Original Article

Flow stress prediction using hyperbolic-sine Arrhenius constants optimised by simple generalised reduced gradient refinement

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ABSTRACT

The generalised reduced gradient refinement was applied to optimise the constitutive constants obtained from hyperbolic-sine Arrhenius equation when describing the flow stress of two titanium alloys subjected to hot compression testing. The results showed that correlation coefficients improved from 0.96 and 0.98 to 0.99, while the average absolute relative error and the root mean square error reduced by more than 30%. The simple generalised reduced gradient refinement can be used to improve the prediction of flow stress when hyperbolic-sine Arrhenius equation or other phenomenological and physical models are used for describing hot working behaviour of metals and alloys.

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1. Introduction

The development of constitutive models which describe the response of materials to imposed strain rate and deformation temperatures during forming processes such as rolling, forging and extrusion [1,2] has continued to attract the interest of researchers. This is ascribed to the importance of the models when used as input code in finite element methods for optimisation of hot working processes [3–5]. Previously, understanding of hot working behaviour of metallic materials was performed by trial and error which was not only costly, but time consuming [6]. The prediction of flow stress with very high accuracy using different constitutive models has become desirable, and finite element methods have used these models during simulations for quick understanding and optimisation of the deformation behaviour of alloys. The different modelling concepts adopted by researchers can be classified into three broad groups:

- the use of one specific type of constitutive model for example, either phenomenological [7] model or physical model [8];
- the use of combinations of constitutive models for example combining two phenomenological models or physical models [9,10]; and
- the use of specific model combined with some optimisation techniques [11,12] for example using phenomenological model and Artificial Neural Network [13,14].
In a recent review, Lin and Chen [15] classified the different constitutive models into three major categories namely phenomenological models, physical models and artificial neural network models. Of the three categories, phenomenological models such as Johnson-Cook [16] and Arrhenius [17] models are mostly used. The hyperbolic-sine Arrhenius equation proposed by Garofalo [18] and later popularised by Sellers and Tegart [17,19] is the commonly used constitutive equation due to its simplicity and small number of required constitutive constants. As a form of modification, the temperature compensated strain rate known as Zener-Hollomon parameter [20] was incorporated into the Arrhenius equation. Consequently, the equation is able to predict the flow stress for a wide range of metallic alloys and metal matrix composites [21,22].

The original Arrhenius equation was initially used for metals with high stacking fault energy where dynamic recovery was the main softening mechanism and the flow stress is independent of strain once the peak stress is attained, hence, the influence of strain was not considered in the model [23,24]. However, in many metallic systems including those with high stacking fault energy, features such as broad peaks, oscillations, jerky patterns or continuous flow softening which are ascribed to either dynamic recrystallisation, flow localisation or dynamic strain aging were widely reported [25–27]. Therefore, the flow stress dependence on strain became non-negligible and various concepts which account for changing stresses as a function of strain were incorporated into the different phenomenological and physical models [28–30]. One major approach that some researchers have adopted is to divide the stress-strain curves into two parts: (i) region on the curve where work hardening, and dynamic recovery dominate the deformation process and (ii) region of the curve where dynamic recrystallisation or flow localisation control the deformation process [31]. While this approach has provided very accurate prediction of flow stress, their complexity and the need to sometimes determine a large number of constitutive constants have been a major disadvantage. Lin and Chen [15] emphasised that simple constitutive models with minimal constitutive constants are often desirable. Therefore, simplified constitutive models with minimal constants were also explored by a number of researchers [32–34].

Lin et al. [35] introduced the concept of strain compensation into the hyperbolic-sine equation to accommodate changing stress values with strain. Thereafter, other researchers have since applied it on different metallic system in the prediction of flow stress [29]. Regression and error analyses from some of these works have shown that the prediction of flow stress was also accompanied with large error values despite the strain compensation. Hence, combination of different constitutive models or the optimisation of constitutive constants [11–13,36] have been the alternative concepts adopted for flow stress prediction with high accuracy.

In this work, flow stress prediction was obtained using hyperbolic-sine Arrhenius equation for two different titanium alloys that were subjected to hot deformation in the dual phase region. A simple optimisation step was introduced to improve the prediction of the flow stress.

2. Experimental

The stress-strain data used in this work was obtained from Ref. [37] where it was established that for most testing condition, the flow curves (Fig. 1) obtained did not satisfy the steady-state stress condition after the peak stress was reached.

The data were generated by axisymmetric compression testing of α + β experimental Ti-6Al-1V-3Fe and Ti-4.5Al-1V-3Fe alloys at deformation temperatures between 750 and 900 °C and under the strain rates of 0.001 to 10 s⁻¹. The alloys were deformed to a global strain of 0.6 on a Glebele 3500 thermomechanical simulator. Nickel paste and graphite foil were placed between the anvils and the samples to minimise the effect of friction. Only deformed samples with barrelling coefficient that was less than 1.1 was considered as a valid test [37]. Correction for adiabatic heating effects were performed on the flow stress data according to Goetz and Semiatin [39].

A hyperbolic-sine constitutive equation based on an Arrhenius-type relationship [11] with a temperature-compensated strain rate parameter (Z), known as the Zener-Hollomon parameter, was used to describe and predict the flow stress [20].

The equations are expressed mathematically as:

\[ \dot{\varepsilon} = AF(\sigma) \exp \left( \frac{Q}{RT} \right) \]  \hspace{1cm} (1)  

\[ Z = \dot{\varepsilon} \exp \left( \frac{Q}{RT} \right) \]  \hspace{1cm} (2)
Fig. 2 – Plots for determining various materials constants for Ti-4.5Al-1V-3Fe alloy.
and:

$$ F(\sigma) = \begin{cases} \sigma^n, & \text{for } \alpha \sigma < 0.8 - \text{low stress} \\ \exp(\beta \sigma), & \alpha \sigma > 1.2 - \text{high stress} \\ [\sinh(\alpha \sigma)]^n \text{ for all } \sigma - \text{low and high} \end{cases} $$

$$ \dot{\varepsilon} = A[\sinh(\alpha \sigma)]^n \exp\left(\frac{-Q}{RT}\right) \quad (3) $$

where $\dot{\varepsilon}$ is strain rate, $\sigma$ is stress, $n$ is the stress exponent, $Q$ is the activation energy, $R$ is the gas constant (8.314 kJ/mol), $T$
is temperature, \( Z \) is the Zener-Hollomon parameter, and \( \alpha, \beta \) and \( A \) are material constants.

From Eq. (3), \( F (\dot{\varepsilon}) \) represents power law which is preferred at low stress while \( F (\exp (\dot{\varepsilon})) \) refers to the exponential law which can be applied at higher stresses. The power law breaks down at high stress as \( \dot{\varepsilon} \) vary with strain rate, while the exponential law breaks down at high temperature below the strain rate of \( 1 \text{s}^{-1} \) [40,41]. The introduction of the hyperbolic-sine function \( F (\sinh(\dot{\varepsilon})) \) allows a wide range of stresses to be described using Eq. (3). The material constant \( \alpha \) is often called stress multiplier which is obtained from \( \sigma = \beta/\dot{\varepsilon} \). The stress multiplier has been reported to be an additional material constant in the hyperbolic-sine equation which brings \( \sigma \dot{\varepsilon} \) in the correct range. Hence the curves in the plot of \( \ln \dot{\varepsilon} \) vs \( \ln [\sinh(\dot{\varepsilon})] \) at constant temperature is often made linear and parallel [40,41]. The different constitutive constants were obtained at incremental stress and each constant was plotted as a function of strain. The predicted stress was determined using Eq. (4). The predictability of the constitutive models was evaluated by average absolute relative error (AARE), root mean square error (RMSE) and correlation coefficient (\( R^2 \)), which are presented in Eqs. (5)-(7). To reduce the AARE and RMSE, the constitutive constants were then optimised using a simple generalised reduced gradient (GRG) algorithm encoded within Microsoft Excel Solver tool. The AARE described in Eq. (5) served as the objective function that was minimised. The solver found a local optimum solution that satisfied the Karush-Kuhn-Tucker (KKT) conditions for local optimality.

\[
\sigma = \frac{1}{\dot{\varepsilon}} \ln \left\{ \left( \frac{Z}{A} \right)^{\frac{1}{n}} + \left[ \left( \frac{Z}{A} \right)^{\frac{1}{n}} + 1 \right]^{\frac{1}{2}} \right\} \tag{4}
\]

\[
\text{AARE} (%) = 1/N \sum_{i=1}^{N} \left| \frac{M_i - \bar{P}_i}{M_i} \right| \times 100 \tag{5}
\]

\[
\text{RMSE (MPa)} = \sqrt{\frac{1}{N} \sum_{t=1}^{N} (M_t - \bar{P})^2} \tag{6}
\]

\[
R^2 = \frac{\sum_{i=1}^{N} (M_i - \bar{M})(P_i - \bar{P})}{\sqrt{\sum_{i=1}^{N} (M_i - \bar{M})^2} \sum_{i=1}^{N} (P_i - \bar{P})^2} \tag{7}
\]

where \( M_i \) is measured stress, \( P_i \) is predicted stress and \( N \) is the number of measurements.

### 3. Results and discussion

The fitting of experimental data for determining the constitutive constants at a strain of 0.1 for the two titanium alloys is shown in Figs. 2 and 3. The data for the different plots in Figs. 2 and 3 were obtained from partial differentiation and rearrangement of Eq. (3) such that the average slopes of the plots of \( \ln \dot{\varepsilon} \) against \( \sigma \) and against \( \ln \sigma \) were used to obtain \( \dot{\varepsilon} \) and \( \beta \) respectively, \( \ln \dot{\varepsilon} \) against \( \ln[\sinh(\dot{\varepsilon})] \) to obtain \( n \) and \( \ln[\sinh(\dot{\varepsilon})] \) against 1000/\( T \) to obtain \( k \). The values of the constitutive constants obtained at strains 0.1 to 0.6 is presented in Tables 1 and 2 for the two titanium alloys. It can be seen from Figs. 2b and 3b that \( \beta \) varies sharply with temperature,
similar trend was seen in Ti-6Al-4V subjected to hot working at different temperatures of 750–900 °C and \(10^{-2}–10^{-1}\) strain rates [10]. The reason for this sharp variation is not clear but may be as a result of the changing physical mechanisms which control the flow behaviour of the alloys under different deformation conditions of temperature and strain rate. Since \(\beta\) is obtained from exponential law, the observed variation may likely be pointing to the breaking of the exponential law at high temperature when the strain rate is lower than \(1\,\text{s}^{-1}\).

Of all the constitutive constants, stress exponents \(n\) and activation energy \(Q\) calculated from Eq. (8) are usually used to suggest mechanisms controlling deformation. Generally, the stress exponents and activation energy values obtained at each incremental strain for both alloys fall within the range of the values reported in most literatures for titanium alloys hot worked within the \(\alpha + \beta\) temperatures [9,13,30,42–46]:

\[
Q = RnK = R \left\{ \frac{\partial \ln \dot{\varepsilon}}{\partial \ln [\sinh (\Delta / T)]} \right\}_T \left\{ \frac{\partial \ln [\sinh (\Delta / T)]}{\partial (\Delta / T)} \right\}_T
\]

(8)

From Tables 1 and 2, it can be seen that the stress exponent \(n\) values were all less than 5 at all strains. This indicates that softening mechanisms other than dynamic recovery was at play during hot deformation of the alloys. Mirzadeh [33] reported that stress exponent is usually taken to be 5 when deformation is controlled by dislocation climb and glide. In another study, it was shown that stress exponent value that is less than 5 can be used to predict the occurrence of dynamic recrystallisation during hot working [47]. The stress exponent obtained from this work already showed that other mechanisms which are not attributable to steady-state stress condition influenced flow softening during deformation of both alloys.

The values of the activation energy for hot working \(Q_{\text{HW}}\) of both alloys decreased with increasing strain, but in all cases, were higher than the activation energy for self-diffusion \(Q_{\text{SD}}\) of titanium, 150 KJmol\(^{-1}\) for \(\alpha\)-Ti and 153 KJmol\(^{-1}\) for \(\beta\)-Ti [48]. McQueen and Ryan [41] reported that activation energy for hot working are usually higher than the activation energy for self-diffusion by 20% and may be up to 50% should the alloy being deformed contain precipitates, secondary phases or other inclusions. Additionally, titanium alloys with more solute contents had higher \(Q_{\text{HW}}\) when compared with alloys having less solute contents [49,50], this is seen in the trend of the activation energy of the two alloys considered in this work. The \(Q_{\text{HW}}\) at all strain (Tables 1 and 2) was higher in Ti-6Al-1V-3Fe than in Ti-6Al-1V-3Fe.

The decrease in activation energy with increasing strain implies that deformation became easier as strain increased due to generation of more slips by mobile dislocations. In some studies [51,52], higher \(Q_{\text{HW}}\) than \(Q_{\text{SD}}\) was ascribed to the occurrence of dynamic recrystallisation during hot working. However, it should be noted that the high \(Q_{\text{HW}}\) values obtained in this work would make any atomistic mechanism almost impossible during deformation and are thus considered apparent. Seetharaman and Semiatin [53] concluded that \(Q_{\text{HW}}\) obtained during hot working of Ti-6Al-4V at sub-transus region were apparent and did not have any physical meaning. For this reason, physical models are preferred by some researchers as they provide physical meaning for the constitutive constants and the overall mechanisms controlling
the deformation process [31, 54]. Recently, some researchers have explored the possibility of attributing physical meaning to materials constants, especially n and Q that are obtained from hyperbolic-sine equation. This approach which is commonly referred to as physically based hyperbolic-sine method, involves incorporating the Young's modulus and self-diffusion coefficient into the hyperbolic-sine equations, thus allowing the $Q_{SD}$ to be used in place of the apparent $Q_{SW}$ [55, 56]. This then gives physical meaning to the activation energy and other material constants. The physically-based hyperbolic-sine equation has been used to describe the flow behaviour of steel, aluminium and magnesium alloys. However, to the best of the author’s knowledge, published articles on the application of the simple physically-based hyperbolic-sine model on titanium alloys are rarely available and this is now being considered this in another work. Additionally, the application of physically-based hyperbolic-sine equation or other physical models may not necessarily guarantee flow stress prediction with low RMSE and AARE values [57].

Since the objective of this study was not to establish flow softening mechanisms but to evaluate the predictability of flow stress using the Arrhenius equation on titanium alloys that do not satisfy the steady-state stress condition, the constitutive constants presented in Tables 1 and 2 were used in predicting the flow stress. Thereafter, the accuracy of prediction was deduced from the correlation coefficient, average absolute relative error and the root mean square error. As shown in Fig. 4, $R^2$, AARE and RMSE for Ti-4.5Al-1V-3Fe are 0.96, 16.9 and 28.4 MPa, while the values are 0.98, 10.1 and 21.1 MPa for Ti-6Al-1V-3Fe alloy. Although the $R^2$ values already showed that reasonable prediction of flow stress can be obtained from the model, but the AARE and RMSE values are still high and can be reduced using the generalised reduced gradient refinement.

The MS Excel solver tool offer a simple and quick optimisation process for obtaining improved predictability of flow stress. It was reported that the high AARE and RMSE error obtained in the conventional Arrhenius equation was due to experimental scatter when fitting data to obtain $\alpha$ and $\beta$ values [34]. These values are used to obtain the stress multiplier, $\alpha$ which allows the Arrhenius equation to be used for both high and low stresses. Therefore, finding optimum value of $\alpha$ may help improve the accuracy of flow stress prediction.

**Fig. 6 – Constitutive constants as a function of strain for Ti-4.5Al-1V-3Fe alloy.**
The GRG refinement done in this study used the AARE as the objective function to be minimised. All constitutive constants presented in Tables 1 and 2 were optimised except $\beta$ and $n$ since $\alpha$ was obtained from both constants. The molar gas constant, $R$, which has a fixed value was constrained during the refinement. The values of the optimised constitutive constants for both alloys are presented in Tables 3 and 4, it is observed that the optimised stress exponent and activation energy followed similar trend as those previously presented in Tables 1 and 2. The constitutive constants were then used to predict the flow stress, and the $R^2$, AARE and RMSE that were obtained are shown in Fig. 5. It is observed that for both alloys the $R^2$ increased to 0.99 indicating an improvement in the prediction of flow stress. The AARE and the RMSE for both alloys reduced as well. For the Ti-6Al-1V-3Fe, the AARE and RMSE reduced by 36% and 30% respectively while for Ti-4.5Al-1V-3Fe alloy, the reduction in AARE and RMSE was 44% and 31% respectively. This reduction in the AARE and RMSE values confirmed that the GRG refinement provided a more accurate prediction of the flow stress.

The $R^2$ and AARE values obtained from this work was compared to those in recently published articles [14,31,54,57,58]. The GRG could be used to minimise the AARE and the RMSE to levels comparable to some of these works.

Figs. 6 and 7 show the plots of constitutive constants as a function of strain, it can be seen that for most cases the relationship can be fitted with good correlation coefficients using a straight-line equation. This differs from most studies where the relationship between constitutive constants and strain are fitted on 3rd to 5th order polynomial curve where over fitting of the data is very likely. Fig. 6a, b and e shows polynomial relationship between constitutive constants ($\alpha$, $n$ and $k$) and strain for Ti-6Al-1V-3Fe alloy. Fitting with lower order poly-
nominal for these constants led to poor prediction of the flow stress.

4. Conclusion

The hot working behaviour of two α + β titanium alloys was studied through constitutive analysis based on the hyperbolic-sine Arrhenius equation. The constitutive constants were obtained at incremental strain and were optimised using generalised reduced gradient refinement. The result showed that good prediction of the flow stress with reasonable correlation coefficient, but high average absolute relative error and root mean square error were obtained without the generalised reduced gradient refinement. The average absolute relative error and root mean square error were reduced by 30 to 40% in both alloys when the constitutive constants were optimised using the generalised reduced gradient refinement. Also, the correlation coefficients of 0.96 for Ti-4.5Al-1V-3Fe and 0.98 for Ti-6Al-1V-3Fe both increased to 0.99 due to the refinement. The generalised reduced gradient refinement offers a simple way of improving the prediction of flow stress during hot working of titanium alloys when using the hyperbolic-sine Arrhenius equation, and may be applied to other phenomenological and physical models when describing hot working behaviour of metals and alloys.

Conflict of interest

The author declares no conflicts of interest.

Appendix A. Supplementary data

Supplementary material related to this article can be found, in the online version, at doi:https://doi.org/10.1016/j.jmrt.2019.12.070.

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