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# Compositional optimization of glass forming alloys based on critical dimension by using artificial neural network

An-hui CAI[1,2], Xiang XIONG[2], Yong LIU[2], Wei-ke AN[1], Guo-jun ZHOU[1], Yun LUO[1], Tie-lin LI[1], Xiao-song LI[1], Xiang-fu TAN[1]

1. College of Mechanical Engineering, Hunan Institute of Science and Technology, Yueyang 414000, China;
2. State Key Laboratory of Powder Metallurgy, Central South University, Changsha 410083, China

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**Abstract:** An artificial neural network (ANN) model was developed for simulating and predicting critical dimension $d_c$ of glass forming alloys. A group of Zr−Al−Ni−Cu and Cu−Zr−Ti−Ni bulk metallic glasses were designed based on the $d_c$ and their $d_c$ values were predicted by the ANN model. Zr−Al−Ni−Cu and Cu−Zr−Ti−Ni bulk metallic glasses were prepared by injecting into copper mold. The amorphous structures and the determination of the $d_c$ of as-cast alloys were ascertained using X-ray diffraction. The results show that the predicted $d_c$ values of glass forming alloys are in agreement with the corresponding experimental values. Thus the developed ANN model is reliable and adequate for designing the composition and predicting the $d_c$ of glass forming alloy.
**Key words:** critical dimension; glass forming alloy; artificial neural network; metallic glasses

## 1 Introduction

Metallic glasses have drawn a lot of interests because of their superior physical, mechanical and chemical properties compared with the corresponding crystalline counterparts [1,2]. In particular, the development of bulk metallic glasses (BMGs) widens their applications and extensively triggers the investigation of glass forming ability (GFA) of alloys.

There are many methods for estimating the GFA of glass forming alloys. One includes empirical rule proposed by INOUE and ZHANG [3] and the electron concentration rule proposed by CHEN et al [4]. These rules can not quantitatively estimate the GFA of the alloys and even there are opposite cases [5]. The second method is the characterization parameters, such as $K_{gl}$ [6], $\Delta T_x$ [7], $T_{rg}$ [8,9], $\gamma$ [7, 9], $\gamma^*$ [10] and $v$ [11]. These parameters can be obtained after the amorphous alloy has been prepared and/or even there are opposite cases [12]. The third method is the mathematical and/or physical equation [9,13−16]. For example, INOUE et al [15] provided an equation for the estimation of critical cooling rate $R_c$. LU and LIU [9,16] proposed some empirical relationships for the prediction of the $R_c$. However, the equation includes some parameters which are difficult to obtain and/or their reliability depends on the number of the data. CAI et al [17,18] tried to relate the $R_c$ with the physical and/or chemical parameters. Although better results were obtained and these parameters were also easily calculated, these relationships can not characterize in the commonality. Finally, researchers proposed some models from the thermal, topological and physical points of view. For example, the composition located at deep eutectic point was designed by thermodynamics [19]. It is clear that its result would deviate from the practical case because the formation of the metallic glass is a non-equilibrium solidification procedure. From the topological structure, it was found that the atomic size ratio [20], the average electronegativity difference [21], and the local packing efficiency [22] were strongly related with the GFA of alloys. However, these parameters are difficult to be calculated for the multi-component alloy. PANG et al [23] have recently designed the composition of Ni−Hf amorphous alloys based on the cluster whose type and magnitude are difficult to be defined. GUO and LIU [24], and CAI et al [25] have recently estimated the $R_c$ for the

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**Corresponding author:** An-hui CAI; Tel: +86-730-8648848; E-mail: cah1970@sohu.com
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formation of amorphous alloys from the $d_c$ from the thermodynamic point of view. However, the thermodynamic model contains many parameters which are difficult to be measured and depend on the temperature. Among above mentioned parameters, the $d_c$ can be directly used to evaluate the GFA of glass forming alloys. However, the $d_c$ of the glass forming alloy can be obtained through a large number of the experiments and depends on the experimental condition. Can it be quickly and reliably estimated ahead of the experiments?

It is well known that the $d_c$ is influenced by physical and chemical factors. The relationships between the $d_c$ and these factors are very complex, resulting in the difficult description of the relationships by a mathematical and/or physical model. Artificial neural network (ANN) technique is thought to be a reliable method for the resolution of the complex system and has been effectively used for the composition design, technology optimization, and performance prediction [26−33] due to its perfect performance, such as self-organization, self-adaption, strong learning and anti-interference capacity. Moreover, the ANN technique has been used to predict parameters for the metallic glasses and reliable results are obtained. For example, KEONG et al [34] established an ANN model for reliably predicting the crystallization temperatures of the Ni−P based metallic glasses. CAI et al [35−37] established ANN models for predicting $T_{rg}$, $\Delta T_x$ and $R_c$ of glass forming alloy, respectively. But there are no reports for the prediction of the $d_c$ of glass forming alloy by ANN technique.

In the present work, a computer model based on radial basis function artificial neural network (RBFANN) is designed for prediction and simulation of the $d_c$ of metallic glass. In addition, a group of Zr−Al−Ni−Cu bulk metallic glasses are designed and their $d_c$ values are predicted by the RBFANN model. It is found that the predicted $d_c$ values are in good agreement with the corresponding experimental values.

## 2 Experimental

Zr−Al−Cu−Ni and Cu−Zr−Ti−Ni shown in Tables 1 and 2 alloys with nominal compositions (mole fraction, %) were pre-alloyed more than five times by arc melting pure metal elements in a Ti-gettered argon atmosphere. These master ingots then were surface-polished, followed by induction-melting inside quartz tubes in argon atmosphere, then injected into copper mold to obtain $d$1−10 mm conical samples. The amorphous structures and the determination of the $d_c$ of as-cast alloys were ascertained using X-ray diffraction (XRD) with a XD-3A diffractometer with Cu $K_\alpha$.

**Table 1** Predicted and tested $d_c$ values for Zr−Al−Ni−Cu bulk metallic glasses developed in this work

| Bulk metallic glass | $d_c$/mm | | Error/% |
|---|---|---|---|
| | Tested | Predicted | |
| $Zr_{54}Al_{13}Cu_{18}Ni_{15}$ | 6.5 | 6.6 | 1.5 |
| $Zr_{60.5}Al_{12.1}Cu_{10.95}Ni_{16.45}$ | 7.5 | 8.0 | 6.7 |
| $Zr_{61.5}Al_{10.7}Cu_{13.65}Ni_{14.15}$ | 5.5 | 5.8 | 5.5 |
| $Zr_{62}Al_{10}Cu_{15}Ni_{13}$ | 5.0 | 5.2 | 4.0 |
| $Zr_{62.5}Al_{12.1}Cu_{7.95}Ni_{17.45}$ | 7.5 | 8.1 | 8.0 |
| $Zr_{63.5}Al_{10.7}Cu_{10.7}Ni_{15.1}$ | 6.0 | 6.5 | 8.3 |
| $Zr_{64}Al_{10.1}Cu_{11.7}Ni_{14.2}$ | 5.0 | 5.2 | 4.0 |
| $Zr_{65}Al_{8.7}Cu_{14.4}Ni_{11.9}$ | 4.0 | 4.5 | 12.5 |

**Table 2** Predicted and tested $d_c$ values for Cu−Zr−Ti−Ni bulk metallic glasses developed in this work

| Bulk metallic glass | $d_c$/mm | | Error/% |
|---|---|---|---|
| | Tested | Predicted | |
| $Cu_{50}Zr_{40}Ti_{10}$ | 2.0 | 2.3 | 15.0 |
| $Cu_{50}Zr_{40}Ti_{9.5}Ni_{0.5}$ | 3.0 | 3.2 | 6.7 |
| $Cu_{50}Zr_{40}Ti_{9}Ni_{1}$ | 4.0 | 3.8 | 5.0 |
| $Cu_{50}Zr_{40}Ti_{8}Ni_{2}$ | 5.0 | 5.2 | 4.0 |
| $Cu_{50}Zr_{40}Ti_{7}Ni_{3}$ | 3.0 | 2.8 | 6.7 |
| $Cu_{50}Zr_{40}Ti_{6}Ni_{4}$ | 2.0 | 1.8 | 10 |

## 3 ANN model

Back-propagation artificial neural network (BPANN) and radial basis function artificial neural network RBFANN are thought to be general methods for simulation and prediction modeling. The BPANN has stronger generalization capacity, but it has some shortcomings. It is difficult to determine learning rate, initial weight, objective error, and the numbers of hidden layers and of neurons in hidden layer. Moreover, it would result in the decrease of convergent rate and even be trapped in a local minimum if these parameters can not be suitably and coordinately selected. Nevertheless, the RBFANN has some merits, such as only one adjusted parameter, rapid training procedure and zero error [26−29,35−37]. In addition, the RBFANN is advantageous of the BPANN for better approximating and sorting capacity, and quick learning rate. The base functions among the nodes of the hidden layers for the RBFANN characterize in locality, indicating that the RBFANN is suitable for solving the complex, nonlinear, and local problems. Thus, MATLAB 7.0 package (Neural Network Toolbox from The Math Works Inc.) was used to create the RBFANN model in the present work. The modeling procedures are as follows. Firstly, the data is collected, analyzed and pre-processed. Then the pre-processed data are divided into two kinds of data,