A Prediction of Atomic Occupation Probability and Order Parameter Changes in the Precipitation Process of $Ni_{75}Al_{2.5}V_{22.5}$Alloy was Carried Out Using a BP Neural Network

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Abstract: The Ni75Al2.5V22.5 alloy was used as the research object, and the precipitation process of the alloy at different temperatures was simulated by the microscopic phase-field method. We found that it takes a long time to change the temperature conditions many times. Therefore, for the first time, this paper proposes to use the simulated data of the microscopic phase-field method as a data set to construct an artificial neural network model to directly and quickly predict the results: The back propagation (BP) neural network model is established. When the total prediction step is 50000, the result is about 970 times shorter than the micro-phase field simulation calculation time. Under the premise of ensuring that the maximum error is 0.00672, the calculation efficiency is greatly improved.

Keywords: $Ni_{75}Al_{2.5}V_{22.5}$ alloy,Back propagationneural network,Microscopic phase-field, Precipitation.

1 Introduction

Microstructure determines macroscopic properties. Computer simulation technology and artificial intelligence technology are widely used in materials science [1]. We can observe the microstructure evolution process of alloy materials at different time and space scales, and can also directly predict the microstructure under different process conditions[2].The machine learning method has been applied to find and identify phase transition models in material physics [3], extracting properties based on material microstructure [4] and accelerate the prediction of material properties [5], which provides ideas for our research. Therefore, we try to combine BP neural network technology with the microscopic phase-field phase field method.

2 Experimental procedure

Firstly, a large amount of data is established by microscopic phase-field simulation, and then the data set is randomly divided into training set and test set. The training set is used to construct the BP neural network model, and the test set is used to evaluate the model. Finally, the fitting results of BP neural network are used to optimize.

The microscopic phase-field model

The phase field method mainly describes the microstructure evolution by obtaining the changes of field variables in time and space. The microscopic phase-fieldequation

$$\frac{dP(r,t)}{dt}=\frac{C_0(1-C_0)}{k_BT}\sum_{r'}L(r-r')\frac{\partial F}{\partial P(r',t)}\#(1)$$

The Back propagationneural network model

The most significant feature of BP neural network is the function of error back propagation [8]. The calculation method of BP neural network algorithm is:
training data input value:

$$X=(x_1,x_2,\dots,x_m)$$

the actual output value of the model :

$$Y=(y_1,y_2,\dots,y_n)$$

the expected output value:

$$T=(t_1,t_2,\dots,t_n)$$

For the k^{th} pair of calculated data $(X_k,T_k)$of the BP neural network, the error of the k^{th} pair of calculated data, that is, the error between the actual output and the expected output, is defined as:

$$E_k=\frac{1}{2}\|Y_k-T_k\|^2=\frac{1}{2}\sum_{z=1}^{n}(y_z-t_z)^2\#(2)$$

Simulation process

The atomic evolution images of $Ni_{75}Al_{2.5}V_{22.5}$ at 1050K and 1350K were obtained by microscopic phase-field model simulation, Fig.1, asa reference.Each la (50,33),(52,34),(54, 35)…

Data collection.The input variable is temperature 1000K~1500K, and the output variable is atomic occupation probability.Select a complete θ phase, a total of 15 lattice points,A total of 101 sets of data were collected.
Algorithm selection.The BP neural network algorithm in the artificial neural network system is selected.

Modeling.Training data 70%, validation data 15%, test data 15%.

Model analysis.Themean square error

$$E(W,b)=\frac{1}{m}\sum_{i=1}^{m}\frac{1}{k}\sum_{j=1}^{k}\left(\hat{y}_{ij}-y_{ij}\right)^2 \#(3)$$

$m$the number of nodes in the input layer.

Finally, the goodness of fit index R is used to evaluate the model.

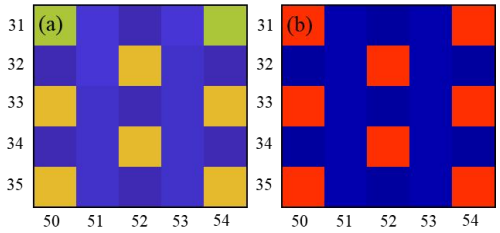

Fig. 1Local the simulation area.(a)1050K(b)1350K,there is aθ precipitated phase structures, completly.

3 Result and discussion

After the training is completed, the mean square error MSE < 6.72E-03, the average error of the training set is 1.33%, the maximum error of the training set is 5.88%, the average error of the verification set is 1.23%, and the maximum error of the verification set is 5.96 %, the error of R value is not more than 0.9%,indicating that the BP neural network of the structure can achieve a better prediction effect.

In order to objectively evaluate the generalization ability of the model, 10 sets of data are used to predict and compare with the reference value.$R^2 = 0.9832$, the fitting degree is good.

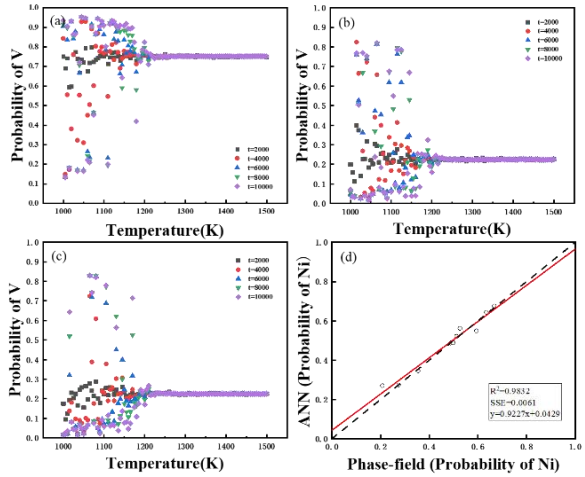

Fig. 2Lattice data sets and prediction results. (a)lattice (50,33) (b) lattice (52,34) (c) lattice(54,35) (d)There is a linear relationship between the atomic occupation probability predicted by BP neural network and the atomic occupation probability calculated by microscopic phase- field.

Predict the order parameters

We use a similar method, only need to change the output value.The R value is concentrated near 0.85, and the prediction effect of the model is general, so more data need to be collected.

Conclusion

The BP neural network is a feed-forward supervised network model, which can better replace the microscopic phase-field model.The BP neural network model takes about 0.6 seconds to perform a prediction, and the calculation time is about 970 times shorter than the phase field model.

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