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Developing of an expert system for nonferrous alloy design①

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Abstract: Expert systems have been used widely in the predictions and design of alloy systems. But the expert systems are based on the macroscopic models that have no physical meanings. Microscopic molecular dynamics is also a standard computational technique used in materials science. An approach is presented to the design system of nonferrous alloy that integrates the molecular dynamical simulation together with an expert system. The knowledge base in the expert system is able to predict nonferrous alloy properties by using machine learning technology. The architecture of the system is presented.

Key words: nonferrous alloy; molecular dynamics; machine learning; expert system
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1 INTRODUCTION

Computational Materials Science uses computers to model, understand and predict material properties[1-3]. This approach often yields unique insights into experimental data, and is used to guide experimenters toward new materials with unique and important properties. Expert systems have been used widely in the predictions and design of alloy systems. But the expert systems are based on the macroscopic models that have less physical meanings. On the other hand, microscopic simulations such as quantum ab initio methods and molecular dynamics are also very useful for the design of the material[4-6]. Microscopic models also have some shortcomings. These kinds of models need a lot of computer CPU times and not valid for some cases. How to integrate the macroscopic models with the microscopic models is a very interesting problem. In the molecular dynamical simulations, there are a lot of interatomic potentials to choose[7]. In the development of the nonferrous alloy design, how to select a proper interatomic potential is a key problem. Different potentials are suitable for the interactions of different kinds of atoms[8, 9]. Usually, we decide the proper inter- atomic potential by our experiences and the comparison with the experiments. There are no rigorous ways to decide which potential is the best. With the development of machine learning, the artificial intelligence provides a route to solve these problems. In this paper, an expert system that integrates the macroscopic models and microscopic models is discussed. In the expert system, neural network models are used for the machine learning.

2 MICROSCOPIC MODELS

Dynamical simulations using particles represent an indispensable tool for many areas of modern scientific research and engineering[10]. In materials science, the method of molecular dynamics and related simulation techniques provide unique microscopic information that is not accessible by experimental methods. Molecular dynamics is a standard computational technique used in condensed matter physics, materials science, chemistry and other fields, consisting of following the temporal evolution of a system of N particles, interacting with each other by means of a certain law[11-13]. In classical molecular dynamics, the evolution is based on the Newton's law, $F = ma$, and the forces are obtained as gradients of a certain potential which is a function of all the particle coordinates. The several interatomic potentials used in the molecular dynamical simulations include classical bond-order potentials, the force matching potentials, Lennard-Jones potentials, and EAM(Embedded atom method) potentials[10, 14, 15].

In this system, we construct an interatomic potential library. Fig. 1 depicts the structure of the interatomic potential library. The interatomic potential library includes different kinds of potential. There are several parameters for each kind of potential. The key problem in the expert system is to decide which kind of interatomic potential will be used to do molecular dynamical simulations and the exact value of the parameters in the selected interatomic potential. In this paper, we take the potential energy within the TB-SMA mode[12, 13] as an example.

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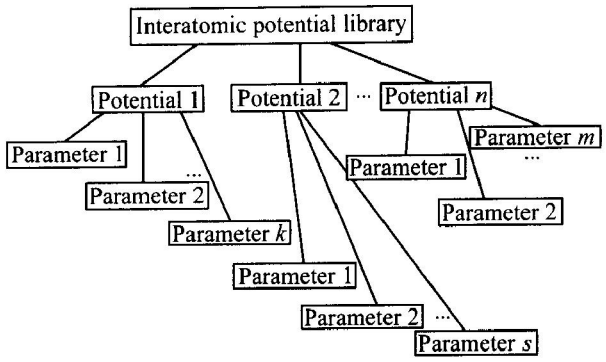

Fig. 1 Structure of interatomic potential library

In the interatomic potential library, there is a class of many-body potentials which is based on local density approximation (LDA) calculations and the second moment approximation(SMA). The total potential energy within the TB-SMA mode[12, 13, 15] could be written as

$$U_{\mathrm{coh}} = \sum_i \varepsilon_0 \sum_{j \neq i} \exp[-p(\frac{r_{ij}}{r_0} - 1)] - \sum_i \{ \sum_{j \neq i} \xi_0^2 \exp[-2q(\frac{r_{ij}}{r_0} - 1)] \} \quad (1)$$

where the first sum corresponds to the pair-potential repulsive term of Born-Mayer type and the second sum to the band structure term, which has a many-body character due to its square root form. In expression (1), r_{ij} is the interatomic distance, and r_0 is usually fixed to the value of the first-neighbor distance. In the case, r_0 is an additional free parameter, as suggested in Ref. [12]. Sums were taken over neighbors within 12 coordination shells in a crystal and over all atoms in clusters. Thus the above potential has five parameters. The parameters of the above potential were fitted to a LDA database that consists of the total energy as a function of the lattice constant. Therefore, these potentials are based on rigorous first-principles LDA results. The five parameters ξ_0, ε_0, q, p and r_0, which have been determined from expression (1) by fitting to the APW total-energy results as a function of lattice constant for different nonferrous element[16]. For example, for single Au crystal of FCC structures, the fitting parameters are ξ= 10.925 eV, ε_0= 13.595 9 eV, q= 2.738 1, p= 6.346 9, r_0= 0.175 17 nm.

In this potential model, there are five parameters for the neural network to identify. There are also other kinds of interatomic potential with different numbers of parameters.

3 MACHINE LEARNING USING NEURAL NETWORK

Machine learning investigates the mechanisms by which knowledge is acquired through experience[17, 18]. Fig. 2 shows the main architecture of the machine learning mechanism of the nonferrous alloy design system.

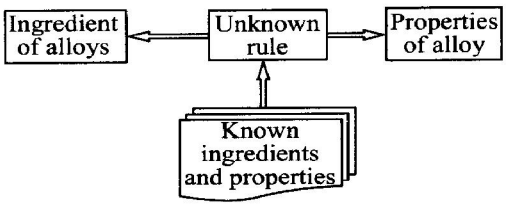

Fig. 2 Architecture of machine learning mechanism of nonferrous alloy design system

The field of neural networks has arisen from diverse sources, ranging from the fascination of mankind with understanding and emulating the human brain, to broader issues of copying human abilities such as speech and the use of language, to the practical commercial, scientific, and engineering disciplines of pattern recognition, modeling, and prediction. Neural networks consist of layers of interconnected nodes, each node producing a non-linear function of its input. The input to a node may come from other nodes or directly from the input data. Also, some nodes are identified with the output of the network[19, 20]. The complete network therefore represents a very complex set of interdependencies which may incorporate any degree of nonlinearity, allowing very general functions to be modelled. In the simplest networks, the output from one node is fed into another node in such a way as to propagate "messages" through layers of interconnecting nodes. More complex behaviour may be modelled by networks in which the final output nodes are connected with earlier nodes, and then the system has the characteristic of a highly nonlinear system with feedback[21].

Fig. 3 shows the neural network models for the expert system for the design of two-components alloy design. The inputs of the neural network model is the name of each element, proportion of each element, each kind of property (such as the lattice constant, melting temperature, the vibration mode and the bulk modulus) including the results from the molecular dynamical simulations and the experiments. The outputs of the neural network is the serial number of the best fitted interatomic potential and the best parameters that fit in with the experimental results. We set a serial number for each kind of interatomic potential. We use some experimental properties of the nonferrous alloy to be the training samples of the neural network. For the known experimental properties, we calculate the results of the molecular dynamical simulation by each kind of interatomic potential. The initial parameters of the interatomic potentials are chosen by the experiences. Then we let the neural net-

work learn by itself. More training the neural networks have, the results are more accurate[22].

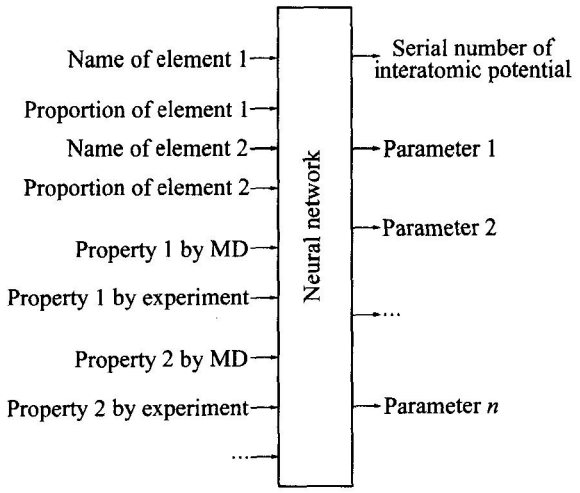

Fig. 3 Neural network models for expert system for design of two-components alloy

A B-P model is used in our network. It has multi-layered sensory structure. Besides an input and an output layer, it also contains one intermediate hidden layer. There are N inputs and L outputs[23]. Its nonlinear activation function $f(u)$ is:

$$f(u) = \frac{1}{1+\exp(-u)} \tag{2}$$

And the output of each layer unit can be calculated by

$$Y_j = f\left(\sum W_{ij}X_i - \theta_j\right), \quad j = 0, \cdots, M-1 \tag{3}$$

$$Z_k = f\left(\sum W_{jk}Y_j - \theta_k\right), \quad k = 0, \cdots, L-1 \tag{4}$$

where X_i represents the output of the ith unit in the input layer; Y_i represents the output of the jth unit in the hidden layer; Z_k represents the output of the kth unit in the output layer; W_{ij} represents the connection mass of the ith unit in the input layer to the jth unit in the hidden layer; W_{jk} represents the connection weight of the jth unit in the hidden layer to the kth unit in the output layer; θ_j represents the threshold of the jth unit in the hidden layer; θ_k represents the threshold of the kth unit in the output layer.

The self-learning algorithm of B-P neural network model is an iterative procedure[24]. At first, a set of initial weights of the network is given, then a sample is input to the network and its output is calculated. The error between the calculated output and the expected output are used to update its weights so that the error can be reduced. This updating process will be repeated until the error is smaller than a specified error value. After the neural network is trained in the self-learning way by sufficient samples, the final weights are its correct interior representation[25].

4 CONCLUSIONS

In this paper, an intelligent design system is designed based on the microscopic models and macroscopic models. Microscopic models and macroscopic models both have some advantages and shortcomings. In this system, we combine these two kinds of models organically. The shortcomings of both kinds of models are overcomed. The results of the microscopic molecular dynamical simulation are used for the input for the training of macroscopic models. The neural network model is used for the machine learning of the macroscopic models. If the trainings are done using a lot of sample data and simulation results, the machine can get more intelligence to reflect the true nature of the nonferrous alloy. The expert system can aid metallurgists in the design of new nonferrous alloys. The system can be operated in several modes which includes a decision support system and a design assistant.

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