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Improvement and application of neural network models in development of wrought magnesium alloys

LIU Bin[1], TANG Ai-tao[1, 2], PAN Fu-sheng[1, 2], ZHANG Jing[1, 2], PENG Jian [1, 2], WANG Jing-feng[1, 2]

1. College of Materials Science and Engineering, Chongqing University, Chongqing 400030, China;
2. National Engineering Research Center for Magnesium Alloys, Chongqing University, Chongqing 400030, China

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Abstract: Neural network models of mechanical properties prediction for wrought magnesium alloys were improved by using more reasonable parameters, and were used to develop new types of magnesium alloys. The parameters were confirmed by comparing prediction errors and correlation coefficients of models, which have been built with all the parameters used commonly with training of all permutations and combinations. The application was focused on Mg-Zn-Mn and Mg-Zn-Y-Zr alloys. The prediction of mechanical properties of Mg-Zn-Mn alloys and the effects of mole ratios of Y to Zn on the strengths in Mg-Zn-Y-Zr alloys were investigated by using the improved models. The predicted results are good agreement with the experimental values. A high strength extruded Mg-Zn-Zr-Y alloy was also developed by the models. The applications of the models indicate that the improved models can be used to develop new types of wrought magnesium alloys.

Key words: magnesium alloy; artificial neural network; model; mechanical property

1 Introduction

Magnesium alloys are becoming increasingly attractive for potential use in a wide range of structural applications, including the automotive, transportation, aeronautical and aerospace industries, due to their low density, good machinability, favorable recycling capability and excellent damping capacity. However, the mechanical properties of magnesium alloys still could not satisfy the demands of some important application fields. For example, only some parts can be produced by using magnesium alloys in vehicles currently[1−5]. In order to improve the mechanical properties of magnesium alloys, new types of magnesium alloys have been being developed, but conventional methods for developing new alloys need to spend a lot of effort and time[6−9].

Because of the non-linear relationship among alloy composition, processing parameters and mechanical properties, it is hard to describe the functional relationship of these variants using only one equation. In this case, artificial neural network (ANN) seems to be suitable for modeling non-linear processes by means of a large-scale parallel-distributed information processing system, which contains many interconnected neurons[10]. It may be helpful in predicting mechanical properties of magnesium alloys.

In recent years, the models based on neural network technique are used increasingly in magnesium alloy research field[6,11−14]. However, the modeling parameters are mainly dependent on human experience. It is very difficult to establish high precision models systematically. In the present work, a new method to obtain parameters with all permutations and combinations training has been developed for improving ANN models. And then, the models have been used to investigate the mechanical properties of Mg-Zn-Mn alloys and Mg-Zn-Y-Zr alloys successfully.

The aim of the present study was to apply ANN models to predicting mechanical properties for developing new types of magnesium alloys. Considering the common mechanical properties types of magnesium alloys, three ANN models for predicting ultimate tensile

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Corresponding author: PAN Fu-sheng; Tel: +86-23-65112635; E-mal: fspan@cqu.edu.cn
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strength (UTS), yield strength (YS) and elongation (ELO) were built, respectively. All of the models have the same structure: three layers with a full connected multilayer feed forward neural network. The general scheme of the models is given in Fig.1. The input parameters of ANN models are processing parameters and alloy composition, including the commonly used alloying elements in magnesium alloys, namely Al, Zn, Mn, Zr, Y, Ce, Si, Be, Cu, Ni, Fe and Ca, etc. Meanwhile, the output parameters for models are UTS, YS and ELO, respectively.

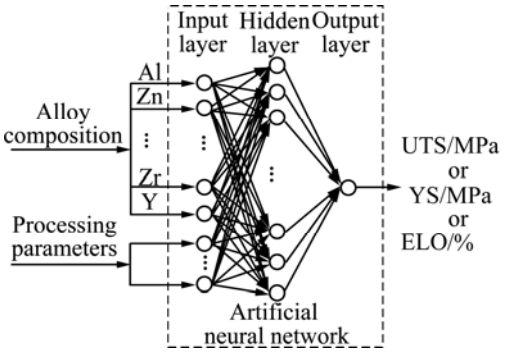

Fig.1 Schematic diagram of models for prediction of mechanical properties of magnesium alloys

The performance of an ANN model depends upon the dataset used for its training. Therefore, for reliable neural network model a significant amount of data as well as powerful computing resources are necessary[15]. In the present work, all the data of magnesium alloys for model training are from the database of the National Engineering Research Center for Magnesium Alloys of China. The neural network models were designed and trained by using the Matlab 7.4 version on a personal computer with 4-core CPU and 2G memory.

2 Improvement of ANN models

2.1 Improved parameters

Different modeling parameters have important influence on the predicted results. The improved parameters, including preprocessing styles, number of hidden layer neurons, transfer functions and algorithms, have been confirmed by comparing prediction errors and relativity values of models, which have been built with all the parameters used commonly (see Table 1) with training of all permutations and combinations. Therefore, there is a total of 2 016 (4×28×3×3×2) combinations of the common parameters.

Each kind of parameter combination was trained five times by computer programming. Then, the average errors and the mean relativity values of models were calculated according to the five results for each combination. Finally, the improved parameters can be obtained by comparing the average errors and the mean relativity values of models. It can be seen that all of the improved parameters for models are the same except the number of hidden layer neurons is 7 for UTS, 15 for YS, and 14 for ELO, respectively. If using these parameters, the models can achieve the average accuracy shown in Table 2 easily. Moreover, it also can be seen that the ELO model has the lowest average accuracy. This may be due to the different discrete degrees of UTS, YS and ELO data for training. The ELO data are generally concentrated between 0 and 20%, while the UTS and YS data are concentrated between 250 MPa and 350 MPa. The fitting is more difficult for the data with greater discrete degree, so it is the lowest average accuracy for ELO.

Table 1 Selected common parameters for training of all permutations and combinations

Parameter	Common value	Number
Preprocessing style	[0.15, 0.90], [0.10, 0.90], [0.01, 0.99], [0, 1]	4
Number of hidden layer neurons	From 3 to 30, interval 1	28
Transfer function (input layer-middle layer)	logsig, tansig, purelin	3
Transfer function (middle layer-output layer)	logsig, tansig, purelin	3
Algorithm	trainbr, trainlm	2

Table 2 Improved parameters

Parameter	UTS	YS	ELO
Preprocessing style	[0, 1]	[0, 1]	[0, 1]
Number of hidden layer neurons	7	15	14
Transfer function (input layer-middle layer)	tansig	tansig	tansig
Transfer function (middle layer- output layer)	logsig	logsig	logsig
Algorithm	trainlm	trainlm	trainlm
Average error of five times/%	2.13	2.38	14.52
Mean relativity value of five times	0.92	0.96	0.89

2.2 Improved models

The UTS, YS, ELO models have been built by using the improved parameters. After training several times, many improved UTS, YS, ELO models can be obtained, respectively. Most of the average errors of

models are lower than those shown in Table 2 and the relativity values are higher than the corresponding values in Table 2 at the same time.

The best models are shown in Fig.2. It can be seen that all the three ANN models have good performance on predicting mechanical properties of magnesium alloys, especially the YS model has the best fitting results. The relativity values are 0.96 for UTS, 0.97 for YS, and 0.92 for ELO. Obviously, the three values are higher than the corresponding average ones shown in Table 2.

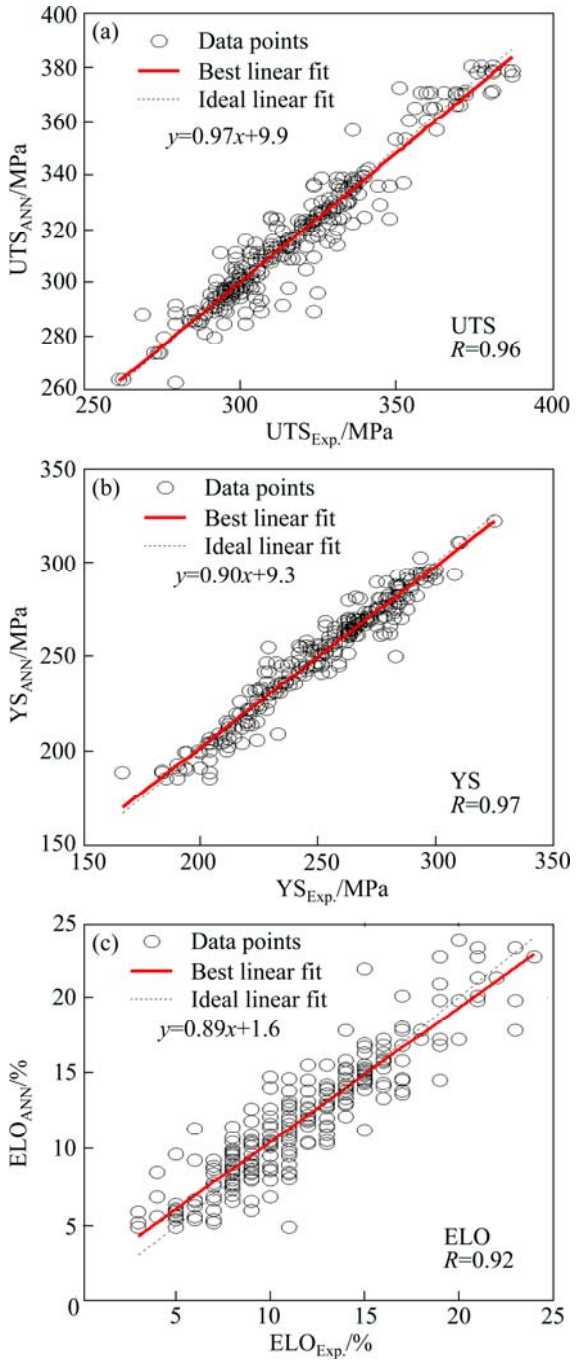

Fig.2 Predicted mechanical properties for magnesium alloys with improved models vs experimental data: (a) UTS; (b) YS; (c) ELO

2.3 Comparison of previous models and improved models

Compared with the previous best models using parameters from conventional random selection [16], the models have higher accuracy and can be built systematically by using parameters from training of all permutations and combinations. Table 3 lists the different results from the previous and improved models. It is easy to see that the accuracy of models can be improved further if using the parameters from training of all permutations and combinations.

Table 3 Results from previous models and improved models

Mechanical property	Type	Relativity value, R	Mean error/%
UTS	Previous	0.95	1.80
	Improved	0.96	1.49
YS	Previous	0.97	2.10
	Improved	0.97	1.99
ELO	Previous	0.91	14.60
	Improved	0.92	13.60

The improved models also were used to predict the mechanical properties of Mg-Zn-Zr alloys in order to compare with previous models. Fig.3 shows the predicted results from the previous models and improved models as well as experimental work. T6-500-3 means that the solution temperature is 500 °C and the holding time is 3 h. For all the T6 treatment, the aging temperature is 180 °C and the holding time is 24 h. The predicted results from the improved models were found to have better agreement with the experimental data, which reveals that the improved model can be used to develop new types of magnesium alloys.

3 Application of improved models

3.1 Prediction of mechanical properties of Mg-Zn-Mn alloys

The improved models were used to predict the mechanical properties of Mg-Zn-Mn alloys. The alloy composition and processing parameters are designed, as listed in Table 4.

Table 5 lists the results from the improved models as well as experimental work. Good results can be

Table 4 Composition and processing parameters of Mg-Zn-Mn alloys

w/%			Temperature/	Extrusion	Mole
Zn	Mn	Mg	°C	rate/(m·min^{-1})	ratio
5	1	Bal.	390	1.5	25

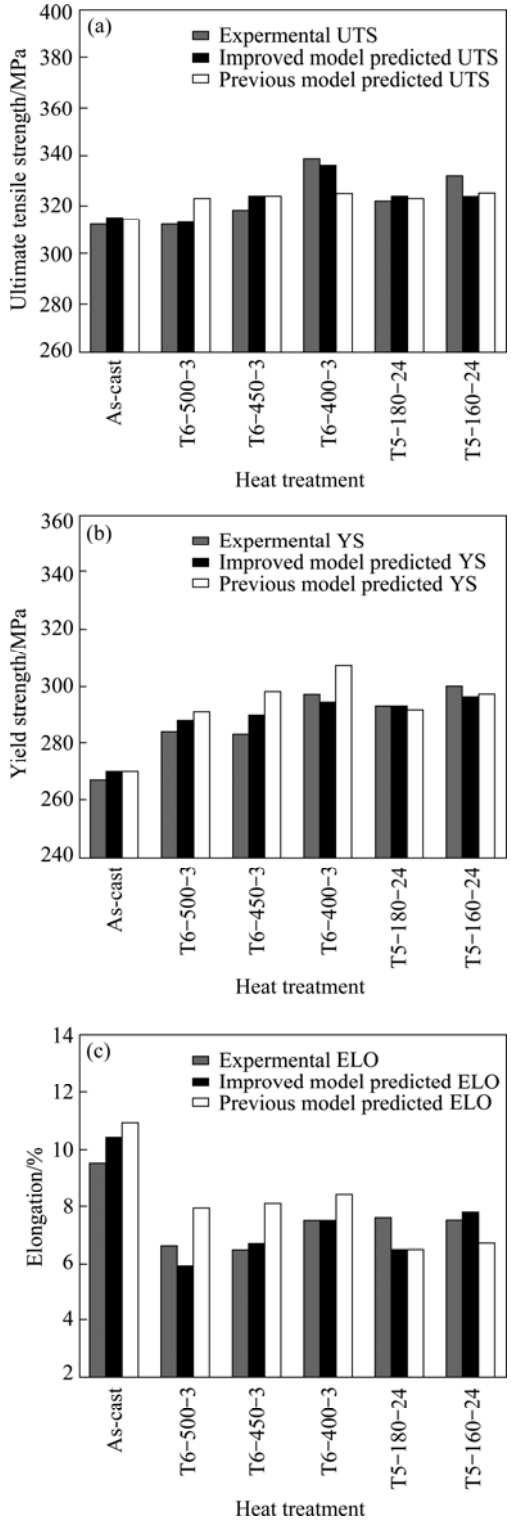

Fig.3 Predicted and experimental values of mechanical properties of Mg-6Zn-0.5Zr alloys under different conditions

Table 5 Predicted and experimental values of mechanical properties of Mg-5Zn-Mn alloys

Mechanical property	Prediction	Experiment	Error/%
UTS/MPa	356	312	14
YS/MPa	232	235	1
ELO/%	13.0	13.3	2.3

obtained for the prediction of YS and ELO, and acceptable results can be predicted for UTS. It is suggested that the models can be used to develop new types of wrought magnesium alloys by predicting mechanical properties.

3.2 Effects of mole ratios of Y to Zn on strength of Mg-Zn-Y-Zr alloys

The improved models also were used to investigate the effects of mole ratios of Y to Zn on the strength of Mg-Zn-Zr-Y alloys. As listed in Table 6, three Mg-Zn-Zr-Y alloys were chosen for the study. The mole ratio of Y to Zn is 0 for Mg-6Zn-0.5Zr, 0.1 for Mg-6Zn-0.4Zr-Y and 0.8 for Mg-4.6Zn-0.6Zr-4.7Y. The processing parameters of extrusion for Mg-Zn-Zr-Y alloys are the same: temperature is 400 °C, extrusion rate is 1.25 m/min and mole ratio is 25.

Table 6 Mg-Zn-Y-Zr alloys with different mole ratios of Y to Zn

n(Y):n(Zn)	w/%			
	Zn	Zr	Y	Mg
0	6.0	0.5	0	Bal.
0.1	6.0	0.4	1.0	Bal.
0.8	4.6	0.6	4.7	Bal.

According to Ref.[16], the coexisting of Y and Zn atoms will introduce *W* phase (*W*-Mg3Y2Zn3), long period structure (LPS-Mg12YZn) and quasicrystalline phase (*I*-Mg3YZn6). All of these phases and MgZn2 have contribution to mechanical properties, and the contributions from high to low are: *W*+LPS, *W*+*I*, MgZn2. According to their results, the phases in Mg-Zn-Y-Zr alloys with different Y to Zn mole ratios are given in Table 7.

Figure 4 shows the predicted UTS and YS results by the improved model as well as experimental work of Mg-Zn-Zr-Y alloys. It can be seen that the predicted strengths are consistent with the experimental data, and the UTS and YS are continuously improved as the Y to

Table 7 Phases in wrought Mg-Zn-Y-Zr alloys with different Y to Zn mole ratios

n(Y):n(Zn)	Alloy	Phase
0	Mg-6.0Zn-0.5Zr	α-Mg+$MgZn_2$
0.1	Mg-6.0Zn-0.4Zr-Y	α-Mg+*W*-Mg3Y2Zn3+*I*-Mg3YZn6(quasicrystal)
0.8	Mg-4.6Zn-0.6Zr-4.7Y	α-Mg+*W*-Mg3Y2Zn3+LPS-Mg12YZn

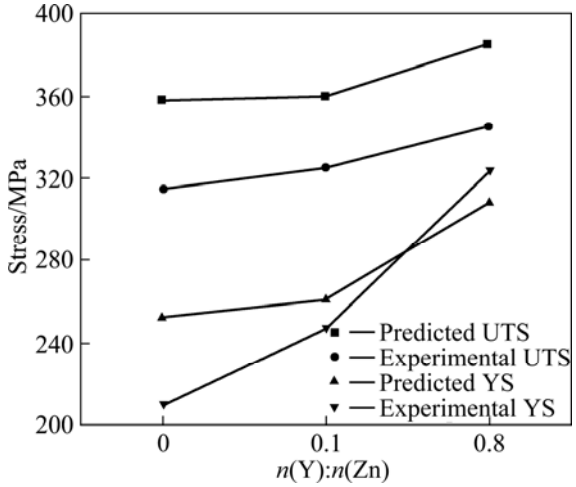

Fig.4 Predicted mechanical properties vs experimental data of Mg-Zn-Zr-Y alloys with different mole ratios of Y to Zn

Zn mole ratio increases. The results reveal that the improved models can be used to develop new types of high strength extruded Mg-Zn-Zr-Y alloys by investigating the effects of Y to Zn mole ratios on the strengths.

3.3 Development of high strength extruded Mg-Zn-Zr-Y alloys

In order to obtain the best mechanical properties and the corresponding alloy compositions for high strength extruded Mg-Zn-Zr-Y alloys, the improved models were used to investigate the relationships between alloy compositions and mechanical properties under fixed experimental conditions. Considering the actual situation of experiment and production, the design for Mg-Zn-Zr-Y alloys is given in Table 8.

Fig.5 shows the trend graphs according to the predicted results, which show the changes of mechanical

Table 8 Design for Mg-Zn-Zr-Y alloys

w/%				Processing parameter		
Zr	Zn	Y	Mg	Homogenization	Extrusion	Aging
0.45	0−10.0, interval 1.0	0−4.0, interval 0.2	Bal.	Temperature 390 °C, time 24 h	Temperature 390 °C, Extrusion rate 1.75 m/min, mole ratio 55	Temperature 170 °C, time 24 h

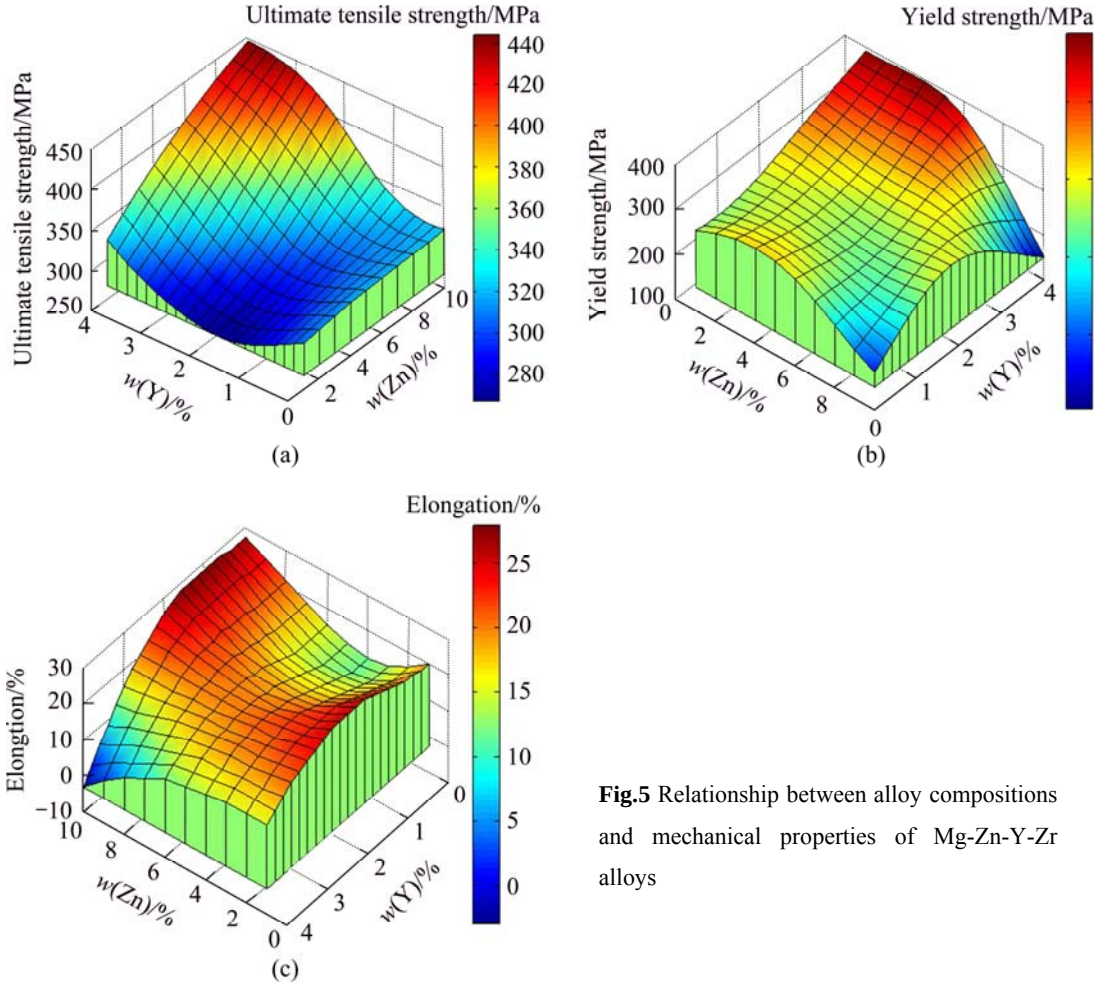

Fig.5 Relationship between alloy compositions and mechanical properties of Mg-Zn-Y-Zr alloys

properties of Mg-Zn-Zr-Y alloys with different Y and Zn contents. Therefore, the satisfactory mechanical properties and the corresponding alloy compositions can be concluded from Fig.5. Thus, the best mechanical properties shown in Table 9 under the fixed experimental conditions can be obtained when the alloy compositions are Mg-7.0Zn-0.45Zr-3.0Y. In this case, the optimum mechanical properties are 376 MPa for UTS, 318 MPa for YS and 19% for elongation, which need to be verified in the future experiment.

Table 9 Relationship between alloy compositions and mechanical properties of Mg-Zn-Zr-Y alloys

Condition	Composition	
	w(Zn)/%	*w*(Y)/%
Experiment	7.0−9.0	2.5−3.5
	<7.0	3.0−3.5
	<8.0	2.0−3.0
Optimum	7.0	3.0

Condition	Mechanical property		
	UTS/MPa	YS/MPa	Elongation/%
Experiment	>350	>300	20
Optimum	376	318	19

4 Conclusions

1) The improved parameters of ANN models for predicting UTS, YS, and ELO of magnesium alloys are obtained by training of all the parameters used commonly with all permutations and combinations.

2) The prediction models with higher accuracy for UTS, YS, ELO of magnesium alloys can be built systematically by using the improved parameters.

3) The improved models were used to predict the mechanical properties of Mg-Zn-Zr alloys. Compared with previous works, the predicted results are found to be better agreement with the experimental data.

4) The improved models were applied to predicting the mechanical properties of Mg-Zn-Mn alloys and Mg-Zn-Y-Zr alloys successfully. All the applications of improved models indicate that the models can be used to develop new types of wrought magnesium alloys.

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改进的神经网络模型在变形镁合金发展中的应用

刘 彬[1], 汤爱涛[1,2], 潘复生[1,2], 张 静[1,2], 彭 健[1,2], 王敬丰[1,2]

1. 重庆大学 材料科学与工程学院，重庆 400030；
2. 重庆大学 国家镁合金工程技术研究中心，重庆 400030,

摘 要：采用更为合理的建模参数，将预测变形镁合金力学性能的神经网络模型进行改进，并将此模型用于发展新型镁合金；对所有建模参数以全排列组合训练的方式构建模型，并通过比较这些模型的预测误差及相关系数来确定最合理的建模参数。模型的应用主要有 Mg-Zn-Mn 和 Mg-Zn-Y-Zr 两种合金。运用改进后的模型对 Mg-Zn-Mn 合金的力学性能进行预测，研究 Mg-Zn-Y-Zr 合金中 Y/Zn 摩尔比对强度的影响。最后，还利用此模型发展了一种高强挤压态的 Mg-Zn-Y-Zr 合金。结果表明：模型预测值与实验值吻合较好，改进后的模型可以用于发展新型变形镁合金。

关键词：镁合金；人工神经网络；模型；力学性能

(Edited by LI Xiang-qun)