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ScienceDirect
Trans. Nonferrous Met. Soc. China 31(2021) 2978−2985
Transactions of Nonferrous Metals Society of China
www.tnmsc.cn

Development of viscosity model for aluminum alloys using BP neural network

Heng-cheng LIAO[1], Yuan GAO[1], Qi-gui WANG[2], Dan WILSON[2]

1. Jiangsu Key Laboratory for Advanced Metallic Materials,
School of Materials Science and Engineering, Southeast University, Nanjing 211189, China;
2. Materials Technology, GM Global Product Group, 30003 Fisher Brothers Road, Warren, MI 48093, USA

Received 1 November 2020; accepted 18 April 2021

Abstract: Viscosity is one of the important thermophysical properties of liquid aluminum alloys, which influences the characteristics of mold filling and solidification and thus the quality of castings. In this study, 315 sets of experimental viscosity data collected from the literatures were used to develop the viscosity prediction model. Back-propagation (BP) neural network method was adopted, with the melt temperature and mass contents of Al, Si, Fe, Cu, Mn, Mg and Zn solutes as the model input, and the viscosity value as the model output. To improve the model accuracy, the influence of different training algorithms and the number of hidden neurons was studied. The initial weight and bias values were also optimized using genetic algorithm, which considerably improve the model accuracy. The average relative error between the predicted and experimental data is less than 5%, confirming that the optimal model has high prediction accuracy and reliability. The predictions by our model for temperature- and solute content-dependent viscosity of pure Al and binary Al alloys are in very good agreement with the experimental results in the literature, indicating that the developed model has a good prediction accuracy.

Key words: BP neural network; aluminum alloy; viscosity; genetic algorithm; prediction model

1 Introduction

Casting aluminum alloys are widely used in the automotive and aerospace industries, due to their low density, high specific strength, and good thermal conductivity [1−3]. Their thermophysical properties such as viscosity, surface tension, and latent heat play a significant role in alloy microstructure characteristics and component quality soundness. Among those thermophysical properties, the viscosity significantly affects the alloy castability, and thus the characteristics of the mold filling, solidification shrinkage, hot tearing and formation of impurities, and thus the quality and soundness of the cast products [4]. In order to develop lightweight and high-performance cast aluminum alloys and products, it is important to know the viscosity of a new aluminum alloy and its influence on the castability.

There are many techniques to measure the viscosity, including the capillary rheometer, oscillating vessel viscometer, and rotational crucible [4]. In recent years, though with the technology advancement and progressing standardization for the method to measure the viscosity, there are still great differences in the measured values of viscosity for the same alloy, because the measurement of viscosity is very complicated and difficult, and different measurement methods will lead to a great difference of data even for the same alloy [4−6].

The viscosity of an alloy melt is affected by many factors. Among those, the alloy compositions

Corresponding author: Heng-cheng LIAO, Tel/Fax: +86-25-52090686, E-mail: hengchengliao@seu.edu.cn
DOI: 10.1016/S1003-6326(21)65707-2

and metal temperature are the most important ones. DINSDALE and QUESTED [6] studied the effect of the alloying elements on the viscosity of aluminum alloys, and reported that the viscosity increased with the content of Cu, Fe, Mn, Ni and Cr, but decreased with the increase of Si content. For pure aluminum melt, the relationship between the viscosity and temperature can be well expressed by the Arrhenius equation. For binary alloys, Moelwyn−Hughes model can give a reasonable prediction [6]. However, for multicomponent alloys, there are very few accurate models to predict the viscosity.

With the advance of computing and artificial intelligent (AI) techniques, some excellent machine-learning algorithms and especially artificial neural network methods have been applied in materials science and engineering. There are many types of models for viscosity prediction. Back-propagation (BP) neural networks have been developed well in recent years, as one of AI algorithm. It is readily to combine with other algorithms, like genetic algorithm. Of more importance, BP neural network is suitable for models with multiple input variables and multiple data sets. XIA et al [7] used the elements Zn, Ca, Zr, Gd, and Sr in Mg alloys as input values to establish a BP neural network, and successfully predicted the hardness and corrosion rate of Mg alloys. HAN et al [8] established an artificial neural network model for the constitutive relationship of Al−0.62Mg− 0.73Si alloy, with a smaller error than the traditional Arrhenius-type model. Based on the artificial neural network, OZERDEM and KOLUKISA [9] predicted the tensile properties of Cu−Sn−Pb−Zn−Ni casting alloy. Although the prediction error of the elongation is high, the ultimate tensile strength and yield strength are well predicted with the average errors of 7.6% and −2.1%, respectively. GAO et al [10] predicted the fluidity of casting aluminum alloys based on BP neural network and the average error of the model is 6.6%. However, there is currently no report on the prediction of the viscosity of aluminum alloys based on the artificial neural networks.

In this study, the viscosity experimental data collected from the literatures were used to develop the viscosity prediction model. The melt temperature and contents of Al, Si, Fe, Cu, Mn, Mg and Zn elements in aluminum alloys were selected as the model input. The influence of the different training algorithms and the number of hidden neurons on the model prediction accuracy was studied in detail. The initial weight and bias values were optimized using Genetic Algorithm. The predicted viscosity results of various alloys were compared with the experimental data from the literatures.

2 Method

2.1 Dataset processing

The dataset used to develop the viscosity model was collected from the literatures [11−17]. According to the suggestion of ASSAEL et al [18], the collected viscosity data were divided into the primary data and secondary data based on a number of factors such as the measurement method, formula for deriving viscosity, alloying element purity, and uncertainty. The viscosity data that are measured by the Oscillating vessel viscometer are chosen as the source data to construct the prediction model for the viscosity of aluminum alloys. Therefore, the selected data in this study have the following characteristics: (1) the mass fraction of Al in the alloy is greater than 50%; (2) the viscosity value is measured by the oscillating vessel viscometer; (3) there is purification operation during research; (4) the viscosity value is kinematic viscosity η, but not dynamic viscosity, of which the unit is mPa·s.

Among the collected data, 7 sets of viscosity values of different Al−Si−Cu based alloys at 1375 K were obtained by KOBATAKE et al [11], 85 sets of viscosity data of hypoeutectic Al−Cu alloys at the temperature of 900−1200 K obtained by PLEVACHUK et al [12], 69 sets of viscosity values of Al−7Si, Al−7Si−Mg, and Al−8Si−3Cu alloys from SKLYARCHUK et al [13], 81 sets of viscosity values of different Al−Fe alloys from SUN [15], and 43 sets of viscosity values of three Al−Si alloys from GENG et al [16] in which Si contents are respectively 5%, 12.5%, 16% in the temperature range of 900−1200 K. In addition, 24 sets of the viscosity values of pure Al, A201, A319 and A356 alloys measured by WANG and OVERFELT [14], and 6 sets of the viscosity values of LM25 alloy (nearly A356) measured by BROOKS et al [17] were collected.

Table 1 summarizes the input and output

variables of the alloying elements and measured viscosity values for the total 315 sets of the experimental data collected from the literatures. For the model development, we randomly divided the data into the training samples and test samples, 280 sets and 35 sets respectively. The training samples were used to train the neural network model and the test samples were used to verify the accuracy and reliability of the model prediction.

Table 1 Ranges of input and output variables

Variable	Feature	Min	Max
Input	*w*(Si)/%	0	50
	w(Fe)/%	0	4
	w(Cu)/%	0	30
	w(Mn)/%	0	0.71
	w(Mg)/%	0	0.46
	w(Zn)/%	0	1.2
	T/K	836	1375
Output	Viscosity/(mPa·s)	0.38	2.46

2.2 Back-propagation (BP) neural network

BP neural network is one of the most common artificial neural networks. It is a kind of multilayer feedforward neural network. In this network, the error feed-forward during the forward propagation of the output and input variables are passed from the input layer through one or more hidden layers to the output layer. If the error between the expected and predicted ones does not satisfy the requirements, the weight value and bias value of the network are optimized according to the fed-forward error, so that the predicted output is gradually close to the expected one.

The number of the hidden layer neurons is one of the important parameters that needs to be considered. If a few of hidden layer neurons are used, the network is not strong enough to make good predictions. On the contrary, the redundant hidden layer neurons will cause overfitting. Based on the study by PIOTROWSKI and NAPIORKOWSKI [19], Levenberg−Marquardt training algorithm and Bayesian Regularization training algorithm were selected in our study. In order to transfer the input variables interval into (−1, 1), we applied the sigmoid function as the transfer function between the input layer and hidden layer while the pure linear transfer function was used between the hidden layer and output layer. Moreover, the core parameters of the network, the weight values and the bias values, were optimized using genetic algorithm. All the algorithms mentioned above were implemented on MATLAB software.

2.3 Genetic algorithm

First, the genetic algorithm, of which the basis is the theory of evolution in nature, determines the parameters that need to be optimized. In each iteration of the optimization, the population composed of different parameters is called a generation. Common fitness function used to evaluate the quality of each generation is reciprocal of the difference between the expected and predicted ones. Then, the population is evolved through the random selection, crossover, and mutation operations. The algorithm terminates until a satisfactory fitness appears in one iteration.

The parameters that need optimization are the initial weight value and bias value. The equations for the number of the initial weight value and bias value are as follows:

$$n_{iw}=n_i n_h+n_h n_o \quad (1)$$

$$n_{ib}=n_h+n_o \quad (2)$$

where n_{iw} and n_{ib} are the numbers of the initial weight value and initial bias value, respectively, and n_i, n_h, n_o are the numbers of the input neurons, hidden neurons and output neurons, respectively. The sum of n_{iw} and n_{ib} is the gene of an individual in a generation, and the length of the genetic code is processed by the real-number encoding ($10n_h$+1) because the number of the input neurons is 8 and the number of output neurons is 1. Then the proper gene crossover probability and mutation probability are chosen, so that the population starts to evolve, and finally gets the best initial weight and bias values.

3 Results and discussion

3.1 Model optimization

3.1.1 Training algorithms and number of hidden neurons

Both Levenberg-Marquardt training (Trainlm) algorithm and Bayesian Regularization training (Trainbr) algorithm have good performances. The Trainlm algorithm is the most widely used

nonlinear least squares algorithm, combining the steepest descent method and linearization method. When the parameters are few, the Trainbr algorithm can avoid overfitting by modifying the loss function. Figure 1 shows the comparison of mean absolute error (MAE) of the test samples changing with the different numbers of the hidden neurons for the model trained by the Trainlm and Trainbr algorithms. Apparently, the obtained MAE values by the Trainbr algorithm are much smaller than those by the Trainlm algorithm, no matter what the number of the hidden neurons is used. This means that the Trainbr algorithm is the best choice for our BP neural network. Also, for the model trained by the Trainlm algorithm, the MAE values of the test samples are nearly random when the number of hidden neurons is greater than 8. The reason for this irregular result is thought to be that the Trainlm algorithm can easily fall into local optimal solution during the iteration, particularly when the dimensions are very large. However, the result trained by the Trainbr algorithm is more stable compared with the Trainlm algorithm.

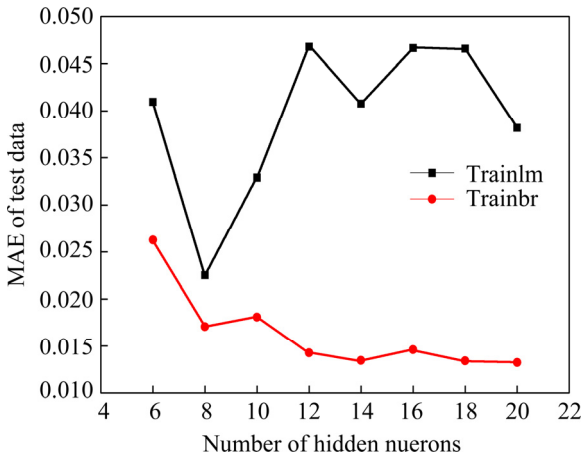

Fig. 1 MAE values of test data for different numbers of hidden neurons trained by Trainlm and Trainbr algorithms

Figure 2 shows that when the number of the hidden neurons is further expanded, the MAE value by the Trainbr algorithm will have a sudden increase, even though it is almost unchanged when the number of the hidden neurons is below 22. Because of the negligible profit of more hidden neurons and the advantage of the simpler model with fewer hidden neurons, the number of the hidden neurons in our BP neural network model is determined as 8.

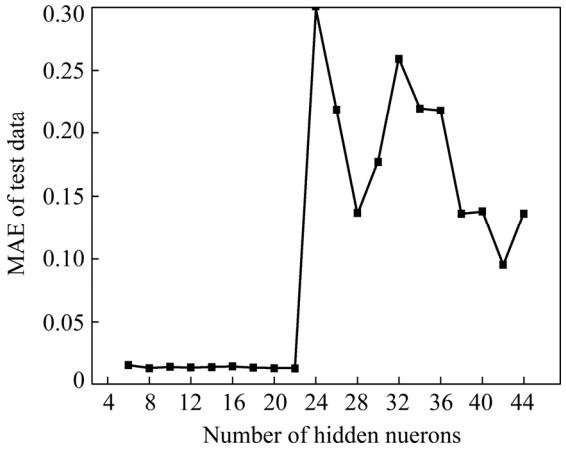

Fig. 2 MAE values of test data for much expanded number of hidden neurons trained by Trainbr algorithm

3.1.2 Initial weight and bias values

If not optimized by an algorithm, the initial weight and bias values are usually given randomly by MATLAB and thus the models are not stable because of the random parameters used. The difference between the MAE values of the initial model and the optimized model is shown in Fig. 3. Although the results of each simulation vary with the number of the hidden neurons, the optimized model has a better performance consistently.

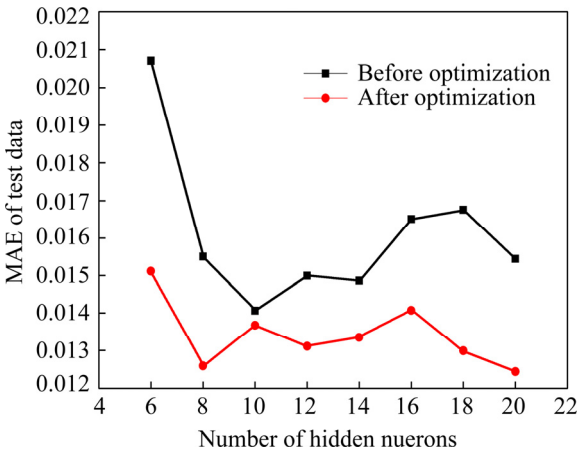

Fig. 3 MAE of predictions of test data before and after optimization

The fitness (F) of every generation is the reciprocal of total MAS predicted by each model in this population. With the increase in the iteration numbers, the reciprocal of fitness is getting smaller, which means that the network models are getting closer to the optimal one. As shown in Fig. 4, in this case the population is 100, the average fitness of the population is increased with the iteration. This

indicates that the average MAE is getting smaller and the best model can be obtained in the last generation.

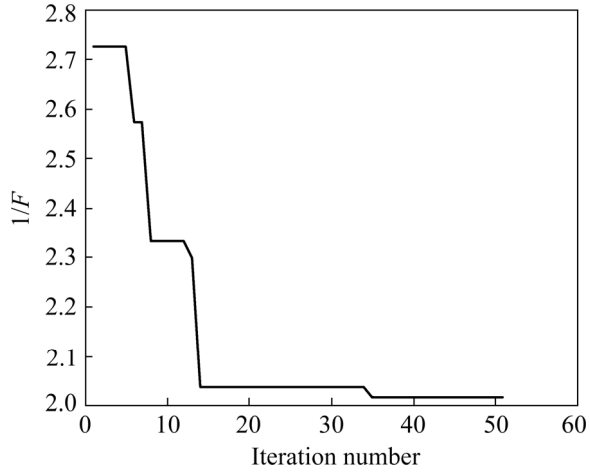

Fig. 4 Optimization process by genetic algorithm

3.2 Model validation

Using our optimized BP neural network model, the predicted viscosity values are compared with the test data, as shown in Fig. 5. They are much closed each other. About two thirds of predictions have a relative error (the difference of the predicted and experimental values/the experimental value) less than 3%, and the relative errors of all predictions are less than 5% (see Fig. 6(a)). As shown in Fig. 6(b), the predicted viscosity values have very good correlation with measurement data within the viscosity value ranging from 0.5 to 2.3 mPa·s (R^2=0.96). This indicates that the developed BP model for the viscosity of aluminum alloys has a high prediction accuracy.

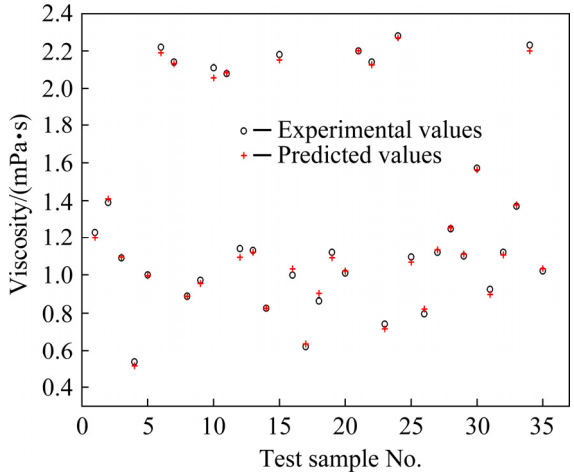

Fig. 5 Comparison between predicted and experimental viscosity values for test samples

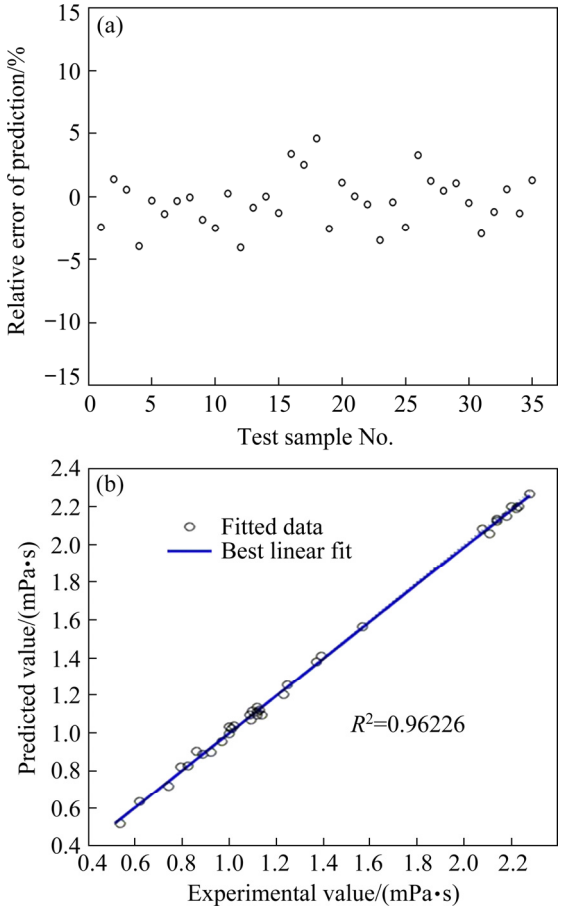

Fig. 6 Relative error of predictions for all test samples by optimal BP model (a), and linear fitting of predicted viscosity values with experimental ones for all test samples (b)

3.3 Application of viscosity BP model

3.3.1 Influence of temperature

The Arrhenius equation is most frequently used to represent the effect of temperature on viscosity: $\eta=\eta_0\exp[E/(RT)]$, where T is the temperature in K, E is the activation energy for viscous flow, η_0 is the pre-exponential viscosity, and R is the mole gas constant.

Figure 7 shows the predicted viscosity values of the pure Al, and Al−7Si and Al−4Cu alloys with the temperature using the optimized model and the comparison of them with the experimental values. The predicted temperature dependence of the viscosity of the pure Al can be seen in Fig. 7(a), which is consistent with the results in Refs. [15,16]. The predicted viscosity values of Al−7Si alloy are also very close to ones measured by SKLYARCHUK et al [13] and the trend fits the Arrhenius equation very well in the temperature range from 900 to 1200 K (Fig. 7(b). Similarly, the

results of Al−4Cu alloy predicted by our model are very consistent with those by PLEVACHUK et al [12], as shown in Fig. 7(c).

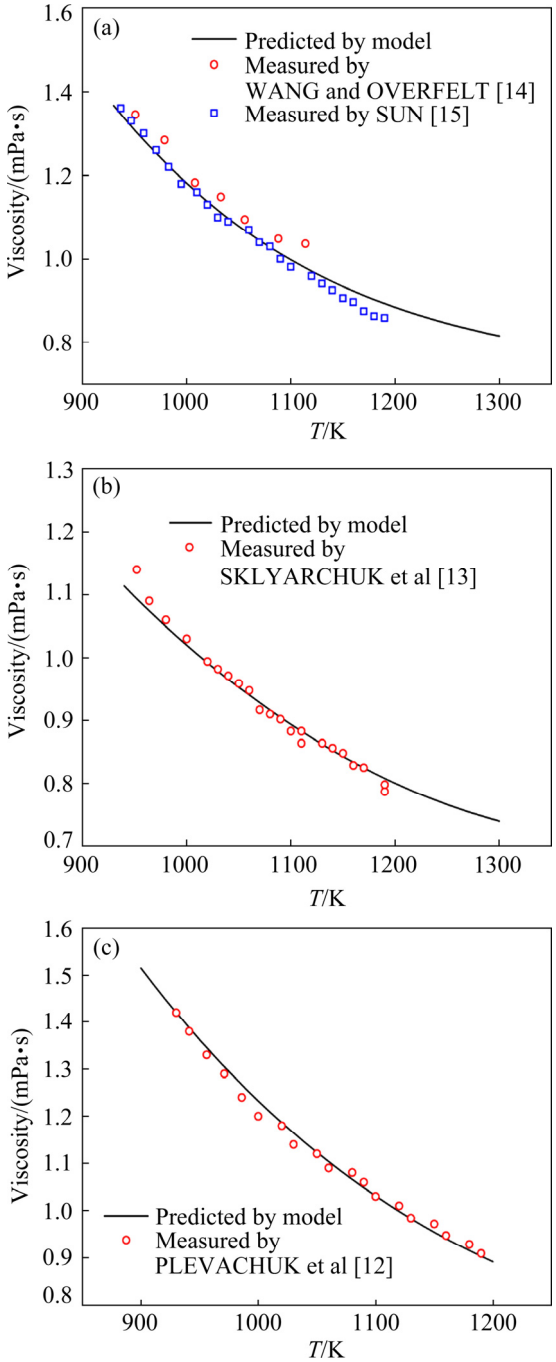

Fig. 7 Predicted temperature dependence of viscosity of pure Al (a), Al−7Si (b) and Al−4Cu (c) alloys and comparison with corresponding results in Refs. [12−15]

As shown in Table 2, the parameters obtained by fitting the predicted viscosity values with the Arrhenius equation are compared with those in the literatures. The parameters calculated from the BP neural network model are close to Ref. [12] for Al−4Cu alloy. Meanwhile, there is only very small difference between our study and Ref. [13] for pure Al and Al−7Si alloy. This indicates a good prediction accuracy of our BP model for the viscosity of aluminum alloys.

Table 2 Comparison of parameters of Arrhenius equation between this study and references

Alloy	η_0/(mPa·s)	E/(kJ·mol^{-1})	Source
Pure Al	0.197	14.97	This study
	0.16	16.63	Ref. [13]
Al−7Si	0.247	11.77	This study
	0.206	13.38	Ref. [13]
Al−4Cu	0.179	16.01	This study
	0.196	15.21	Ref. [12]

3.3.2 Binary alloys

As mentioned above, DINSDALE and QUESTED [6] reported that the viscosity of aluminum alloys increases with the increase of Cu and Fe, but conversely with Si content. The effect of the solute content on the viscosity of Al binary alloys is predicted by our model, as shown in Fig. 8. The Si content is 7−20 wt.% (see Fig. 8(a)), which is a little narrow due to the limitation of the available dataset. For Al−Si alloys, there is a good agreement between the predicted viscosity values and the ones measured by SKLYARCHUK et al [13]. The viscosity first decreases rapidly with increasing Si content and then it declines slowly when Si content is greater than 12 wt.%. For the effect of Cu solute content, as seen in Fig. 8(b), the viscosity is positively correlated with Cu content in the alloy. The predicted viscosity values are very close to those measured by PLEVACHUK et al [12]. The addition of 0.2 wt.% Fe in Al can sharply increase the viscosity from about 1.0 to 2.0 mPa·s, which is an interesting phenomenon. SUN [15] stated that Fe is harmful to Al alloys because it can cause a rapid increase of the viscosity. For binary Al alloys, the predictions by our model also agree very well with results in the literature.

3.3.3 Ternary alloys

Figure 9 exhibits the contour map of the viscosity of Al−Si−Cu alloys predicted by our viscosity model, where Si content varies from 6 to 20 wt.% and Cu content from 6 to 20 wt.% at 1000 K. For the contour map of Al−Si−Cu alloy system, there exist a region with large viscosity (orange area, bottom right corner) and a region with

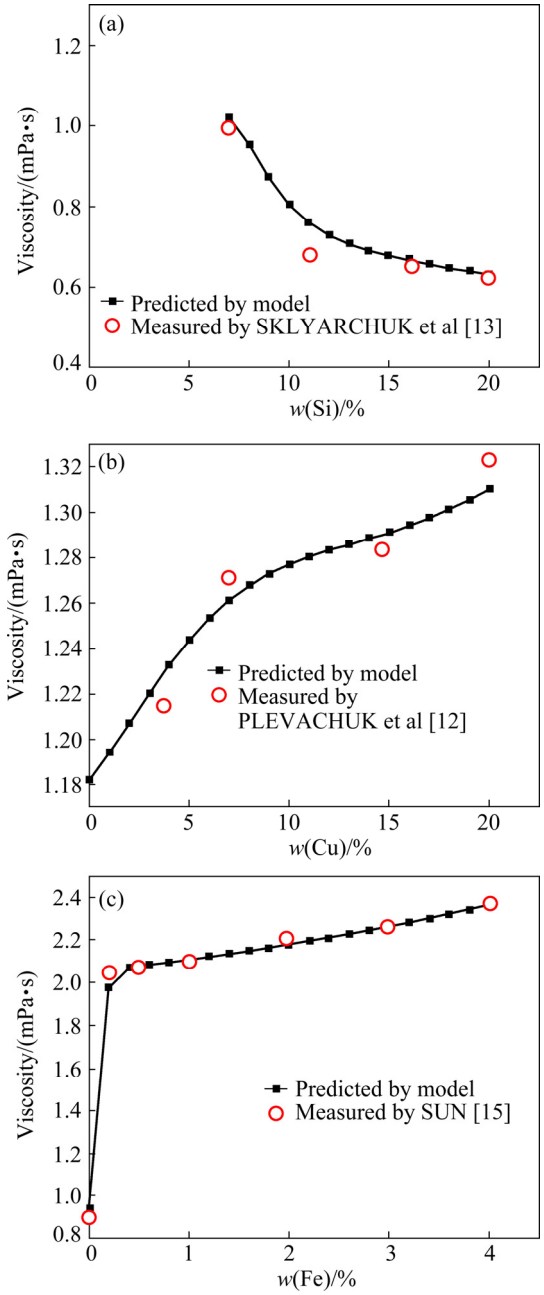

Fig. 8 Predicted and experimental viscosity values of Al−Si alloys (a), Al−Cu alloys (b) at 1000 K and Al−Fe alloys at 1150 K (c) and comparison with corresponding results in Refs. [12,13,15]

small viscosity (blue area, top left corner). As seen from the contour plot, when the Si content is low, contour lines are very dense and parallel to the Cu content axis, indicating Si solute content plays a vital role in determining viscosity. In addition, the slope of the contour line approaches 1 when Si content is more than about 14 wt.% in the alloy. This implies that if the same amount of Si and Cu is added into the alloy the viscosity value will keep constant. This is due to the neutralization effect of the combined Si and Cu contents on the viscosity. The results above suggest that the developed BP viscosity model can be applied to the design of multicomponent Al alloys.

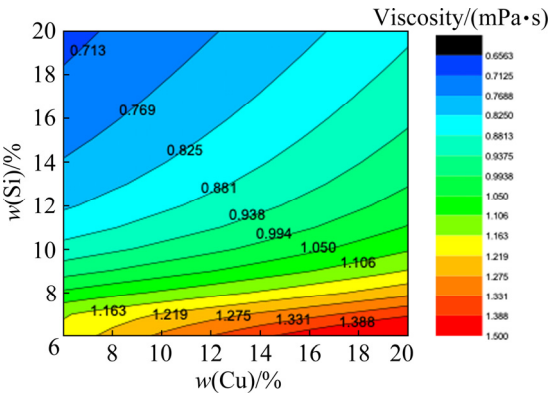

Fig. 9 Prediction of viscosity of Al−*x*Cu−*y*Si alloys at 1000 K

4 Conclusions

(1) The Bayesian Regularization algorithm provides a better training results than the Levenberg−Marquardt algorithm in our model and the best number of the hidden neurons is 8 in this study.

(2) The initial weight and bias values are also optimized using genetic algorithm, which improves the model accuracy considerably.

(3) The average relative error between the predicted and experimental viscosity data is less than 5%, exhibiting a good prediction accuracy.

(4) The BP neural network viscosity model can predict the temperature- and solute content-dependency of the viscosity in pure Al, binary, and ternary Al alloys, with a good accuracy.

Acknowledgments

The authors are grateful for the financial supports from the GM Research Foundation, China (No. GAC2094), Jiangsu Key Laboratory of Advanced Metallic Materials, China (No. BM2007204), and the Fundamental Research Funds for the Central Universities, China (No. 2242016K40011)

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基于 BP 神经网络算法的铝合金黏度预测模型

廖恒成[1]，高 源[1]，Qi-gui WANG[2], Dan WILSON[2]

1. 东南大学 材料科学与工程学院，江苏省先进金属材料高技术重点实验室，南京 211189；
2. Materials Technology, GM Global Product Group, 30003 Fisher Brothers Road, Warren, MI 48093, USA

摘 要：黏度是液体铝合金重要的热物性质之一，影响到液体充型与凝固的特征，继而铸件的质量。在本研究中，从文献中收集了 315 组实验测定的黏度数据，用来开发黏度预测模型。采用 BP 神经网络算法构建模型，以熔体温度和合金中 Al、Si、Fe、Cu、Mn、Mg 和 Zn 的含量作为模型输入，并以黏度值作为模型输出。为了改善模型精度，研究不同训练算法和隐含层神经元数的影响。使用遗传算法优化初始权重与赋值，这显著改善了模型精度。模型预测值与实验值间的相对误差小于 5%，证明所构建的优化模型具有高的预测精度与可靠性。用建立的模型对纯 Al 和二元 Al 合金的黏度随温度和溶质含量变化的预测结果与文献中的实验结果非常一致，表明该模型在工程应用中具有较好的预测精度。

关键词：BP 神经网络；铝合金；黏度；遗传算法；预测模型

(Edited by Xiang-qun LI)