Constitutive modeling of commercial pure titanium during hot deformation in alpha and beta phase fields

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The hot working behavior of commercial pure titanium (CP-Ti) in alpha and beta phase fields was studied through constitutive analysis based on a simple physically-based approach. Accordingly, reliable constitutive equations were proposed for hot deformation of titanium above and below the beta transus temperature. It was quantitatively shown that besides the effect of the Zener-Hollomon parameter (which represents the effect of deformation conditions), the deforming phase play a significant role in determining the flow stress of titanium during high-temperature thermomechanical processing.

Keywords: Titanium, Hot deformation, Constitutive equations, Deformation mechanism, Activation energy, Diffusion

Titanium and its alloys offer a unique combination of high specific strength, excellent corrosion resistance, high melting temperature, good weldability, high temperature performance at just half the weight of steels and Ni-based alloys, and biocompatibility, which make them desirable for a variety of applications in the marine, aerospace, automobile, chemical processing, sports, architecture, and biomedical industries.\textsuperscript{1-4}

Titanium exists in two allotropic forms. At low temperatures, it has a hexagonal closed packed (HCP) structure, which is commonly known as $\alpha$; whereas above $883^\circ$C, it has a body centered cubic (BCC) crystal structure termed $\beta$. The alloying elements such as Al, Sn, and O that tend to stabilize the $\alpha$ phase are called alpha stabilizers and the addition of these elements increase the beta transus temperature, while elements such as Mo, V, and Fe that stabilize $\beta$ phase are known as beta stabilizers and addition of these elements depress the $\beta$ transus temperature.\textsuperscript{4} The $\beta$ transus temperature for commercial pure titanium (CP-Ti) has been reported to be around $915^\circ$C.\textsuperscript{5} By addition of alloying elements, three major types of Ti alloys will be resulted: (I) CP-Ti, $\alpha$ and near $\alpha$ alloys,\textsuperscript{7-9} (II) $\alpha+\beta$ alloys such as Ti-6Al-4V,\textsuperscript{10} and (III) $\beta$ and near $\beta$ alloys.\textsuperscript{11}

Due to its HCP crystal structure, $\alpha$-Ti has a limited number of slip systems (i.e. \{$1\bar{1}00\} <11\bar{2}0>$ and \{$1\bar{1}01\} <11\bar{2}0>$) but plastic deformation in $\beta$ phase field takes place by mechanisms characteristic of metals with BCC structure, which are \{110\}<111>, \{112\}<111>, \{123\}<111>.\textsuperscript{12} Therefore, hot deformation processing is a suitable shaping method. The possibility of structural refinement or modification is another important advantage of hot working\textsuperscript{13-16}. Moreover, the typical hot working approach for processing $\alpha$ alloys comprises primary ingot breakdown in the $\beta$ phase field and secondary working to produce a specific shape by either hot forging or rolling below or above the beta transus temperature.\textsuperscript{5} Therefore, both $\alpha$ and $\beta$ phase fields have industrial significance, and hence, it is important to characterize the hot working behavior of CP-Ti in a wide range of deformation temperatures. The understanding of the hot working behavior and the constitutive relations describing material flow are two of the prerequisites for the implementation of shaping technology in the industry.\textsuperscript{17-22} The modeling of hot flow stress is thus important in metal-forming processes because any feasible mathematical simulation needs accurate flow description. Zeng \textit{et al}.\textsuperscript{7} have successfully modeled the flow stress of pure titanium under hot compression test by using the strain-dependent hyperbolic sine equation, which is known as strain-compensation technique.\textsuperscript{22} Tsao \textit{et al}.\textsuperscript{3} proposed a mathematical model using an updated Fields–Backofen (FB) equation to describe the flow stress behavior of CP-Ti during warm tensile testing.

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However, more fundamental constitutive analysis by consideration of microstructural phenomena might be useful for industrial applications and comparative studies.

In the present work, the constitutive behavior of CP-Ti will be studied during hot working in both α and β phase fields, and subsequently, reliable but simple constitutive equations will be proposed for hot deformation of this material.

**Experimental Procedure**

**Constitutive analysis**

A common constitutive equation in hot working for a wide range of temperatures and strain rates is expressed by a hyperbolic sine relation of the form,

\[ Z = \dot{\varepsilon} \exp(Q / RT) = \alpha \sinh(\alpha \sigma)^n, \]

where \( Z \) is the Zener-Hollomon parameter, \( Q \) is the deformation activation energy, \( \dot{\varepsilon} \) is the strain rate, \( T \) is the absolute temperature, and finally \( n \) is the hyperbolic sine constant. The constants \( \alpha \) and \( \beta \) are the material’s parameters.

The stress multiplier \( \alpha \) is an adjustable constant which brings \( \alpha \sigma \) into the correct range that gives linear and parallel lines in \( \ln \dot{\varepsilon} \) versus \( \ln \{\sinh(\alpha \sigma)\} \) plots. The Zener-Hollomon parameter can also be related to flow stress by the power law \( (Z = A'\sigma^n) \) and the exponential law \( (Z = A''\exp(\beta \sigma)) \) at relatively low and high stresses, respectively.

Conventionally, \( n \) and \( Q \) are to be apparent parameters in the hyperbolic sine law, which makes it impractical to conduct the comparative studies to elucidate the effects of alloying elements or second phases. Recently, it has been shown that when the deformation mechanism is controlled by the glide and climb of dislocations (climb controlled), a constant hyperbolic sine power of \( n = 5 \) and self diffusion activation energy \( (Q_{sd}) \) can be used to describe the appropriate stress.

A convenient way to do this is by taking into account the dependences of Young’s modulus \( (E) \) and self-diffusion coefficient \( (D) \) on temperature and modification of hyperbolic sine law as follows:

\[ \dot{\varepsilon} / D = B[\sinh(\alpha' \sigma / E)]^5 \]  

where \( D = D_0 \exp(-Q_{sd} / RT) \), in which \( D_0 \) is a pre-exponential constant. The constants \( \alpha' \) and \( B \) are the modified stress multiplier and the hyperbolic sine constant, respectively. The consideration of hyperbolic sine power of \( 5 \) and self diffusion activation energy gives a physical and metallurgical meaning to Eq. (1) and also reduces the number of unknown parameters and constant to \( 2 \) (\( \alpha' \) and \( B \)). The former results in a more reliable constitutive equation and the latter simplifies the constitutive analysis and makes it possible to conduct comparative hot deformation studies.

### Database and identifying the required constants

The flow stress data of CP-Ti were taken from the literature. The description of flow stress by Eq. (1) is incomplete, because no strain for determination of flow stress is specified. Therefore, characteristic stresses that represent the same deformation or softening mechanism for all flow curves, such as steady state or peak stress, should be used in this equation. Since the peak stress \( (\sigma_P) \) is the most widely accepted one in obtaining the hot working constants, its values were taken with emphasis on the consistency of stress level among different references.

The values of \( D_0 \) and \( Q_{sd} \) can be taken from the Frost and Ashby tables. In these tables, the dependence of the shear modulus \( (G) \) on temperature in the form of \( G / G_0 = 1 + \eta (T - 300) / T_M \) is also available. Here, \( G_0 \) is the shear modulus at 300 K, \( T_M \) is the melting temperature of the material, and \( \eta = (T_M / G_0) dG / dT \) shows the temperature dependence of the shear modulus. According to the relation of \( E = 2G(1+\nu) \), the values of \( E \) can be estimated (\( \nu \) is usually taken as 0.3). Using the available data for \( \alpha \) and \( \beta \) titanium (as shown in Table 1), the following expressions can be derived for \( D_0, D_\beta, E_\alpha, \) and \( E_\beta \):

\[
\begin{align*}
D_\alpha &= 8.6 \times 10^{-10} \times \exp(-150000 / RT) \\
D_\beta &= 1.9 \times 10^{-7} \times \exp(-153000 / RT) \\
E_\alpha &= 113360 \times \{1 - 1.2(T - 300) / 1933\} \\
E_\beta &= 53300 \times \{1 - 0.5(T - 300) / 1933\}
\end{align*}
\]  

The anomalous behavior of titanium has led to a fairly wide range of experimental activation energies for self diffusion in both alpha and beta phases. For instance, the activation energy for lattice diffusion in alpha Ti is 150 kJ/mol, while an apparent activation energy of 242 kJ/mol has been reported for power-law creep. Moreover, the lattice self-diffusion activation
energy of 251.2 kJ/mol has also been indicated for beta Ti. To make the analysis valid, in the current work, the data based on one reference (Table 1) is being used.

As indicated before, above 883°C, α-Ti transforms to β. However, the impurity and alloying elements affect the β transus temperature such that the β transus temperature for CP-Ti has been reported to be around 915 °C. Based on the available data and to avoid any ambiguity, deformation temperatures ranging from 400 to 875°C (subtransus temperatures) and ranging from 925°C to 950°C (supertransus temperatures) were considered for the α and β phase fields, respectively. Note that for CP and α alloys, hot deformation below the β transus occurs in the α phase field. However, for near-alpha alloys, subtransus hot deformation takes place in the α plus beta β field.

Results and Discussion

In Eq. (1), there are only two unknown parameters (B and α’). In order to find the value of α’, the power and exponential laws were modified as

\[
\dot{\varepsilon} / D = B’(\sigma_p / E)^{n’} \quad \text{and} \quad \dot{\varepsilon} / D = B’\exp(\beta’\sigma_p / E),
\]

respectively. In the modified equations, B’, B”, n’, β’ are constants. Therefore, in complete analogy with the case of classical hyperbolic sine law, the value of α’ can be estimated as β’/n’. It follows from these expressions that the slope of the plot of \(\ln(\dot{\varepsilon} / D)\) against \(\ln(\sigma_p / E)\) and the slope of the plot of \(\ln(\dot{\varepsilon} / D)\) against \(\sigma_p / E\) can be used for obtaining the values of n’ and β’, respectively. These plots are shown in Fig. 1. The linear regression of these data resulted in the values of α’ = 606.33 and 1966 for α and β phase fields, respectively. The average correlation coefficient (R²) for these regression analysis was higher than 0.95 and 0.99 in the α and β phase fields, respectively.

According to Eq. (1), the slopes of the plots of \(\dot{\varepsilon} / D\) against \(\sinh(\alpha’\sigma_p / E)\) by fitting straight line with the intercept of zero (\(y = ax + 0\) as shown in Fig. 2) was used for obtaining the values of \(B^{0.2} = 1803.1\) and 317.6 for α and β phase fields, respectively. The resultant constitutive equations can be expressed as:

\[
\begin{align*}
\dot{\varepsilon} / D_\alpha &= 1803.1^5 \times \{\sinh(606.33 \times \sigma_p / E_\alpha)\}^5 \\
\dot{\varepsilon} / D_\beta &= 317.6^5 \times \{\sinh(1966 \times \sigma_p / E_\beta)\}^5
\end{align*}
\]

where the expressions for \(D_\alpha\), \(D_\beta\), \(E_\alpha\), and \(E_\beta\) are shown in Eq. 2. Therefore, the reliable constitutive equations for describing the hot working behaviors in α and β phase fields of CP-Ti can be expressed as:

\[
Z = \left\{ \frac{\dot{\varepsilon} \exp(150000 / RT)}{\sinh(606.33 \times \sigma_p / E_\alpha)} \right\}^5
\]

\[
Z = \left\{ \frac{\dot{\varepsilon} \exp(153000 / RT)}{\sinh(1966 \times \sigma_p / E_\beta)} \right\}^5
\]

Based on Fig. 2, it seems that the consideration of hyperbolic sine power of 5 and the lattice self-diffusion activation energies of α and β titanium as

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Table 1 – Data used to obtain the temperature dependence of \(D\) and \(G\) for Ti.

<table>
<thead>
<tr>
<th>Phase</th>
<th>(D_0) (m²/s)</th>
<th>(Q_{SD}) (kJ/mol)</th>
<th>(n)</th>
<th>(G_0) (MPa)</th>
<th>(T_m) (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alpha-Ti</td>
<td>8.6×10⁻¹⁰</td>
<td>150</td>
<td>-1.2</td>
<td>43600</td>
<td>1933</td>
</tr>
<tr>
<td>Beta-Ti</td>
<td>1.9×10⁻⁷</td>
<td>153</td>
<td>-0.5</td>
<td>20500</td>
<td>1933</td>
</tr>
</tbody>
</table>

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Fig. 1 – Plots used to obtain the values of the modified stress multiplier α’

Fig. 2 – Plots used to obtain the physically-based constitutive equations
the deformation activation energy works well. These equations can be used to describe the hot working behavior of CP-Ti. However, since both of the values of \( B \) and \( \alpha' \) are different for \( \alpha \) and \( \beta \) phase fields, conducting a comparative study based on Eq. (4) is not easy. Therefore, in the following, another approach will be considered to address this point.

To make it possible to compare the flow stress in alpha and beta phase fields, the constitutive analyses based on the power law were conducted. This approach bypasses the complexities raised from the different values of \( \alpha' \). Based on the power law description of flow stress as shown by

\[
\sigma = P Z^{n'},
\]

the plots of \( \ln \sigma_p \) against \( \ln Z \) can be used for obtaining the values of \( n' \) and \( A' \). The corresponding plots, by consideration of \( Q = 150 \text{ kJ/mol} \) for both \( \alpha \) and \( \beta \) phase fields, are shown in Fig. 3, which show that the fitted lines are highly parallel to each other and hence have a same slope of \( \approx 0.2 \). Therefore, the power law analysis was performed again by consideration of slope of 0.2 and the resulting constitutive equations can be expressed as follows:

\[
\sigma_p = \begin{cases} 
2.98 Z^{0.2} & \text{\( \alpha \)-phase} \\
1.17 Z^{0.2} & \text{\( \beta \)-phase}
\end{cases} \quad ... (5)
\]

where \( Z = \dot{\varepsilon} \exp(150000/RT) \). Since the deformation temperatures in \( \alpha \) and \( \beta \) phase fields are different, the equal \( Z \) can be achieved by adjusting the strain rate. It is apparent that, at a given \( Z \), the flow stresses in \( \alpha \) phase field are higher than those encountered in the high-temperature \( \beta \) phase field. This implies that, besides \( Z \), the crystal structure and slip activation in \( \alpha \) and \( \beta \) phases play significant roles in determining the flow stress of titanium. These findings along with the consideration of microstructural phenomena such as softening processes should be considered in high-temperature processing of titanium.\(^{13,34,35}\)

Conclusions

The hot working behavior of commercial pure titanium during hot working in alpha and beta phase fields was studied through constitutive analysis based on a simple physically-based approach, which accounts for the dependence of the Young’s modulus and the self-diffusion coefficient of Ti on temperature. The following conclusions can be drawn from this study:

(i) A reliable constitutive equations for hot deformation of commercial pure Ti at subtransus temperatures can be expressed as

\[
\dot{\varepsilon}/D_\alpha = 1803.5 \times \{\text{Sinh}(606.33 \times \sigma_p / E_\alpha)\}^5,
\]

where

\[
D_\alpha = 8.6 \times 10^{-10} \times \exp(-150000/RT) \quad \text{and} \quad E_\alpha = 113360 \times (1-1.2(T-300))/193.
\]

(ii) A reliable constitutive equation for hot deformation of commercial pure Ti at supertransus temperatures can be expressed as

\[
\dot{\varepsilon}/D_\beta = 317.6 \times \{\text{Sinh}(1966 \times \sigma_p / E_\beta)\}^5,
\]

where

\[
D_\beta = 1.9 \times 10^{-7} \times \exp(-153000/RT) \quad \text{and} \quad E_\beta = 53300 \times (1-0.5(T-300))/1933.
\]

(iii) Besides the effect of the Zener-Hollomon parameter (which represents the effect of deformation conditions), the constitutive analyses were able to quantitatively show that the type of the deforming phase (alpha or beta) play a significant role in determining the flow stress of titanium. As a result, the equations of \( \sigma_p = 2.98 Z^{0.2} \) and \( \sigma_p = 1.17 Z^{0.2} \) were proposed for hot working in the alpha and beta phase fields, respectively.

References


