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Universal multi-objective function for optimising superplastic-damage constitutive equations

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Abstract

Based on the dominated deformation mechanisms of superplastic materials, an assumption for micro-damage evolution is presented. Then, a set of unified viscoplastic-damage constitutive equations is proposed to model material hardening due to the increase of dislocation density and grain growth, as well as material softening due to intergranular void nucleation and growth. The effects of the hardening and softening state variables on superplastic flows are characterised. To overcome the difficulties associated with the difference between predicted and experimental life spans and the variation in scales during multi-objective optimisations of material constants arising in the constitutive equations from experimental data, a unitless objective function has been formulated. This enables all experimental data to be involved in the optimisation. The constitutive equation set has been characterised for two superplastic alloys from experimental data using evolutionary programming (EP) optimisation techniques and the proposed method for formulating objective functions.

Keywords: Superplasticity; Micro-damage; Void growth; Materials modelling; Optimisation

1. Introduction

The superplastic behaviour of structural alloys, such as aluminium and titanium, are being exploited increasingly for producing a range of light-weight components with complex shapes, such as aircraft structural components, electronic equipment cabinets, etc. The superplasticity of a material is highly dependent on temperature and occurs only in a narrow range of strain rates with an optimum value that is unique to each material [1,2]. Therefore, the control of deformation rate in a superplastic forming process is important [3]. The finite element technique has been successfully developed and used to simulate superplastic forming processes [4] and optimise the forming parameters, such as temperature, loading history and the final thickness [3,5]. In order to accurately simulate superplastic forming processes and thoroughly understand the superplastic deformation mechanisms of materials, physically based unified viscoplastic constitutive equations for superplastic alloys need to be established.

One of the most difficult tasks encountered in developing viscoplastic constitutive equations is how to accurately determine material constants arising in the equations from experimental data for a range of temperatures and strain rates. Lin and Hayhurst [6] developed an optimisation technique and successfully determined the material constants for the constitutive equations where stress can be explicitly expressed as a function of strain. However, for a set of unified general viscoplastic constitutive equations, numerical integration is needed for solving the equations. It has been shown that the objective functions for the optimisations are highly non-linear [7–9]. Hence traditional gradient descent methods tend to fail because it is very difficult to choose starting values for the constants to obtain the global minimum. Thus, extra care should be taken to choose starting values of the constants for optimisation. Kowalewski et al. [10] developed a three-step method to determine the starting values of the constants in a set of creep-damage constitutive equations for final optimisation. Zhou and Dunne [8] proposed a four-stage method to determine material constants for a particular set of the superplastic constitutive equations. The starting values of the material constants have to be chosen carefully at each stage of the optimisation, otherwise convergence to a local

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minimum is unavoidable and poor material constants would be obtained.

The techniques developed above are highly problem dependent and usually suitable for only particular sets of constitutive equations. Significant knowledge of material science, mathematics and computational mechanics is required. In order to solve the problem, Lin and Yang [11] proposed a genetic algorithm (GA)-based optimisation technique, which is suitable for both creep-damage models and general unified viscoplastic constitutive equations. This technique has generic features, overcomes the difficulty of choosing starting values for the constants, and provides a better chance to converge to the global minimum. However, the method used was based on the classical binary GA. It is inefficient in solving continuous problems [12], such as those considered in this paper. Hence the computing resources required for solving the optimisation problems are significant.

To solve the optimisation problems in materials modelling, two important aspects need to be considered. One is the nature of the objective (or fitness) functions, which should characterise the particular feature of an optimisation problem. The other is the optimisation algorithms used, which should be consistent with the convergence nature of the formed objective functions. In this paper, effort will be made to (i) develop a set of unified viscoplastic-damage constitutive equations for superplastic alloys, (ii) formulate an unitless objective function for optimisation, and (iii) use evolutionary programming (EP) techniques introduced by Yao et al. [13] to determine the constitutive equations from experimental data for two superplastic alloys.

2. Unified superplastic-damage constitutive equations

2.1. Steady-state viscoplastic material models

For ductile metals and alloys at temperatures less than $0.4T_m$ where plastic deformation occurs through dislocation movement, the non-linear stress–strain relationship, i.e. the material hardening, is conventionally described by [14]

$$\sigma = K\varepsilon_p^N \tag{1}$$

where K is a constant and N is the strain-hardening exponent. When the temperature raises above $0.5T_m$ and thermally activated processes are allowed to intrude, the flow stress is a function of strain rate. Thus there is

$$\sigma = K\varepsilon_p^N\dot{\varepsilon}_p^m \tag{2}$$

where $\dot{\varepsilon}_p$ is the strain rate and m is the strain rate-hardening exponent. The term ε_p^N specifies the material hardening due to plastic deformation and $\dot{\varepsilon}_p^m$ characterises the hardening due to plastic strain rate. To physically model the hardening mechanisms, the plastic flow of the material can be expressed by unified elasto-viscoplastic constitutive equations. The general uniaxial plastic strain rate equation for steady-state flow of the material takes the form

$$\dot{\varepsilon}_{ss} = \left[\frac{\sigma - R - k}{K}\right]^n d^{-u} \tag{3}$$

where d is the average grain size, k the initial yield stress, n and u are the material constants. The strain rate sensitivity parameter m is given by $m = 1/n$. R is the isotropic hardening variable, which is related to the accumulation of dislocation density and expends the yield surface of a material under plastic deformation. The evolution equation for R takes the form [11]

$$\dot{R} = b(Q - R)\dot{\varepsilon}_p \tag{4}$$

where b and Q are the material constants. The evolution equation for average grain size in the thermo-mechanical processing can be modelled by the equation [14]

$$\dot{d} = \alpha d^{-\gamma_0} + \beta\dot{\varepsilon}_p d^{-\phi} \tag{5}$$

The constants γ_0 and ϕ characterise the effects of isothermal and plastic strain-induced grain growth, respectively. α and β are the material constants.

2.2. Damage evolution equations

Eqs. (3)–(5) can be used to model the steady-state flow of a viscoplastic material (Fig. 1). In the early stage of deformation, the overall material hardening is mainly a result of grain growth and the increase of dislocation density. At the late stage of deformation, softening due to micro-damage dominates and decreases the flow stress (Fig. 1).

It is well known that grain-boundary sliding and grain rotation are two important mechanisms in superplastic alloys. The relative movements result in void nucleation and growth at grain boundaries. Thus the modelling of void nucleation and growth mechanisms is key in predicting the softening at the late stage of superplastic deformation. Fig. 2 shows a schematic structure of a cavitated superplastic material, which is similar to the intergranular void growth

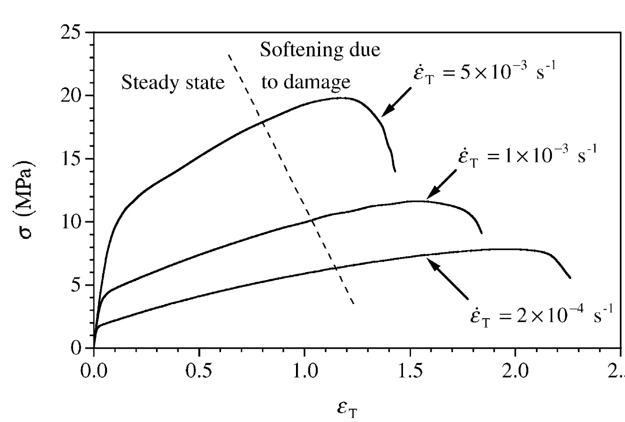

Fig. 1. Characteristics of stress–strain relationship for a superplastic alloy.

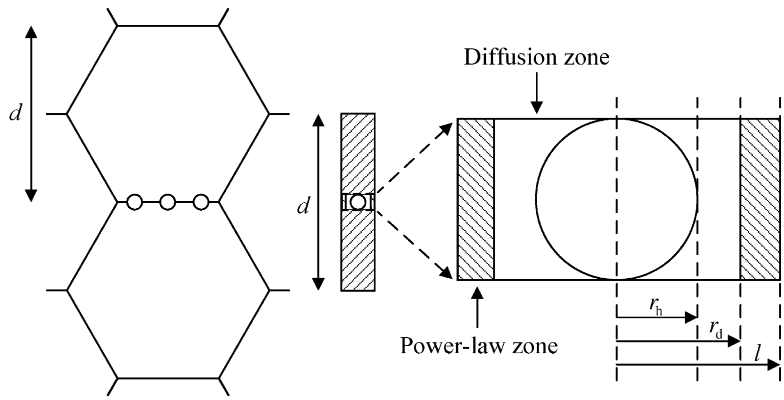

Fig. 2. Void growth at grain boundaries.

under high stress creep, as discussed by Cocks and Ashby [15]. The deformation of the cavitated material can be described by a cavitated cylinder shown in the figure, of which the radius is equal to the cavity spacing l. For the top and bottom parts of the cylinder, their behaviour can be directly described by the power-law equation (Eq. (3)). However, for the behaviour of the slab containing a spherical cavity of radius r_h, it needs to account for the size of the cavity and the extent of the diffusion zone indicated by r_d. Such a model possesses an important feature: if r_d extends to as large as the cavity spacing l, cavity growth is purely by diffusion; but if it shrinks until $r_d = r_h$, then the surrounding area ($r_d < r < l$), or simply the power-law zone, totally controls the rate of void growth. This allows void growth to be regarded as a combined result of both diffusion and power-law deformation.

Assuming that the load shed by the diffusion zone is negligible, the slab can be seen as containing a hole of an "effective" size r_d, and therefore, subjected to an "effective" stress of $\sigma/(1-f_d)$, where f_d is the area fraction defined as $f_d \equiv r_d^2/l^2$. Subsequently, based on Eq. (3), the plastic strain rate for the slab is obtained as

$$\dot{\varepsilon}_{zz} = \left[\frac{\sigma/(1-f_d) - R - k}{K}\right]^n d^{-\mu} \tag{6}$$

Making use of the results obtained by Cocks and Ashby [15], the overall plastic strain rate for the whole cylinder becomes

$$\dot{\varepsilon}_p = \dot{\varepsilon}_{ss}\left[1 + \frac{2lf_h^{1/2}}{d}\left(\frac{\dot{\varepsilon}_{zz}}{\dot{\varepsilon}_{ss}} - 1\right)\right] \tag{7}$$

The evolution law for the area fraction $f_h \equiv r_h^2/l^2$ can be obtained by imposing volume conservation and considering the rigid body translation of the grains on either size, giving

$$\dot{f}_h = \frac{f_h}{d}\dot{d} + \left(f_d - \frac{2lf_h^{3/2}f_d}{d}\right)\dot{\varepsilon}_{zz} \tag{8}$$

On the other hand, the evolution law for the area fraction f_d can be expressed in terms of $\dot{\varepsilon}_p$, ε_p, and f_d:

$$\dot{f}_d = D_1 f_d^{d_1}\dot{\varepsilon}_p^{-d_2} + D_2\dot{\varepsilon}_p^{-d_3}\cosh(D_3\varepsilon_p) \tag{9}$$

where D_1, d_1, d_2, D_2, d_3, and D_3 are the material constants. The evolution law for the radius of the cylinder l, which is also the cavity spacing, is obtained following the results of Cocks and Ashby [15]: for $f_h = 0$,

$$\dot{l} = \tfrac{1}{2} l\dot{\varepsilon}_{zz} \tag{10}$$

which is a function of only the strain rate experienced by the slab; for $f_h > 0$, the effects of f_h need to be incorporated and hence results in

$$\dot{l} = \frac{l}{2f_h}(f_d\dot{\varepsilon}_{zz} - \dot{f}_h) \tag{11}$$

Consolidating the above, the set of constitutive equations for superplastic materials with consideration of micro-damage is given as

$$\dot{\varepsilon}_p = \dot{\varepsilon}_{ss}\left[1 + \frac{2lf_h^{1/2}}{d}\left(\frac{\dot{\varepsilon}_{zz}}{\dot{\varepsilon}_{ss}} - 1\right)\right] \tag{12}$$

$$\dot{\varepsilon}_{ss} = \left[\frac{\sigma - R - k}{K}\right]^n d^{-u} \tag{13}$$

$$\dot{\varepsilon}_{zz} = \left[\frac{\sigma/(1-f_d) - R - k}{K}\right]^n d^{-\mu} \tag{14}$$

$$\dot{R} = b(Q - R)\dot{\varepsilon}_p \tag{15}$$

$$\dot{d} = \alpha d^{-\gamma_0} + \beta\dot{\varepsilon}_p d^{-\phi} \tag{16}$$

$$\dot{f}_h = \frac{f_h}{d}\dot{d} + \left(f_d - \frac{2lf_h^{3/2}f_d}{d}\right)\dot{\varepsilon}_{zz} \tag{17}$$

$$\dot{f}_d = D_1 f_d^{d_1}\dot{\varepsilon}_p^{-d_2} + D_2\dot{\varepsilon}_p^{d_3}\cosh(D_3\varepsilon_p) \tag{18}$$

$$\text{for } f_h = 0, \quad \dot{l} = \tfrac{1}{2} l\dot{\varepsilon}_{zz} \tag{19}$$

$$\text{for } f_h > 0, \quad \dot{l} = \frac{l}{2f_h}(f_d\dot{\varepsilon}_{zz} - \dot{f}_h) \tag{20}$$

$$\dot{\sigma} = E(\dot{\varepsilon}_T - \dot{\varepsilon}_p) \tag{21}$$

where E is the Young's modulus (e.g. $E = 1000$ MPa for Al–Zn–Mg at 515 °C), and ε_T is the true total strain. Both damage variables f_h and f_d vary from 0, the virgin state, to 1, the failure state. The damage is initiated due to high-temperature grain-boundary diffusion that is related to Eq. (18), which is a function of plastic strain and plastic strain rate. As deformation progresses, f_d increases from zero and the non-zero value of f_d encourages the growth of f_h. The weakening of a superplastic material is a combined result of the damage mechanisms. In particular, f_h dominates the weakening process at the late stage of deformation and determines the failure of the material. The radius of the cylinder l indicates the average number of voids at a grain boundary; it varies from an initial value l_0 to 0, the theoretical limit.

Including Young's modulus and l_0, there are 18 material constants within the unified viscoplastic-damage equations (Eqs. (12)–(21)). These material constants need to be determined from experimental data of a material using an optimisation technique. In the following, a method for formulating a universal multi-objective function is proposed for the optimisation.

3. Objective functions for optimisation

3.1. The conventional least-squares

Suppose one is fitting N data points $(x_i, y_i), i = 1, \ldots, N$, to a model y that has M adjustable parameters $a_j, j = 1, \ldots, M$, and y predicts a functional relationship between the measured independent and dependent variables,

$$y(x) = y(x; a_1 \cdots a_M) \tag{22}$$

where the dependence on the parameters is indicated explicitly on the right-hand side. When determining $a_1 \cdots a_M$, it is common to express the problem as

$$\text{minimise over } a_1 \cdots a_M : \quad \sum_{i=1}^{N} [y_i - y(x_i; a_1 \cdots a_M)]^2 \tag{23}$$

The practitioners seldom query the origin of this least-squares formulation nor do they examine the basic principles it is based on and, more importantly, the underlying assumptions. Actually, Eq. (23) comes from the subject of maximum likelihood estimators, and it is determined based on normal distribution. Normal distribution is the distribution of a random variable y with a frequency function

$$f(y) = \left[\frac{1}{s\sqrt{2\pi}}\right] \exp\left[-\frac{(y-\mu)^2}{2s^2}\right] \tag{24}$$

where μ is the mean, s the standard deviation, and y is described as $\eta(\mu, s^2)$. Eq. (24) is symmetric about $y = \mu$, and is often described as bell-shaped. Now, if each y_i has a measurement error Δy_i that is independently random and distributed as a normal distribution around $y(x_i)$, there exist a statistical universe of data sets, which can be drawn from $y(x_i)$. Assuming the standard deviations for the normal distributions are the same for all data points, $s_i = s$, and the measurement errors at each data point are the same, $\Delta y_i = \Delta y$, the probability of getting the data set

$$P = \left[\frac{\Delta y}{s\sqrt{2\pi}}\right]^n \prod_{i=1}^{n} \exp\left\{-\frac{[y_i - y(x_i)]^2}{2s^2}\right\} \tag{25}$$

Maximising Eq. (25) is equivalent to minimising the negative of its logarithm, namely,

$$-n \log\left[\frac{\Delta y}{s\sqrt{2\pi}}\right] + \left[\sum_{i=1}^{n} \frac{[y_i - y(x_i)]^2}{2s^2}\right] \tag{26}$$

Since n, Δy and s are all constants, minimising Eq. (26) is equivalent to minimising the conventional least-squares (Eq. (23)).

Notice the stringent assumption and constraint in the least-squares formulation: that the standard deviations are defined as the same at all points, and the error calculations are always performed at the same x_i's. When dealing with constitutive models of which the life spans are implicitly characterised by some of the material parameters, this inevitably gives rise to the problem mentioned by Li et al. [16]. If the life span of a predicted behaviour is shorter than the data points', such as fitting curve 1 in Fig. 3, data beyond the predicted life span are not involved in the least-squares. For a prediction with a life span that is longer than the data points', such as fitting curve 2 in Fig. 3, the resulted residual can be misleading as well.

3.2. Universal multi-objective function

When dealing with predictions with various life spans, the judgement is made not only based on the distances from the data set, the trends of predictions also give credits to the final decision. This, therefore, makes the conventional least-squares which only takes errors at the same x_i's into account

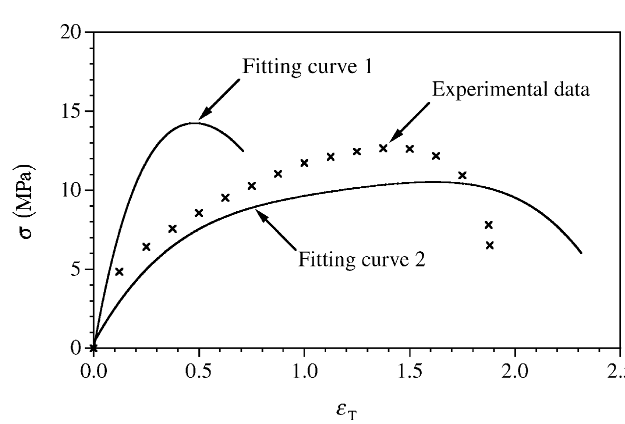

Fig. 3. Assessment of residuals between predicted and experimental results for different life spans.

becomes inefficient. To reduce the effect of the inconsistent life spans on the residuals, correction terms are introduced to fitness functions by Kowalewski et al. [10] and Li et al. [16] for determining creep-damage constitutive equations. The convergence has been proved, but it is very difficult to choose weightings, which are different from one problem to another.

By virtue of the trend and life span, the universal objective function is expressed as

$$f_U = f_1 + f_2 \tag{27}$$

where f_1 depicts the likelihood between the predicted and model's trends, and f_2 is the likelihood between the predicted and model's life spans. Their detailed formulations are as follows:

$$f_1 = \left(\frac{1}{N}\right)\sum_{i=1}^{N}\left\{\frac{y_i - y(x^c_{max}x_i/x_{max})}{s_{1,i}}\right\}^2 \tag{28}$$

$$f_2 = \left[\frac{x_{max} - x^c_{max}}{s_2}\right]^2 \tag{29}$$

where x^c_{max} is the predicted life span, $x_{max} = x_n$, $s_{1,j}$ the standard deviation for data point y_i, and s_2 is the standard deviation for life span prediction.

When optimising f_1 alone, it ensures that the prediction behaves in the same way as that exhibited by the data points at significant stages of their life spans. Since the frequency of performing such an examination is directly dependent on the density of data points, one should provide a density that is sufficient to characterise the behaviour that is sought for. Notice that Eq. (28) does not assume that the standard deviations are constant for all data points. The association of the standard deviations in Eq. (28) essentially provides a means of normalisation and transforms the errors to unitless numbers, which is important when dealing with multiple objectives. Another attribute of Eq. (28) is that the sum of the errors is also normalised against the number of data points. This enforces the compatibility with f_2 such that both play an equally important role and f_U does not give a representation biased towards the criterion that received more counts.

The formulation of f_2 is relatively simpler, however, it is equally as important as f_1 in representing the overall quality of a prediction. The error in f_2 is normalised against s_2, which again results in a unitless error count. When optimising with f_2 alone, it ensures that the predicted life span is as close as the data points'. This x-direction effect is all pervasive to the entire prediction, because pushing x^c_{max} towards x_{max} ultimately means pushing all the predicted points towards their corresponding counterparts of the model's. Furthermore, due to the generic features of Eq. (27), the residuals for multiple objectives can be combined directly to form a multi-objective function without introducing weighting factors, in contrast to the formulations given by Lin and Yang [11].

4. Determination of viscoplasticity-damage constitutive equations

4.1. Overall objective function

The objective function used for determining the material parameters arising in Eqs. (12)–(21) is expressed as the sum of

$$f = f_\sigma + f_D \tag{30}$$

$$f_\sigma = \sum_{j=1}^{n_1}\left\{\frac{1}{m_j}\sum_{i=1}^{m_j}\left\{\frac{(\sigma^e_i)_j - (\sigma^c(\varepsilon^c_{T,max}\varepsilon^e_{T,i}/\varepsilon^e_{T,max}))_j}{(s_{1_\sigma,i})_j}\right\}^2 + \left[\frac{(\varepsilon^e_{T,max})_j - (\varepsilon^c_{T,max})_j}{(s_2)_j}\right]^2\right\} \tag{31}$$

$$f_D = \sum_{k=1}^{n_2}\left\{\frac{1}{m_k}\sum_{i=1}^{m_k}\left\{\frac{(d^e_i)_k - (d^c_i(\varepsilon^c_{T,max}\varepsilon^e_{T,i}/\varepsilon^e_{T,max}))_k}{(s_{1_d,i})_k}\right\}^2 + \left[\frac{(\varepsilon^e_{T,max})_k - (\varepsilon^c_{T,max})_k}{(s_2)_k}\right]^2\right\} \tag{32}$$

where f_σ is the residual for stress and f_D is the residual for grain size, both formulated based on Eq. (27), $s_{1_\sigma,i} = \max(1.0, 0.1\sigma^e_i)$, $s_2 = 0.1\varepsilon^e_{T,max}$, $s_{1_d,i} = 0.1d^e_i$, n_1 the number of strain rates considered in f_σ, n_2 the number of strain rates considered in f_D, m_j and m_k are the number of experimental data points for the corresponding strain rate.

4.2. Determination of constitutive equations for superplastic alloy Al–Zn–Mg

To determine the material constants in Eqs. (12)–(21) for Al–Zn–Mg at 515 °C from experimental (symbols) stress–strain and grain size–strain data (Fig. 4) [17], an optimisation are carried out using the multi-objective functions

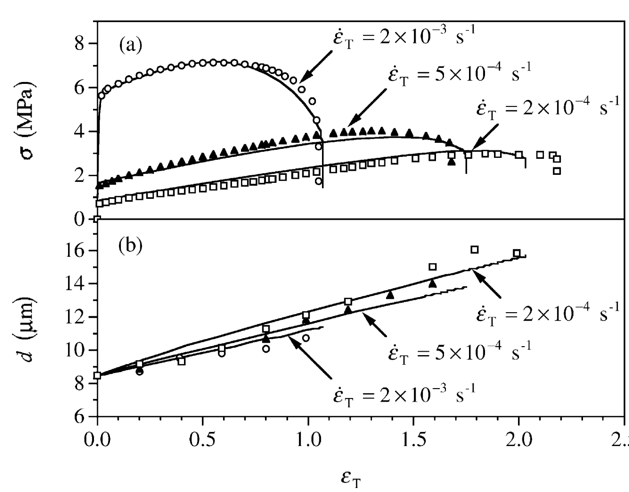

Fig. 4. Comparison of the predicted (solid curves) and experimental (symbols) for Al–Zn–Mg at 515 °C for different strain rates: (a) stress–strain relationship; (b) grain size–strain relationship.

Table 1
Optimised material constants for Al–Zn–Mg at 515 °C

k	K	n	μ	b	Q	α	γ_0	β
0.2912	85.1712	1.0000	1.6236	0.1537	7.6744	6.9000E−2	2.4000	2.6000
ϕ	D_1	D_2	D_3	d_1	d_2	d_3	E	l_0
5.5000E−5	8.1445E−9	69.5748	1.0000	30.0013	3.3300	1.7658	1.000E+3	3.6347

Table 2
Optimised material constants for Al 7475 at 515 °C

k	K	n	μ	b	Q	α	γ_0	β
4.3917E−2	7.6385	1.7204	2.4179	0.8422	5.5170	99.0815	1.0877E+2	55.3596
ϕ	D_1	D_2	D_3	d_1	d_2	d_3	E	l_0
0.8729	24.6681	7.1677	1.9716	88.4659	3.0426	1.6609	1.5128E+2	2.9857

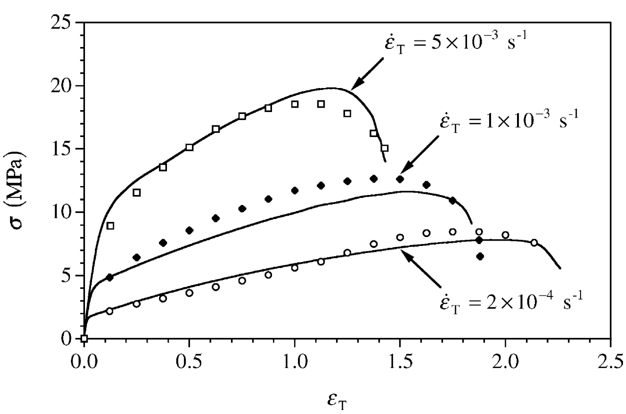

Fig. 5. Comparison of the predicted (solid curves) and experimental (symbols) stress–strain relationships for Al 7475 at 515 °C for different strain rates.

(Eqs. (30)–(32)) and the EP-based optimisation technique introduced by Li et al. [16]. EP has been shown to be an effective global optimisation algorithm for a wide range of different problems [13,16]. The optimised material constants are listed in Table 1 and the computed results (solid curves) are shown in Fig. 4. It can be seen that both the predicted stress–strain relationships and grain growth show a good agreement with the corresponding experimental data for strain rates $\dot{\varepsilon}_T = 2\times10^{-4}$, 5×10^{-4} and $2\times10^{-3}\,s^{-1}$ and initial grain size $d_0 = 8.47\,\mu m$.

4.3. Determination of constitutive equations for superplastic alloy Al 7475

Experimental stress–strain data (symbols) for Al 7475 at 515 °C shown in Fig. 5 are used for the optimisation. The determined material constants are listed in Table 2. The computed stress–strain relationships are shown by the solid curves in Fig. 5 for different strain rates. It can be seen that a close agreement between the experimental data and computed results is obtained.

5. Conclusions

The universal multi-objective function formulated from the work ensures that all the experimental data points are involved in the error assessment. This is especially useful for determining constitutive equations such as creep-damage and viscoplastic-damage material models, of which the life spans are of significance. The introduction of weightings to compensate for the different units in objective functions has been completely eliminated. It is also convenient to deal with multi-objective optimisation problems. The unified viscoplastic-damage constitutive equations developed in the work are able to model material hardening due to the accumulation of dislocation density and grain growth, as well as material softening due to micro-void nucleation and growth at grain boundaries. The equation set can model the deformation of Al–Zn–Mg and Al 7475 at 515 °C for complete life spans and a range of straining rates.

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