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Modeling constitutive relationship of 6013 aluminum alloy during hot plane strain compression based on Kriging method

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Abstract: Hot plane strain compression tests of 6013 aluminum alloy were conducted within the temperature range of 613−773 K and the strain rate range of 0.001−10 s^{-1}. Based on the corrected experimental data with temperature compensation, Kriging method is selected to model the constitutive relationship among flow stress, temperature, strain rate and strain. The predictability and reliability of the constructed Kriging model are evaluated by statistical measures, comparative analysis and leave-one-out cross-validation (LOO-CV). The accuracy of Kriging model is validated by the *R*-value of 0.999 and the AARE of 0.478%. Meanwhile, its superiority has been demonstrated while comparing with the improved Arrhenius-type model. Furthermore, the generalization capability of Kriging model is identified by LOO-CV with 25 times of testing. It is indicated that Kriging method is competent to develop accurate model for describing the hot deformation behavior and predicting the flow stress even beyond the experimental conditions in hot compression tests.

Key words: aluminum alloy; hot deformation; constitutive model; Kriging method

1 Introduction

Al−Mg−Si alloys have been extensively studied because of their superior yield strength and ultimate tensile strength obtained by precipitation hardening. 6013 Al alloy developed by Alcoa is one potential substitute for the 2024 alloy [1]. It has been widely used in aircraft structures and transportation industry because of the high specific mechanical properties [1,2]. In practical manufacturing process, hot forming has been extensively performed on alloys, such as converting a cast ingot into a wrought product [3]. Constitutive relationship is a mathematical representation for describing the dependence of flow stress on the coupled influences of temperature, strain rate and strain. Modeling the constitutive relationship of a given alloy is significant for designing the hot deformation process and optimizing the microstructure and mechanical properties of its final products [4]. Numerous efforts have been devoted to finding out the effective way to build the accurate constitutive model [4−7]. Several classifications of constitutive models, such as physical-based, phenomenological and empirical model, have been proposed to date. However, the applications of these constitutive models are limited by their own drawbacks. For the physical-based models, a large number of material constants are difficult to obtain, which inevitably impose serious constraints on their practical applications [5]. The phenomenological and the empirical constitutive models are unreliable to predict the flow stress beyond experimental conditions, as the modeling process is merely on the basis of specific deformation mechanisms [8,9]. Moreover, the development of modeling material flow behavior in the conventional way is usually time consuming and relies on amounts of experimental data. Therefore, the research work for searching the new modeling methods has obtained great attention.

The deformation behaviors of alloys at elevated temperature are always associated with various metallurgical phenomena and thereby complicated in

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nature. That is, modeling the constitutive relationship is substantially solving highly complex non-linear engineering problems. In the previous work, artificial neural network (ANN) was widely employed as a novel approach to deal with this type of non-linear problems [8−11]. ANN is actually one type of metamodeling method which is a valuable tool to support a wide scope of activities in the modeling process for engineering design [12]. Besides ANN, some other types of metamodeling method were maturely developed in the past, such as Kriging method, multivariate polynomial method and radial basis function method [13]. Among them, Kriging method is the most popular approach to model the low-dimensional non-linear problems for its high accuracy and efficiency [12]. Comparing with other methods like ANN, the important advantage of Kriging method in application is the lower demand in the amount of modeling data [14]. Therefore, the new application of Kriging method may be a significant attempt in effectively modeling the hot deformation behavior of alloys.

The objective of the present work is to investigate the applicability and effectiveness of Kriging method in modeling the constitutive relationship of 6013 aluminum alloy during hot deformation. The hot plane compression tests for simulating hot rolling process, were carried out on Gleeble−3500 thermo mechanical simulator to obtain the flow stress data. Considering deformation heating integrated with heat transfer, the experimental flow stress data are corrected at relatively high strain rates. Based on the experimental and corrected data, Kriging method is utilized to model the flow behavior, and the performance of the developed Kriging model is evaluated by statistical measures, comparative analysis and leave-one-out cross-validation (LOO-CV).

2 Experimental

2.1 Materials and experimental procedure

The chemical composition of the commercial 6013 aluminum alloy in this work was as follows: 0.95 Mg, 0.75 Si, 0.9 Cu, 0.35 Mn (mass fraction, %) and Al balance. The cast ingot was processed by homogenizing at 813 K for 15 h and then water quenched. The specimens with dimensions of 20 mm × 15 mm × 10 mm were machined from the cast ingot for test. The hot plane strain compression tests were carried out using Gleeble−3500 thermo mechanical simulator at five different temperatures (613, 653, 693, 733 and 773 K) and five different strain rates (0.001, 0.01, 0.1, 1, and 10 s^{-1}). The specimens were heated to the deformation temperature at a rate of 10 K/s and held for 120 s to eliminate thermal gradient before compression, and the experimental procedure is shown in Fig. 1. All the specimens were compressed to a true strain of 0.8. In order to minimize the frictions between specimens and press indenters, the ends of specimens were covered by graphite lubricant.

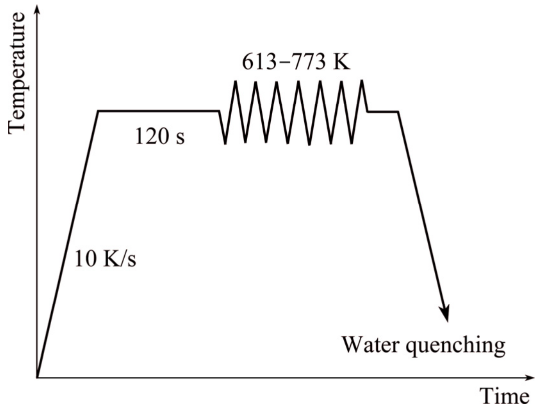

Fig. 1 Experimental procedure for hot plane strain compression tests

3 Results

The true stress−true strain curves obtained from tests are shown in Fig. 2. The flow stress is greatly influenced by temperature and strain rate. The yield stress increases with the decrease of temperature and the increase of strain rate. During the deformation process, the work hardening and the flow softening occur simultaneously. At first, the flow stress rapidly increases due to work hardening. After reaching the peak stress, the flow stress gradually decreases into a steady-state stress level, showing the characteristic of flow softening.

Up to now, it has been accepted that the experimental data measured directly from the tests are always affected by the temperature rise induced by deformation heating [6,15,16]. The temperature rise of specimen undoubtedly leads to the experimental flow stress being lower than the actual one. Moreover, the heat transfer, which occurs among the deformed region, the undeformed region and the press indenter during hot plane strain compression, would significantly affect the temperature rise. In order to compensate the effect of the temperature rise, the experimental flow stress needs to be corrected based on the coupled influences of deformation heating and heat transfer. Considering these coupled influences, the temperature rise ΔT (K) of the deformed region of specimen can be calculated according to the law of energy conservation [16]:

$$\Delta T=\frac{\eta_0 V_{\text{def}}\int_0^{\varepsilon}\sigma \mathrm{d}\varepsilon}{2\eta_1 S_1 ht+2\eta_2\dfrac{S_2\lambda t}{d}+\rho C V_{\text{def}}} \tag{1}$$

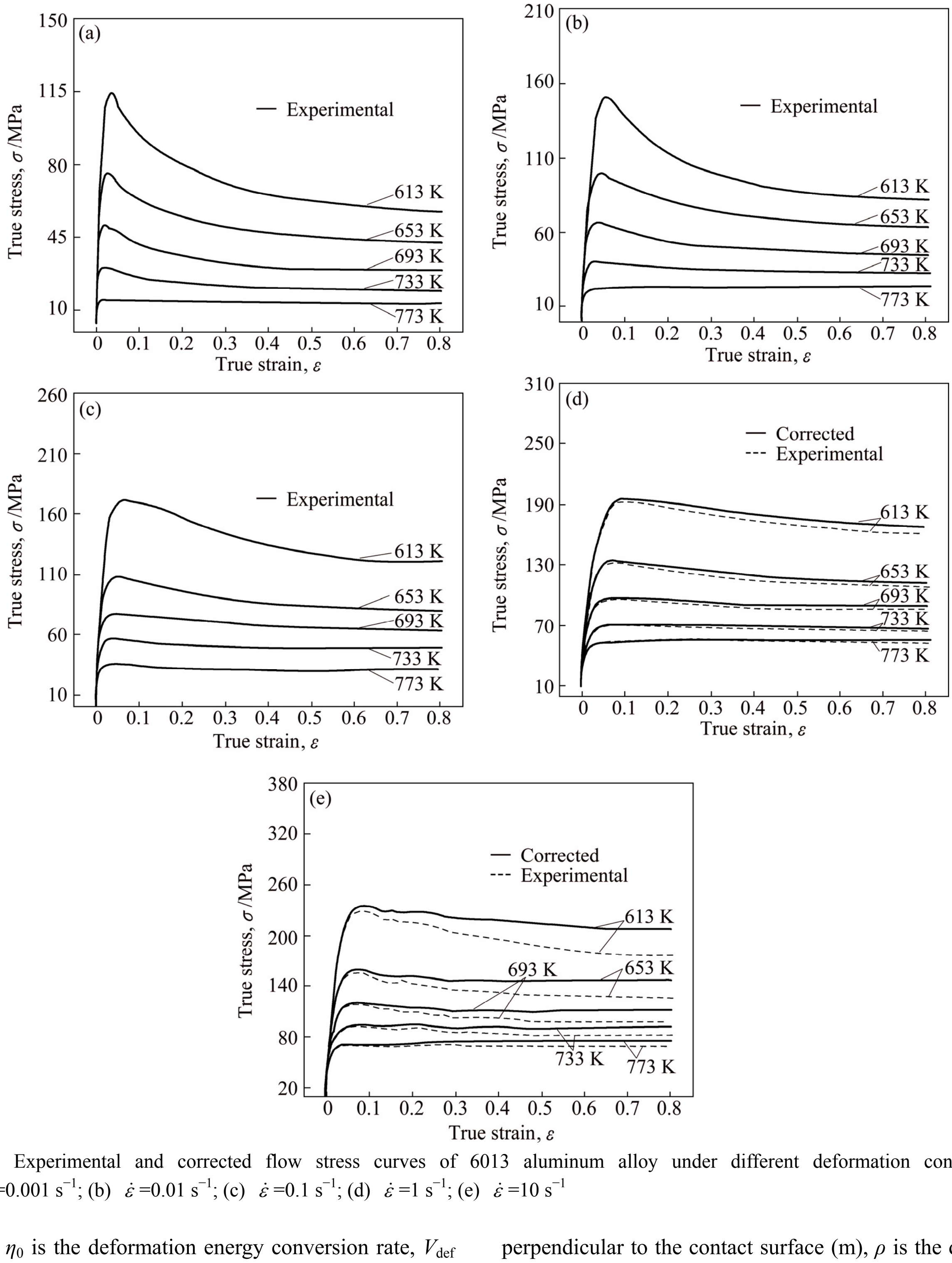

Fig. 2 Experimental and corrected flow stress curves of 6013 aluminum alloy under different deformation conditions: (a) $\dot{\varepsilon}=0.001\ s^{-1}$; (b) $\dot{\varepsilon}=0.01\ s^{-1}$; (c) $\dot{\varepsilon}=0.1\ s^{-1}$; (d) $\dot{\varepsilon}=1\ s^{-1}$; (e) $\dot{\varepsilon}=10\ s^{-1}$

where η_0 is the deformation energy conversion rate, V_{def} is the volume of the deformed region (m^3), ε is the true strain, σ is the true stress (MPa), η_1 and η_2 are the correction factors of heat transfer, S_1 is the contact area between the deformed region and the press indenter (m^2), S_2 is the contact area between the deformed and the undeformed region of the specimen (m^2), h is the contact heat exchange coefficient between the specimen and the press indenter ($W\cdot m^{-2}\cdot K^{-1}$), λ is the thermal conductivity of the alloy ($W\cdot m^{-1}\cdot K^{-1}$), t is the time of the heat transfer process (s), d is the specimen thickness in the direction perpendicular to the contact surface (m), ρ is the density of alloy ($kg\cdot m^{-3}$), and C is the specific heat capacity ($J\cdot kg^{-1}\cdot K^{-1}$).

The stress decrease $\Delta\sigma$ (MPa) due to the temperature rise is usually calculated by [15,16]

$$\Delta\sigma=\frac{Q}{n\alpha R}\left(\frac{1}{T}-\frac{1}{T+\Delta T}\right) \tag{2}$$

where Q is the activation energy for hot deformation ($kJ\cdot mol^{-1}$), n and α are the material parameters, R is the mole gas constant ($J\cdot mol^{-1}\cdot K^{-1}$), T is the preset temperature (K).

Based on Eqs. (1) and (2), the experimental flow stress data at 1 s^{-1} and 10 s^{-1} can be corrected, and the results are shown in Fig. 2. It can be seen that the corrected flow stress is higher than the experimental one. This also indicates that the temperature rise has a more significant effect on experimental flow stress at higher strain rates. The effect at relatively low strain rates ($\dot{\varepsilon} \le$ 0.1 s^{-1}) is not considered in this work.

4 Application and assessment of Kriging method in constitutive modeling

4.1 Modeling foundation and preparation

The Kriging method, which was originated from the geostatistics community [17], was proposed by SACKS et al [18] for modeling sampled data from any fields that satisfy the appropriate mathematical assumptions. In Kriging method, the random output is assumed to be obtained from a linear combination of regression functions plus a random process factor as follows:

$$Y = \sum_{j=1}^{m} b_j f_j(\boldsymbol{x}) + Z(\boldsymbol{x}) \tag{3}$$

where m is the number of regression functions, $f_j(\cdot)$ is a regression function, b_j is the coefficient for $f_j(\cdot)$, $\boldsymbol{x}$ is the design point, and $Z(\cdot)$ is the random process function. It is assumed in Kriging method that the random factor is from a random process, and a correlation function defined by the following equation:

$$\mathrm{Cov}(Z(\boldsymbol{x}_1), Z(\boldsymbol{x}_2)) = r(\theta, \boldsymbol{x}_1, \boldsymbol{x}_2) \tag{4}$$

where $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$ are design points, and θ is a structural parameter to be optimized. The correlation function could be expressed in several different ways such as exponential, Gaussian and spherical [19].

The best linear unbiased predictor is used here, which satisfies the following three requirements [20]: 1) it is a linear combination of the training data outputs:

$$\hat{g}(\boldsymbol{x}) = \sum_{i=1}^{M} c_i(\boldsymbol{x}) y_i \tag{5}$$

where $\hat{g}$ is the estimated output value, M is the number of design points in the training data, y_i is an output in the training data, and c_i is the coefficient for y_i; 2) it is unbiased in prediction; and 3) it has the least prediction variance.

The schematic of Kriging method for modeling the hot deformation behavior of 6013 aluminum alloy is shown in Fig. 3. The inputs of the model are log temperature (lg T), log strain rate (lg $\dot{\varepsilon}$) and strain (ε) whereas flow stress (σ) is the output.

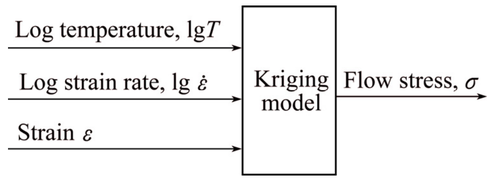

Fig. 3 Schematic of Kriging method for modeling hot deformation behavior

A total of 300 points have been selected from the 25 experimental (or corrected) flow stress curves for model training and testing, as shown in Table 1. Among them, the data at true strain between 0.1 and 0.8 with the interval of 0.1 are used for model training, while the left data at true strain between 0.15 and 0.75 with the interval of 0.2 are selected for testing.

In order to provide a statistical view regarding the predictability of developed models, the correlation coefficient (R) and average absolute relative error (AARE) are employed. The correlation coefficient R can provide information on the strength of linear relationship between the experimental and the predicted values. However, a high R-value does not always indicate the satisfactory performance as the tendency of the model to be biased often leads to high or low values [9]. Therefore, the AARE has also been used in this work as an unbiased statistical measure to evaluate the predictability.

$$R = \frac{\sum_{i=1}^{N}(E_i - \overline{E})(P_i - \overline{P})}{\sqrt{\sum_{i=1}^{N}(E_i - \overline{E})^2 \sum_{i=1}^{N}(P_i - \overline{P})^2}} \tag{6}$$

Table 1 Experimental data for model training and testing

Data	Number of points	Model inputs	Level	Condition
Training	200	Temperature/K	5	613, 653, 693, 733, 773
		Strain rate/s^{-1}	5	0.001, 0.01, 0.1, 1, 10
		Strain	8	0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8
Testing	100	Temperature/K	5	613, 653, 693, 733, 773
		Strain rate/s^{-1}	5	0.001, 0.01, 0.1, 1, 10
		Strain	4	0.15, 0.35, 0.55, 0.75

$$\mathrm{AARE} = \frac{1}{N}\sum_{i=1}^{N}\left|\frac{E_i - P_i}{E_i}\right| \times 100\% \quad (7)$$

In Eqs. (6) and (7), N is the number of testing samples, E is the experimental value, P is the predicted value, and $\overline{E}$ and $\overline{P}$ are the mean values of E_i and P_i, respectively.

4.2 Predictability assessment

The predictability of the model which is developed from the newly applied Kriging method, cannot be sufficiently reflected just by statistical measures (i.e., R and AARE). In fact, the comparative analysis is usually employed to identify the effectiveness of one specific method. Among the classical constitutive models, Arrhenius-type model has been widely recognized and frequently applied for describing the hot deformation behaviors of different materials [21]. Compensating the material parameters with functions of strain, the improved Arrhenius-type model is more complete and excellent than the original one [22,23]. For this reason, the improved Arrhenius-type model is selected in this section as a standard for reference to assess the predictability of Kriging model based on the same training and testing data.

4.2.1 Improved Arrhenius-type model

In Arrhenius-type model, the relationship among the flow stress, temperature and strain rate during hot deformation at a given strain can be expressed as [23]

$$\dot{\varepsilon} = Af(\sigma)\exp(\frac{-Q}{RT}) \quad (8)$$

where $\dot{\varepsilon}$ is the strain rate (s^{-1}), A is a material parameter, the function of stress $f(\sigma)$ is defined by the following three forms:

$$f(\sigma) = \sigma^n \quad (\alpha\sigma < 0.8) \quad (9)$$

$$f(\sigma) = \exp(\beta\sigma) \quad (\alpha\sigma > 0.8) \quad (10)$$

$$f(\sigma) = [\sinh(\alpha\sigma)]^n \quad (\text{for all } \sigma) \quad (11)$$

In Eqs. (9)−(11), β is material parameter, and $\alpha=\beta/n$. Substituting Eq. (11) into Eq. (8), then

$$\dot{\varepsilon} = A[\sinh(\alpha\sigma)]^n \exp(\frac{-Q}{RT}) \quad (12)$$

Introducing the Zener−Hollomon (Z) parameter, Eq. (12) can be changed as

$$Z = \dot{\varepsilon}\exp(\frac{Q}{RT}) = A[\sinh(\alpha\sigma)]^n \quad (13)$$

In the previous research, the original Arrhenius-type model used to be improved by compensating the material parameters with functions of strain [22,23]. The values of α, n, Q and A can be calculated based on the training data from Table 1. The results show that α is lying in the range from 0.0142 to 0.0146. Thus, it can be determined as 0.0145 here by averaging the eight values of α at different strains. Meanwhile, the fitted curves of $n(\varepsilon)$, $Q(\varepsilon)$ and $A(\varepsilon)$ using exponential functions are shown in Fig. 4.

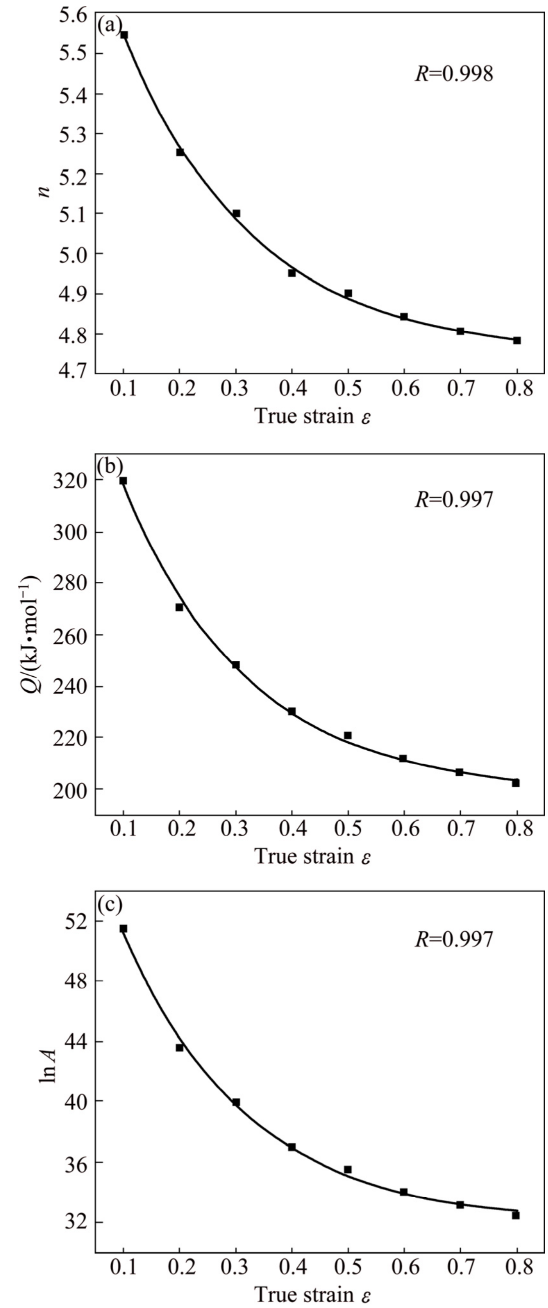

Fig. 4 Relationships among n (a), Q (b), A (c) and ε of 6013 aluminum alloy

According to the preceding results, the improved Arrhenius-type model of 6013 aluminum alloy can be expressed as follows:

$$Z = \dot{\varepsilon}\exp(\frac{Q(\varepsilon)}{RT}) = A(\varepsilon)[\sinh(0.0145\sigma)]^{n(\varepsilon)} \quad (14)$$

where $Q(\varepsilon)$, $A(\varepsilon)$ and $n(\varepsilon)$ are represented as

$$Q(\varepsilon)=198.683+186.954\exp\left(\frac{-\varepsilon}{0.222}\right) \quad (15)$$

$$\ln A(\varepsilon)=31.871+30.340\exp\left(\frac{-\varepsilon}{0.222}\right) \quad (16)$$

$$n(\varepsilon)=4.747+1.223\exp\left(\frac{-\varepsilon}{0.233}\right) \quad (17)$$

4.2.2 Comparative analysis of predictability

The prediction results from the Kriging model and the improved Arrhenius-type model are obtained based on the testing data given in Table 1. As shown in Fig. 5, the R-value is 0.999 from the Kriging model, which is higher than 0.989 from the improved Arrhenius-type model. Meanwhile, compared with the AARE of 5.529% from the improved Arrhenius-type model, the prediction accuracy of the Kriging model is again validated by the much smaller AARE of 0.478%.

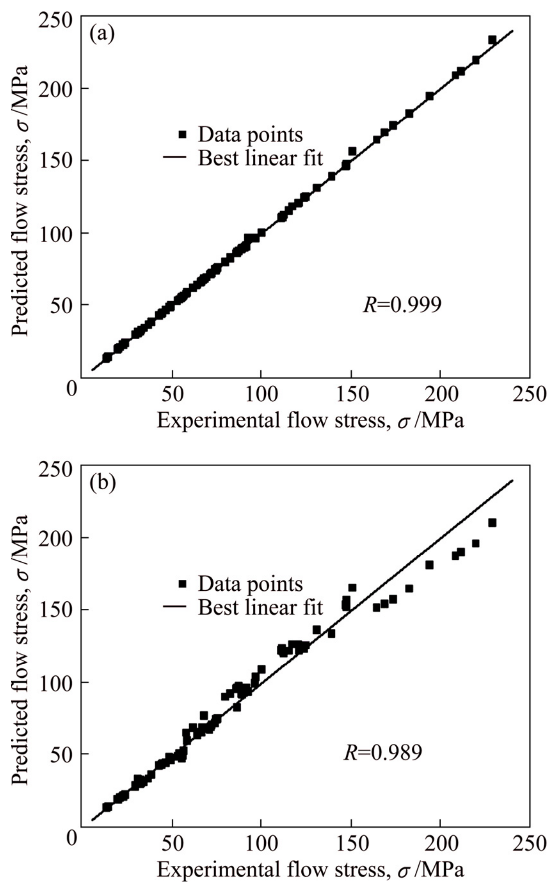

Fig. 5 Correlation between experimental (corrected) and predicted flow stress values: (a) Kriging; (b) Arrhenius-type

In Fig. 6, the comparisons of the prediction accuracy between the Kriging model and the improved Arrhenius-type model are displayed in details. As shown in this figure, the prediction deviations from the Kriging model are smaller than the ones from the improved Arrhenius-type model. According to the results of the statistical analysis and the comparative study, the excellent performance of Kriging model has been demonstrated. It is indicated that Kriging method is competent in modeling the constitutive relationship of 6013 aluminum alloy during hot deformation.

Like most of the conventional constitutive models, the improved Arrhenius-type model cannot provide the complete physical interpretation in wide scopes of temperature, strain rate and strain, where various physical mechanisms of deformation occur [3,8,9]. It is difficult for this constitutive model to exactly track the experimental data during the hot compression. Fortunately, Kriging method can deal with the problem mentioned above very well, as it is not subjected to the constraints from describing physical mechanisms. Moreover, it is not necessary to determine a number of material parameters for developing Kriging model, which contributes to simple steps and short time required for model construction. Comparing with the conventional constitutive modeling method, there are reasons to believe that the newly applied Kriging method provides a more effective approach for solving the problems associated with hot deformation process.

4.3 Generalization capability assessment

Although the predictability of the developed Kriging model has been verified in Section 4.2, the applicability and superiority of Kriging method in modeling hot deformation behavior are still not completely demonstrated. Therefore, further evaluation is required and the implementation process is provided in this section.

Generalization capability is usually considered as one of the crucial properties related to the applicability and reliability of modeling methods [24], and it is mainly reflected in the prediction capability outside the model training conditions. Leave-one-out cross-validation (LOO-CV) which is a special case of the cross-validation technique [25], is a meaningful method to evaluate the generalization capability [24]. In this work, LOO-CV is selected and the assessing process is explained as follows.

Given N samples available in a data set, the model from Kriging method is trained with $N-1$ samples and then is tested on the sample that was left out. This process ends when every sample in the data set has been used once as a cross-validation instance. Finally, the R-value and the mean AARE from all the N tests are taken as the criteria for evaluating the generalization capability of modeling method.

In this work, N equals the number of data groups 25 (8 points per group from the training data in Table 1). Based on the 25 times of testing, the correlation between the experimental flow stress and the predicted values from Kriging models is shown in Fig. 7. With the

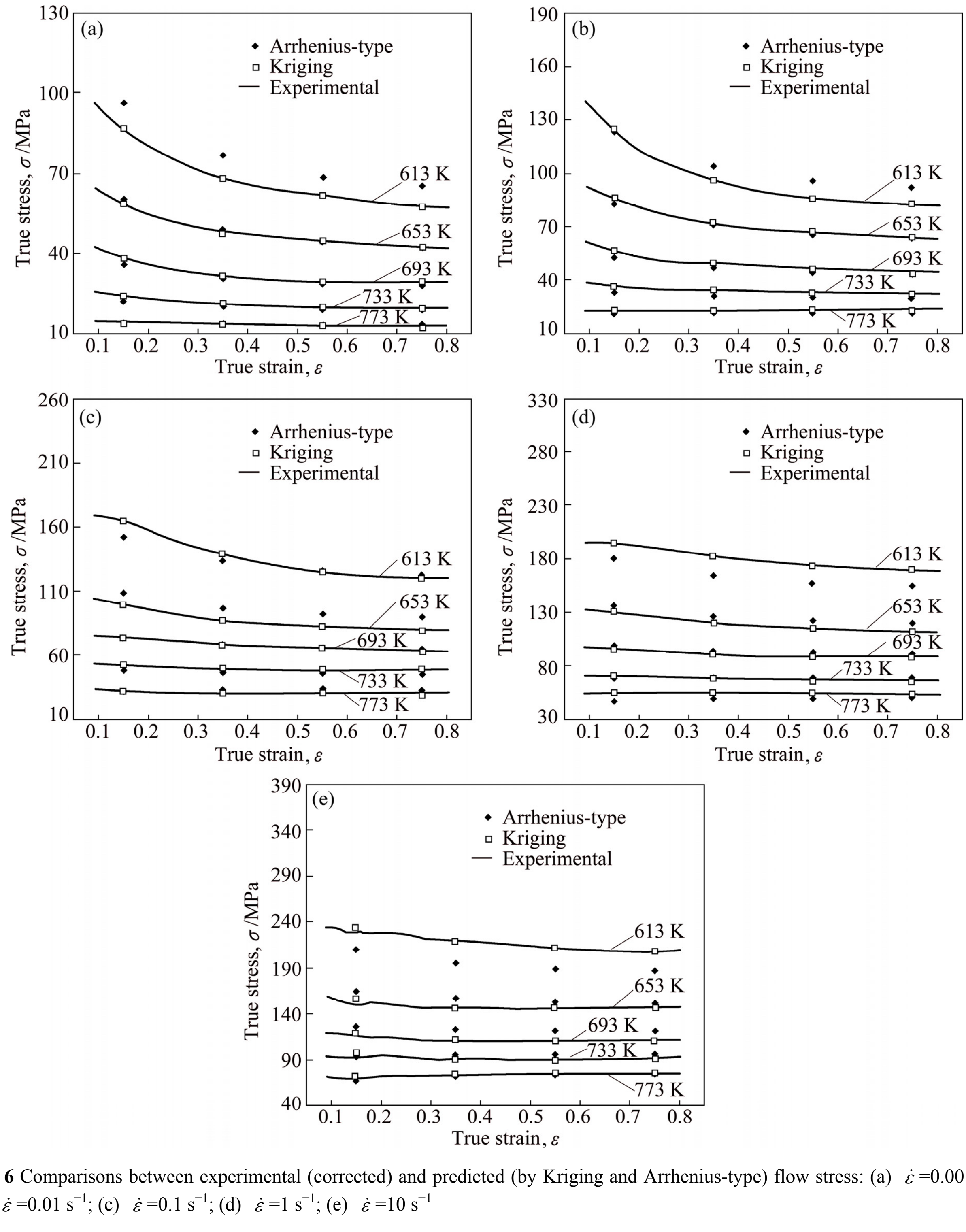

Fig. 6 Comparisons between experimental (corrected) and predicted (by Kriging and Arrhenius-type) flow stress: (a) $\dot{\varepsilon}$=0.001 s^{-1}; (b) $\dot{\varepsilon}$=0.01 s^{-1}; (c) $\dot{\varepsilon}$=0.1 s^{-1}; (d) $\dot{\varepsilon}$=1 s^{-1}; (e) $\dot{\varepsilon}$=10 s^{-1}

R-value 0.996 and the mean AARE 5.093%, the generalization capability of Kriging model is thus validated. It is also illustrated in the comparison figure on the basis of five representative conditions, as shown in Fig. 8. In a word, the potentiality of Kriging model has been revealed in predicting the flow stress of 6013 aluminum alloy beyond the experimental conditions in the hot compression tests.

5 Conclusions

1) The predictability of the constructed Kriging model is validated by the high *R*-value of 0.999 and the small AARE of 0.478%. Since this value of AARE is one order of magnitude less than 5.529% from the improved Arrhenius-type model, the superiority of Kriging model

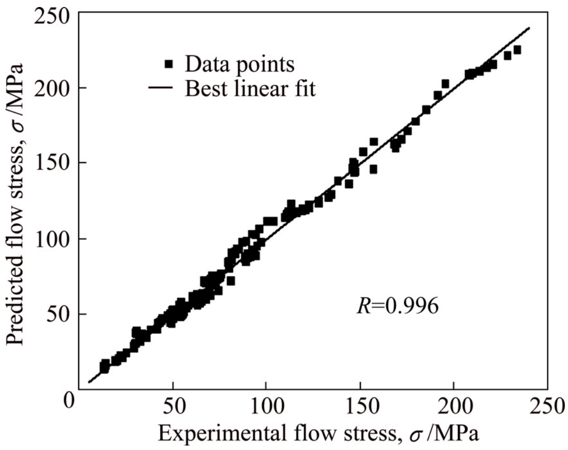

Fig. 7 Correlation between experimental (corrected) flow stress and predicted values from LOO-CV

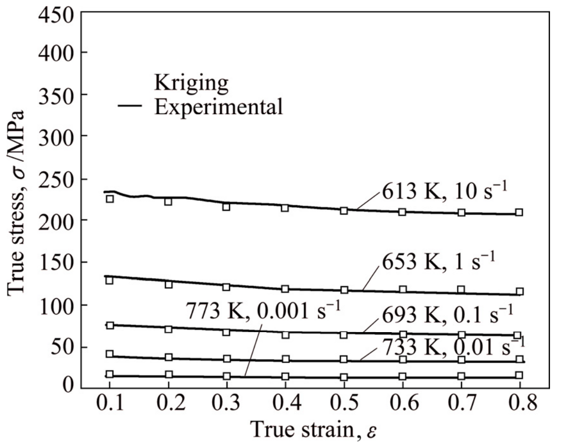

Fig. 8 Comparison between experimental (corrected) flow stress curves and predicted values from LOO-CV

is demonstrated in the comparative analysis. The competence of Kriging method is basically proved in developing model to describe the hot deformation behavior of 6013 aluminum alloy.

2) According to the model evaluation technique leave-one-out cross-validation, the generalization capability of Kriging model is finally identified by the R-value of 0.996 and the mean AARE of 5.093% from 25 times of testing. With the satisfactory performance of the models in prediction even beyond the experimental conditions, the applicability of Kriging method in modeling the hot deformation behavior of 6013 aluminum alloy is completely validated.

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基于 Kriging 方法的 6013 铝合金平面热压缩变形本构关系建模

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摘　要：采用 Gleeble−3500 热模拟机测试了 6013 铝合金在 613~773 K、0.001~10 s^{-1} 下的平面应变流变力学行为，并基于变形温升修正了试验测量的流变应力数据。选取 Kriging 方法对该热变形过程本构关系进行建模，并通过统计学分析、对比分析和舍一交叉验证法对所建模型的预测能力与可靠性进行评价。结果表明：构建的 Kriging 模型预测精度较高，其预测值与实验值对比得到的 R 值为 0.999、AARE 值为 0.478%，相较于修正的 Arrhenius-type 模型具有显著优势。通过基于舍一交叉验证法设计的 25 次测试与验证，充分说明了 Kriging 模型具有较好的泛化能力。由此可知，通过 Kriging 方法可高效构建精确模型以描述合金热变形流变行为并有效预测试验条件范围以外的流变应力。

关键词：铝合金；热变形；本构模型；Kriging 方法

(Edited by Yun-bin HE)