Constitutive modelling with a novel two-step optimization for an Al-Zn-Mg-Cu alloy and its application in FEA

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Abstract
The modified Johnson-Cook constitutive model was developed for describing the flow behavior of Al-7.8Zn-1.65Mg-2.0Cu (wt%) alloy based on the flow curves in the temperature range of 300 °C~450 °C and strain rate range of 0.01 s^-1 ~ 10 s^-1 which were obtained by isothermal compression tests conducted on a Gleeble-3500 isothermal simulator. A two-step optimization method was proposed to optimize the prediction precision according to the evaluation of average absolute relative error (AARE). By using a traversal procedure for calculating the model under different reference conditions, this evaluator was found varying in the range of 4.1837% ~ 11.105%, revealing the great influence of reference condition on the precision, then the reference condition optimization (RCO) was conducted. Genetic algorithm (GA) was introduced as the second step of the two-step optimization (TSO) to optimize the material constants of the model, which furtherly improved the precision by reducing the AARE-value to 3.801%. The models before and after optimization were written into subroutines for the software DEFORM and the compression tests were investigated through finite element analysis (FEA). The simulated results (forming load and temperature rise) revealed that the model after TSO has the highest agreement with the experimental.

1. Introduction
Due to the property advantages such as high specific strength-to-weight ratio and good ware resistance, Al-Zn-Mg-Cu series alloys have been widely applied in the industries of automobile, aerospace and shipping [1–3].

Forging is one of the main processing technologies to obtain qualified components in these fields. To better guide the design of forging process, finite element analysis (FEA) was proposed and occupied an important position. It has been a consensus that the deformation property should be investigated to provide more precision materials data for FEA. Among these materials data, constitutive model is one of the most important factors in the FEA process [3, 4]. Constitutive model describes the stress-strain relationship of metals and alloys during hot working [5–8]. The stress-strain relationship was affected by the deformation parameters as well as the composition of alloying elements. As a novel aluminum alloy, the constitutive relationship of Al-7.8Zn-1.65Mg-2.0Cu (wt%) alloy was rarely reported. In order to provide better guidance for the forging process of this alloy, a suitable constitutive model is necessary.

So far, the investigations on constitutive model were divided into phenomenological constitutive model (e.g. Arrhenius model [9], Johnson-Cook model [10] etc), physical constitutive model (e.g. Zerilli-Armstrong model [11], dynamic recrystallization model [12] etc) and artificial neuron network model [13–15]. The most important point being focused on is the prediction precision of the model in describing flow behavior [16]. Among these models, Johnson-Cook model was extensively investigated. Since it was firstly proposed in 1983 [10], researchers had taken enormous effort trying to enhance the prediction precision through modifying the
structure and parameters [17–21]. Among them, the modified Johnson-Cook model proposed by Lin et al [20] was believed to be better in describing the flow behavior of alloys with softening effect. To modelling this model, the reference condition needs to be selected in advance. However, in previous researches [20, 22–24], the selection of reference condition was generally random and without optimization. Hence, to acquire better precision, it is necessary to discuss the effect of reference condition on the prediction precision. Moreover, genetic algorithm (GA) has been proved to be efficient in optimizing the prediction precision of Johnson-Cook model [22]. Therefore, combining the optimization of reference condition and further GA optimization, higher prediction precision of the modified Johnson-Cook model is hopeful.

In this work, the flow curves of homogenized Al-7.8Zn-1.65Mg-2.0Cu (wt%) alloy were obtained by isothermal compression tests. The modified Johnson-Cook model was developed and average absolute relative error (AARE) was introduced to evaluate the prediction precision. The effect of reference condition on prediction precision was analyzed and the precision was optimized through an ergodic process written by MATLAB. GA was then applied to furtherly improve the precision and the optimal material constants set was obtained. Moreover, the models before and after optimization were written into subroutines of DEFORM by FORTRAN. The hot compression tests were simulated and compared with the experimental.

2. Experimental procedures

The homogenized Al-7.8Zn-1.65Mg-2.0Cu (wt%) alloy with an initial microstructure as shown in figure 1 and chemical compositions of (wt%): Fe-0.04, Zn-7.80, Cr-0.02, Mg-1.65, Mn-0.02, Cu-2.00, Zr-0.10, Si-0.03, Ti-0.03, and the balance of Al was machined into cylinders with height of 12 mm and radius of 8 mm. The end faces of the specimens were ground to reduce the effect of friction. Before compression, the graphite flakes were used to furtherly reduce the friction between anvils and end faces, meanwhile, the specimen were heated to 300°C~450°C with an interval of 50°C by 5°C s⁻¹, and hold 180 s after reaching the certain temperature to obtain uniformed temperature distribution. Furthermore, thermocouple was weld on the middle of the specimen to monitor the temperature variation during compression. Hot compression tests were then conducted on a Gleeble-3500 simulator with the strain rates of 0.01 s⁻¹, 0.1 s⁻¹, 1 s⁻¹ and 10 s⁻¹ and the height reduction of 60%. The true stress-strain curves were acquired real-timely during the compression tests by the equipped monitor. After compression, the specimens were water quenched immediately to remain the deformed microstructures. After that, the specimens were cut along the compressive axis across the center and the cut faces were ground by sandpapers and mechanical polished. The microstructures were observed by optical microscopy after etched in the Keller solution (H₂O:HNO₃:HCl:HF = 95 ml:2.5 ml:1.5 ml:1 ml) for 30 s.

3. Results and discussion

3.1. Flow curves

The obtained flow curves were shown in figure 2. The flow stress increases with increasing strain rate and decreasing temperature. Moreover, most of the flow curves increase rapidly at the initial stage resulting from
work-hardening and start to decease after reaching the peak value which corresponds the strain values lower than 0.2, indicating the softening effect predominant. As an exception, the flow curve at 300 °C & 0.1 s\(^{-1}\) keeps increasing with straining and enters a steady state after strain higher than approximately 0.5, indicating the work-hardening predominant. Generally, due to high stack fault energy (SEF), during hot deformation, dynamic recovery (DRV) tends to be the main softening effect of aluminum alloys, which theoretically results in that the flow curves enter steady state after reaching the peak value immediately \[3, 25\]. For this alloy, the alloying elements affect the SEF and lead to different softening results. The initial microstructure also affects the dynamic recrystallization (DRX) behavior. The size of particles of homogenized Al-7.8Zn-1.65Mg-2.0Cu (wt\%) alloy are generally larger than 1 μm which may activate the particle stimulated nucleation (PSN) \[26, 27\] and accelerate recrystallization and promote the softening of flow stress. Besides, at the strain rate of 10 s\(^{-1}\), the zigzag morphology of flow curves reveals that discontinuously yield occurred, and it becomes more violently with increasing temperature. Guo et al\[28\] and Sakai et al\[29\] mentioned that the oscillation may result from the coarsen of grain during discontinuous dynamic recrystallization (DDRX). It should be noted that the precondition for this phenomenon is the occurrence of DDRX \[30\]. Liu et al\[31\] also observed the oscillation of flow stress in the study of 7A85 alloy, they believed that the combined effect of the variation of dislocation migration under different temperatures and high strain rate leads to this phenomenon. At high strain rate with lower temperature, the driving force of dislocation migration is much lower than that at higher temperature, hence the flow stress exhibits continuous increasing with straining before reaching critical stress. With the increasing of temperature, the annihilation and migration rates of dislocation are accelerated, but there is no sufficient time for efficient dislocation migration, the flow stress slightly decreased. The new generated dislocation strengthens the work-hardening and increases the flow stress after the short decreasing. This vigorously competition causes the oscillation under high strain rate after work-hardening stage and the oscillation becomes steady with straining due to the balance out of this competition.

Figure 2. The flow curves of the tested alloy.
3.2. Constitutive modeling and optimization

3.2.1. Modified Johnson-Cook model

Johnson-Cook model was firstly proposed by Johnson and Cook [10], which was originally used to predict the hot flow behavior of alloys under severe plastic deformation. But the original model was not widely used because it ignored the interactive effect of strain rate and temperature during hot deformation, which results in the disability in describing the dynamic softening behavior properly. To make it suitable for the alloys with softening behavior, it has been modified to suit different deformation conditions and materials [20, 23, 32, 33], among the modified models, the following version proposed by Lin et al [20] is one of the most widely accepted [22, 24, 34].

\[
\sigma = (A_0 + A_1 \dot{\varepsilon} + A_2 \dot{\varepsilon}^2 + A_3 \dot{\varepsilon}^3)(1 + C \ln \dot{\varepsilon}^* \exp \left[ \left( m_1 + m_2 \ln \dot{\varepsilon}^* \right)(T - T_{\text{ref}}) \right])
\]

Where \( A_0 \sim A_3 \), \( m_1 \) and \( C \) are material constants, \( \dot{\varepsilon}^* = \dot{\varepsilon} / \dot{\varepsilon}_{\text{ref}} \), \( \dot{\varepsilon} \) is strain rate, \( \dot{\varepsilon}_{\text{ref}} \) is reference strain rate, \( T \) is deformation temperature, \( T_{\text{ref}} \) is reference deformation temperature. It should be noted that the reference conditions are generally chosen randomly. Here, it was chosen to be 300 °C & 0.1 s \(^{-1}\).

At the reference deformation temperature and strain rate, equation (1) could be denoted as its Part1 and the values of \( A_0 \sim A_3 \) are determined to be 87.52, 92.29, -142.72, 68.67 respectively through a third ordered polynomial fitting as shown in figure 3(a). At the reference deformation temperature, equation (1) could be denoted as its Part2 and the value of \( C \) is determined to be 0.0895 through linear fitting as shown in figure 3(b).

Moreover, at the reference strain rate, the values of \( m_1 \) in equation (3) can be calculated as -0.007 at 0.01 s \(^{-1}\) by the linear fitted average slopes of \( T^* \) and \( \sigma / (A_0 + A_1 \dot{\varepsilon} + A_2 \dot{\varepsilon}^2 + A_3 \dot{\varepsilon}^3)(1 + C \ln \dot{\varepsilon}^* \exp \left[ \left( m_1 + m_2 \ln \dot{\varepsilon}^* \right)(T - T_{\text{ref}}) \right]) \) as shown in figure 3(c), and this value at 0.1 s \(^{-1}\), 1 s \(^{-1}\) and 10 s \(^{-1}\) were determined to be -0.0062, -0.0044, -0.0029, respectively. After that, \( m_1 \) and \( m_2 \) were obtained as 0.00583 and 0.00062 by the linear fitted slope of \( \ln \dot{\varepsilon}^* \) and \( m \) as shown in figure 3(d).

Here, all the parameters in equation (1) at the reference condition of 300 °C & 0.1 s \(^{-1}\) were obtained and the flow stress is predicted as shown in figure 4. It can be seen that, the predicted results under all the conditions have the similar morphology to that of 300 °C & 0.1 s \(^{-1}\), namely the reference condition. Meanwhile, the prediction...
Figure 4. The comparison between measured flow stress and prediction by modified Johnson-Cook model at the reference condition of 300 °C & 0.1 s⁻¹.

Figure 5. The execution path of the optimization program.
at the reference condition is the most precise, which shows apparently work-hardening with straining. But, at the strain rate of 0.01 s\(^{-1}\) where softening effect is distinct, the prediction cannot properly describe the morphology. Furthermore, to exactly reveal the prediction precision, relative coefficient (R) and absolute average relative error (AARE) were introduced, which are expressed as shown in equations (2) and (3). It is known that, R-value closer to 1 and AARE-value closer to 0 indicate higher similarity between the objects being compared [7].

\[
R = \frac{\sum_{i=1}^{N} (E_i - \bar{E})(P_i - \bar{P})}{\sqrt{\sum_{i=1}^{N} (E_i - \bar{E})^2 \cdot \sum_{i=1}^{N} (P_i - \bar{P})^2}}
\]

\[
AARE(\%) = \frac{1}{N} \sum_{i=1}^{N} \left| \frac{P_i - E_i}{E_i} \right| \times 100\%
\]

Where \(E_i\) is tested value, \(\bar{E}\) is the average tested value, \(P_i\) is the predicted value, \(\bar{P}\) is the average predicted value, \(N\) is the number of tested values. At the reference condition of 300 °C & 0.1 s\(^{-1}\), the R-value and AARE-value are 0.9882% and 6.802%, respectively.
3.2.2. Reference condition optimization (first step of optimization)
As discussed in section 3.2.1, the prediction of flow stress is similar in the morphology to the flow curve of reference condition. Hence, the choice of reference condition can affect the prediction and its precision. However, it is quite time-consuming to successively calculate the parameters in the modified Johnson-Cook model with different reference conditions by the method in section 3.2.1 manually. Thus, a program which can automatically calculate the parameters and optimize the reference condition based on AARE-value was written using MATLAB according to the execution path as shown in figure 5.

In the optimization program, the selection, calculation, prediction and evaluation processes were executed 16 times for this alloy to traverse all the reference conditions. The AARE-values under all the reference conditions were determined as shown in table 1. It can be seen that the AARE-values vary from 4.1837% to 11.105%, and the variation is irregular with the strain rate and temperature. The optimal reference condition is at $350 \, ^{\circ}C \& 0.1 \, s^{-1}$, and the corresponding values of $A_0 \sim A_3$, $m_1$, $m_2$ and $C$ are $72.32$, $11.69$, $-6.60$, $-5.05$, $0.12$, $-0.0058$, $0.00062$, respectively. The comparison between measured flow stress and the predicted flow stress using the optimal reference conditions are shown in figure 6. It is obvious that the optimized prediction can much better describe the measure flow stress compare with the prediction in figure 4.

3.2.3. Optimization by genetic algorithm (second step of optimization)
After reference condition optimization, the optimized material constants were obtained. To furtherly optimize the precision, genetic algorithm (GA) which was an effective solution in parameter optimization was introduced [22, 35, 36]. Figure 7 shows the implementation of the GA in the optimization of material constants. The experimental flow stress was imported firstly and the initial material constants set as an initial generation was randomly generated based on the optimization of reference condition. Meanwhile, the flow stress was predicted and its precision was evaluated. The GA optimization consisting of selection, mutation and crossover were executed and new materials constants set was generated as the next generation and the new prediction executed. This process loop executed until the generations $= 1000$ and the optimized material constants set was obtained. After that, the prediction based on optimized material constants set was evaluated by equation (3) and the AARE-value is $3.801\%$.

The comparison between measured flow stress and the predicted flow stress after the two-step optimization (TSO) is shown in figure 8. Comparing with the prediction in figure 6, the prediction precision at $300 \, ^{\circ}C$, $350 \, ^{\circ}C$, $400 \, ^{\circ}C$ with $0.1 \, s^{-1}$ were pronouncedly enhanced. The comparison of the material constants sets with no optimization (NO), reference condition optimization (RCO) and TSO are listed in table 2. It can be seen that, after the two-step optimization, the AARE-value decreased from $6.802\%$ to $3.801\%$, revealing the efficient optimization effect.
Table 2. The comparison of the material constants sets under different optimization conditions.

| Optimization type | AARE-value | Material constants |
|-------------------|------------|--------------------|
|                   | A₀ | A₁    | A₂    | A₃ | m₁ | m₂ | C    |
| NO                | 6.802% | 87.52 | 92.29 | −142.72 | 68.67 | 0.0058 | 0.00062 | 0.0895 |
| RCO               | 4.184% | 72.32 | 11.69 | −6.60 | −5.05 | 0.12 | −0.0058 | 0.00062 |
| TSO               | 3.801% | 73.32 | 9.73 | −6.74 | −4.04 | 0.13 | −0.0059 | 0.00068 |

Figure 8. The comparison between measured flow stress and the predicted flow stress after the two-step optimization.

Figure 9. The comparisons of (a) forming loads and (b) temperatures between measured and simulated based on NO, RCO and TSO models.

Table 2. The comparison of the material constants sets under different optimization conditions.
3.3. Application of the constitutive models

The constructed constitutive models before and after optimization were written into procedures by FORTRAN language according to the subroutine generation rules of the commercial software DEFORM. Based on that, the compression test at 350 °C & 10 s−1 were simulated and the simulation parameters were listed in table 3. It should be noted that, because the strain rate is relatively high and the forming time is too short, the forming speed of top die could be considered to be linear with time, thus it can be calculated from the following equation.

\[
v_f = \frac{(h_t - h_e)}{\varepsilon_e / \dot{\varepsilon}}
\]

Where \(h_t\) and \(h_e\) are the height of the specimen before and after compression respectively, namely 12 mm and 4.8 mm, \(\varepsilon_e\) is the true strain after compression, \(\approx 0.91\), \(\dot{\varepsilon}\) is strain rate, namely 10 s−1.

Figure 9(a) shows the comparison of forming loads between measured and simulated based on NO, RCO and TSO models. It can be seen that, the forming load of NO model is much higher than measured, RCO and TSO, revealing this model has more error than the rests in predicting the forming load. The forming load curve by TSO model can better describe the measured forming load than RCO model. Hence, the TSO model has been proved to be better in the application of simulation. Moreover, the comparison of temperature between measured and simulated based on NO, RCO and TSO models is shown in figure 9(b). The curves are the temperature variation of the shown tracked point, where the thermocouple weld in the hot compression test. The temperature distributions of NO, RCO and TSO at 0.038 s, 0.057 s, 0.076 s and 0.091 s are giving. The center temperatures are higher than surface due to larger plastic deformation. Meanwhile, its value predicted by RCO model is the lowest but highest by NO model. It is worthy mention that, the temperature rising during hot compression induced by deformation heat is affected by deformation resistance \([37, 38]\), namely flow stress. Hence, more accurate in describing flow behavior can better predict the temperature rising during deformation.

Table 3. The simulation parameters.

| Objects      | Number of elements | Temperature | Friction coefficient | Heat transfer coefficient | Forming speed |
|--------------|--------------------|-------------|----------------------|---------------------------|---------------|
| Workpiece    | 15000              | 350 °C      | 0.4                  | 5 N s−3 mm−1             | /             |
| Top die      | /                  | 350 °C      | 0.4                  | 79.1 mm s−1              | /             |
| Bottom die   | /                  | 350 °C      | /                    | /                         | /             |

Figure 10. The simulation results and OM microstructures at 400 °C.
Here, due to higher agreement with the measured, the TSO model has been furtherly proved to be better in the application of simulation.

Furthermore, the compression tests at the temperature of 400 °C were simulated based on TSO model with a forming speed of 0.0791 mm s\(^{-1}\), 0.791 mm s\(^{-1}\), 7.91 mm s\(^{-1}\) and 79.1 mm s\(^{-1}\) which correspond to the average strain rate of 0.01 s\(^{-1}\), 0.1 s\(^{-1}\), 1 s\(^{-1}\) and 10 s\(^{-1}\) according to equation (4). It can be seen that in figure 10, the temperature and effective strain increase with the increasing strain rate (forming speed). Due to higher forming speed, the temperature rise induced by deformation heat at the track point increases and the rising temperature reduces the deformation resistance at local area, which make this area forming easier and cause larger local strain. Hence, the OM observed areas are not corresponding to the true strain of 0.91 which was widely believed \([31, 39, 40]\), but 1.43, 1.51, 1.55 and 1.62 at the strain rate of 0.01 s\(^{-1}\), 0.1 s\(^{-1}\), 1 s\(^{-1}\) and 10 s\(^{-1}\), respectively.

4. Conclusions

This work proposed a novel two-step optimization method to enhance the prediction precision of modified Johnson–Cook model in the study of hot deformation behavior of homogenized Al-7.8Zn-1.65Mg-2.0Cu (wt%) alloy. Meanwhile, it was applied in the finite element simulation. The following conclusions could be obtained:

1. The reference condition affects the prediction precision of modified Johnson–Cook model significantly. It is of great importance to search for the optimal reference condition for this model.

2. The genetic algorithm optimization as the second optimization step furtherly reduces the AARE-value from 4.184% to 3.801% of modified Johnson–Cook model in describing the hot deformation behavior of the homogenized Al-7.8Zn-1.65Mg-2.0Cu (wt%) alloy.

3. The two-step optimized (TSO) model can better predict the forming load and temperature rise during hot compression when applied in the finite element simulation. Based on the simulation, the actual temperature and true strain at the area where OM observed increase with increasing strain rate, which is not as the widely believed.

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Data availability statement

No new data were created or analysed in this study.

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