \),

\[
\sigma_{a} = \sigma_{a_0} + \sigma_{a_1}(\dot{e}) = 482D^{-1/2} + (410 - 208D^{-1/2})\dot{e}^{(0.6 - 0.3D^{-1})}
\]

Although \( \sigma_{a} \) is often regarded as a material constant,\(^{13,14} \) it is more reasonable to assume it as a variable depending on \( \dot{e} \) in the present case.\(^{15,16} \) The \( \sigma_{a} \) at \( \dot{e} = 0 \) (\( \sigma_{a_0} \)) can be described as a function of \( D^{-1/2} \) as shown in Fig. 2, whose slope \( k (= 482 \) MPa/\( \mu m^{-1/2} \)) in the Hall–Petch equation\(^{24} \) almost agrees with the experimental result.\(^{6} \) The work-hardening component of \( \sigma_{a_1}(\dot{e}) \) in Eq. (10) was also dependent on \( D \), and the constants of \( K \) and \( n \) became smaller with a decrease in ferrite grain size.

Figure 3 shows \( (\sigma - \dot{e})/\mu \) as a function of \( T \) and \( \dot{e} \) in order to determine the \( \sigma_{D_0} \) and \( g_0 \) in Eq. (5). The values 0.5, 1.0, and \( 10^8 \) s\(^{-1} \) were used for the constants of \( p_t, q_t \) and \( \dot{e}_{ult} \), respectively.\(^{20} \) Stress at \( T = 0 \) K in Fig. 3 means the MTS \( \sigma_{D_0} \) and the slope in the figure represents the value of \( g_0 \). The values of \( \sigma_{D_0} \) and \( g_0 \) were determined to be
525 MPa and 0.16, respectively. The estimated \( \sigma_1 \) and \( g_{0I} \) are independent of ferrite grain size.

In order to estimate the parameters of \( \sigma_D \), \( (\sigma-\sigma_a-\sigma_s(\varepsilon, T))/\mu \) is plotted as a function of \( T \) and \( \varepsilon \) at various true strains like Fig. 3, where \( \rho_I = 0.5 \), \( q_I = 1.5 \), and \( \varepsilon_I = 10^8 \text{s}^{-1} \) are assumed. As a result, \( \Theta_D \), \( \sigma_D \), and \( g_{0D} \) in Eq. (6) were determined to be 4500 MPa, 560 MPa and 0.3, which are also independent of ferrite grain size. Table 1 summarizes all of the obtained parameters. It should be noted that the effect of ferrite grain size on the \( \sigma-\varepsilon \) curves contributes only to the athermal stress. The effect of ferrite grain size on the athermal stress can be described as a function of the inverse square root of ferrite grain size \( (D^{-1/2}) \).

Figure 4 shows comparisons between the calculated \( \sigma-\varepsilon \) curves by using the KM model and the measured ones at static tensile tests below room temperature. It can be seen that the calculated \( \sigma-\varepsilon \) curves agree well with the measured ones.

Figure 5 represents the comparison between the calculated \( \sigma-\varepsilon \) curves and the measured ones at a strain rate of \( 10^3 \text{s}^{-1} \). Temperature rise of a specimen during adiabatic deformation was considered in the calculations at \( 10^3 \text{s}^{-1} \). The temperature rise of specimen was calculated based on the assumption that 95% of the work made by plastic deformation was converted into heat, whose work was estimated

**Table 1.** Parameters of the Kocks–Mecking model for the ferrite–cementite and ferrite–pearlrite steels.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Ferrite-Cementite</th>
<th>Ferrite-Pearlite ( \times 10^5 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \sigma_I ) (MPa)</td>
<td>482D(^{1/2})(410-208D(^{1/2}))(6(^{1/2}))</td>
<td>150+185D(^{1/2})+300(D^{1/2})</td>
</tr>
<tr>
<td>( \sigma_D ) (MPa)</td>
<td>525</td>
<td>470</td>
</tr>
<tr>
<td>( g_0 )</td>
<td>0.16</td>
<td>0.16</td>
</tr>
<tr>
<td>( \rho_I )</td>
<td>0.5</td>
<td>0.5</td>
</tr>
<tr>
<td>( q_I )</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>( \varepsilon_I (\text{s}^{-1}) )</td>
<td>( 10^8 )</td>
<td>( 10^8 )</td>
</tr>
<tr>
<td>( \varepsilon_0 )</td>
<td>0.3</td>
<td>0.3</td>
</tr>
<tr>
<td>( \Theta_D ) (MPa)</td>
<td>4500</td>
<td>5000</td>
</tr>
<tr>
<td>( \sigma_{0I} ) (MPa)</td>
<td>560</td>
<td>600</td>
</tr>
<tr>
<td>( \rho_D )</td>
<td>0.5</td>
<td>0.5</td>
</tr>
<tr>
<td>( q_D )</td>
<td>1.5</td>
<td>1.5</td>
</tr>
<tr>
<td>( \varepsilon_{0I} (\text{s}^{-1}) )</td>
<td>( 10^8 )</td>
<td>( 10^8 )</td>
</tr>
</tbody>
</table>

D: ferrite grain size (\( \mu \text{m} \)), \( \varepsilon \): true strain

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1022
by using measured nominal stress–strain curves.

\[
T = T_0 + \frac{0.95}{\rho \cdot C_p} \int_0^e s(\varepsilon)d\varepsilon \quad \text{.................(11)}
\]

where \(T_0\) is the initial temperature, \(\rho\) is the mass density, \(C_p\) is the temperature dependent heat capacity of the specimen, and \(\sigma\) and \(\varepsilon\) are nominal stress and nominal strain, respectively. The calculated \(\sigma–\varepsilon\) curves taking the temperature change into consideration show a good agreement with the measured ones.

It is practicable to calculate tensile strength (TS) and uniform elongation (U.El) from the estimated flow curves. Figure 6 shows comparisons between the calculated TS and U.El and the measured ones. Good coincidence is found between the calculations and the experimental results.

3.2. Effect of Microstructure on Slope in the Hall–Petch Equation

The fine-grained steels have two specific kinds of microstructures, namely ferrite–cementite (FC) and ferrite–pearlite (FP). In the previous study, effects of temperature and strain rate on flow stress in the FC and FP steels obtained by a low carbon steel were compared.\(^6,7\) To discuss the microstructural effect, the \(\sigma–\varepsilon\) curves of FP steels with ferrite grain sizes between 3.6 and 46.2 \(\mu\text{m}\)\(^5,6\) were also analyzed using the KM model. The parameters obtained are tabulated in Table 1. The effect of ferrite grain size on flow stress contributes to the athermal stress as a function of \(D^{-1/2}\). However, some parameters for \(\sigma_a\) and MTS in Eq. (5) are different between the FC steels and the FP ones. This seems to be mainly associated with the difference of microstructure, especially the difference in volume fraction of the second phase. The second phase in the FC steels is cementite with the volume fraction of a few % and that in the FP ones is pearlite with the volume fraction of about 25%.

In order to discuss the effect of volume fraction of the second phase on the slope \(k\) in the Hall–Petch equation, flow curves of FP steels with different pearlite volume fractions and grain sizes are calculated by the secant method based on a micromechanical model.\(^27,28\) In the calculations, flow curves of ferrite and pearlite single microstructure steels are needed and those are calculated by the parameters as shown in Table 2. Because these parameters are obtained by an IF steel (ferrite)\(^{16}\) and a medium carbon steel (pearlite),\(^{29}\) the calculations were made only for demonstration how the pearlite volume fraction may affect the \(k\)-value.

Table 2. Parameters of the Kocks–Mecking model for the ferrite and pearlite single microstructure steels.\(^{16}\)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Ferrite (IF)(^{16})</th>
<th>Pearlite (0.54C)(^{36})</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\sigma_a) (MPa)</td>
<td>50–120(^{4,4})</td>
<td>240–1470(^{25})</td>
</tr>
<tr>
<td>(\delta_f) (MPa)</td>
<td>932</td>
<td>1000</td>
</tr>
<tr>
<td>(\beta)</td>
<td>0.12</td>
<td>0.08</td>
</tr>
<tr>
<td>(\rho_f)</td>
<td>0.5</td>
<td>0.5</td>
</tr>
<tr>
<td>(\theta)</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>(\dot{\varepsilon}_a) (s(^{-1}))</td>
<td>10(^6)</td>
<td>10(^6)</td>
</tr>
<tr>
<td>(\beta_{0\alpha})</td>
<td>0.45</td>
<td>0.12</td>
</tr>
<tr>
<td>(\Theta_f) (MPa)</td>
<td>3000</td>
<td>2400</td>
</tr>
<tr>
<td>(\sigma_{0\alpha}) (MPa)</td>
<td>350</td>
<td>370</td>
</tr>
<tr>
<td>(\rho_f)</td>
<td>0.5</td>
<td>0.5</td>
</tr>
<tr>
<td>(\Phi_f)</td>
<td>1.5</td>
<td>1.5</td>
</tr>
<tr>
<td>(\dot{\varepsilon}_{0\alpha}) (s(^{-1}))</td>
<td>10(^7)</td>
<td>10(^7)</td>
</tr>
</tbody>
</table>

\(\varepsilon\): true strain

Fig. 5. Comparisons between the calculated true stress–strain curves and the measured ones by using the KM model with a strain rate of 10\(^3\) s\(^{-1}\) at 296 K for the FC steels.

Fig. 6. Comparisons between the calculated mechanical properties and the measured ones by using the KM model for tensile strength (a) and uniform elongation (b).
Figure 7 represents the calculated 10% flow stress as a function of the inverse square root of ferrite grain size \(D^{-1/2}\) for FP steels with several pearlite volume fractions of 3%, 25%, and 50%. In Fig. 7, the flow stresses of ferrite and pearlite single microstructure steels are also included. The 10% flow stresses of the FP steels and the ferrite single microstructure steels increase with decreasing of ferrite grain size and that for pearlite is a constant. It is found that the slope in the Hall–Petch equation for the FP steels decreases with an increase in the volume fraction of pearlite. This seems to explain the difference of the slope in the Hall–Petch equation for the athermal stress between the FC steels and the FP ones as seen in Table 1. From Fig. 7, the grain size dependence on flow stress in the multi-phase steels becomes smaller with increasing of the volume fraction of the second phase.

### 3.3. Strain Rate Sensitivity Exponent

In discussion of strain rate sensitivity, the strain rate sensitivity exponent \(m\), which is the engineering parameter measuring strain rate sensitivity, is often used,

\[
m = \frac{\partial \log \sigma}{\partial \log \dot{\varepsilon}}
\]

where \(\sigma\) is the flow stress and \(\dot{\varepsilon}\) the corresponding strain rate. Calculated 10% flow stress at 296 K for the FC steels with different grain sizes are plotted as a function of \(\log \dot{\varepsilon}\) in Fig. 8. The \(m\)-value, which means the slope in Fig. 8, becomes smaller with decreasing of grain size as shown in Table 3. This is consistent with other data for bcc metals and alloys reported elsewhere.\(^{30}\) Because \(\sigma\) in eq. (12) is usually given by the external stress, which is composed of athermal and thermal stresses, the calculated results that the \(m\)-value decreases with decreasing of grain size seem to show the influence of athermal stress with a decrease in grain size.

On the other hand, flow stress may be also described as a function of the athermal stress and the thermal one by using the strain rate sensitivity exponent as follows,\(^{31}\)

\[
s|_{\varepsilon, T} = \sigma_a + c_0 \dot{\varepsilon}^m \quad \text{(13)}
\]

where \(n\) is the flow stress at a constant strain and temperature, \(\sigma_a\) the athermal stress, \(m^*\) the strain rate sensitivity exponent for thermal stress, \(c_0\) a constant. The calculated 10% flow stress at 296 K (\(s|_{\varepsilon=0.1, T=296 K}\)) with the parameters in Table 1 was described by using Eq. (13). As a result, the following equation was obtained,

\[
s|_{\varepsilon=0.1, T=296 K} = 482D^{-1/2} + 410 - 208D^{-1/2} \times (0.1)^{0.6 - 0.3D^{-1/2}} + 348e^{0.053}
\]

The athermal stress, the first and second terms, is identical with Eq. (10) and the \(m^*\)-value in Eq. (14) is 0.053. That is, the strain rate sensitivity exponent for thermal stress is independent of grain size.

### 4. Conclusions

True stress \((\sigma)\)–true strain \((\varepsilon)\) curves for the ferrite–cementite (FC) steels with various ferrite grain sizes were analyzed by using the Kocks–Mecking (KM) model. The followings are main obtaining results.

1. The effect of ferrite grain size on the \(\sigma–\varepsilon\) curves depends on the athermal stress that can be described by the inverse square root of ferrite grain size \(D^{-1/2}\).
2. Equations derived by the KM model can precisely predict the \(\sigma–\varepsilon\) curves of the FC steels in the wide range of experimental parameters like ferrite grain size, strain rate,
and test temperature.

(3) The similar analysis for the $\sigma-\epsilon$ curves of the ferrite-pearlite (FP) steels revealed that the athermal stress also depends on grain size but the dependence is lower. A consideration based on a micromechanic model indicates that the volume fraction of second phase affects the dependence; that is, larger fraction becomes lower dependence.

(4) The strain rate sensitivity exponent ($m$) was discussed by using the 10% flow stress at 296 K. The $m$-value for the external stress became smaller with decreasing of grain size and that for the thermal stress was independent of grain size.

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