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PREDICTION OF HARDNESS AND ELECTRICAL PROPERTIES IN ZRB_2 PARTICLE REINFORCED METAL MATRIX COMPOSITES USING ARTIFICIAL NEURAL NETWORK

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Abstract

In the present study, the hardness and electrical properties of copper based composite prepared by hot pressing of mechanically alloyed powders were predicted using Artificial Neural Network (ANN) approach. Milling time (t, h), particles size of mechanically alloyed powders (d, nm), dislocation density (ρ, m^{-2}) and compressive yield stress ($\sigma_{0.2}$, MPa) were used as inputs. The ANN model was developed using general regression neural network (GRNN) architecture. Cu-based composites reinforced with micro and nano ZrB_2 particles were consolidated via powder metallurgy processing by combining mechanical alloying and hot pressing. Analysis of the obtained results concerning hardness and electrical properties of the Cu-7 vol.% ZrB_2 alloy showed that the distribution of micro and nano ZrB_2 particles and the presence of agglomerates in the Cu matrix directly depend on the milling time. Also, the results show a strong influence of the milling time on hardness and electrical properties of Cu-7 vol.% ZrB_2 alloy. Addition of ZrB_2 particles decreases electrical conductivity of copper, but despite this fact Cu-7 vol.% ZrB_2 alloy can be marked as highly conductive alloy (samples made of mechanically alloyed powders milled longer than 20 h). Experimental results of the samples have shown a consistency with the predicted results of ANN.

Keywords: mechanical alloying, hot pressing process, Cu-ZrB$_2$ alloy, mechanical properties, Artificial Neural Network

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Introduction

Materials with improved mechanical and physical properties are being increasingly used in metal industry. Powder metallurgy enables the production of materials by combining different types of constituents providing the necessary and desired properties. These properties are a result of very fine and uniform microstructure with minimum segregation which cannot be obtained by ingot metallurgical techniques. Metal matrix composite materials with good combination of mechanical and physical properties enable a wide application in aerospace, automotive, military, electrical and nuclear industry [1-5].

Copper matrix composites reinforced with ceramic particles (in this study ZrB_2 particles were used) show improved mechanical and physical properties, such as hardness and strength, high electrical and thermal conductivity, wear and spark resistance [6,7]. During mechanical alloying (MA) particles of Zr and B were mechanically activated which enabled *in situ* forming of ZrB_2 in copper matrix in the course of hot pressing process [8]. Good distribution of ZrB_2 particles in the copper matrix has strong influence on mechanical and physical properties. Reinforcing ZrB_2 particles act as nucleation sites during solidification which leads to increasing dislocation density and decreasing grain size [9]. Therefore, the ZrB_2 particles have higher hardness relative to the copper matrix and tolerate higher loads, consequently the local strain of the copper matrix is lower than the applied, which increases the strength of composite.

Application of artificial neural networks (ANNs) is a newer approach for studying and predicting the properties and behavior of different types of materials. Many studies have been published about predicting one or more properties of metal matrix composites [10-12]. ANNs are biologically inspired systems for data processing, which produce good results in modeling systems with very complex physical processes. An ANN is usually defined as a structure composed of a large number of simple processors (neurons) that are massively interconnected, operate in parallel, and learn from experience (examples) [13]. Hence, most ANNs have some kind of rules for training, thus the coefficients of connections between neurons have being adjusted towards the input data. Summation of the input neuron values multiplied by the corresponding weight coefficients is passed through an activation function which gives output neuron value. Depending upon the number of layers, artificial neural networks can be classified as single or multiple layered. The general regression neural network (GRNN) estimates values for continuous dependent variables through the use of nonparametric estimators of probability density functions [13]. Connecting neurons in a multiple layer network enables processing of very complex (nonlinear) functions, due to the nonlinear activation functions in the hidden layers. Architecture of ANN is determined by the number of neurons, number of neuronal layers and specific arrangement and connectivity of neurons within the network.

In the present study, an attempt has been made to develop a model based on artificial neural network to predict hardness and electrical conductivity of Cu–7 vol.% ZrB_2 composites.

Experimental

Materials

Powder mixture of copper (94.78 wt.%), zirconium (4.1 wt. %) and boron (1.12 wt. %) was used as a starting material. Mechanical alloying of powder mixture was carried out at various times – from 5 up to 30 hours and samples were taken on every five hours. All the specimens of mechanically alloyed powders were hot pressed up to nearly theoretical density, in argon atmosphere, at the temperature of 950˚C, with retention time 2.5 hours and pressure of 35 MPa.

Methods

Nadaraya-Watson kernel regression algorithm was used for modeling and prediction of results with GRNN [14]. As input parameters, mechanical alloying time (t, h), particle sizes (d, nm), dislocation density (ρ, m^{-2}) and yield stress ($\sigma_{0.2}$, MPa) were used, while hardness and electrical conductivity were outputs in GRNN model whose architecture (4/28/3/2) is presented in Fig. 1 [14]. An exponential function has been used as the activation function:

$$f\left(D_j\right) = exp\left(\frac{-D_j}{2\sigma^2}\right) \tag{1}$$

where D_j is the distance of the training patterns in N-dimensional space (N is the number of inputs) and σ is so-called smoothing factor which represents the width of the calculated Gaussian curve for each probability density.

Mechanically alloyed powders and hot-pressed samples were characterized by X-ray diffraction (XRD)-Ultima IV Rigaku, with CuKα Ni filtered radiation. Dislocation density was determined by mathematical analysis of the structural parameters obtained by XRD.

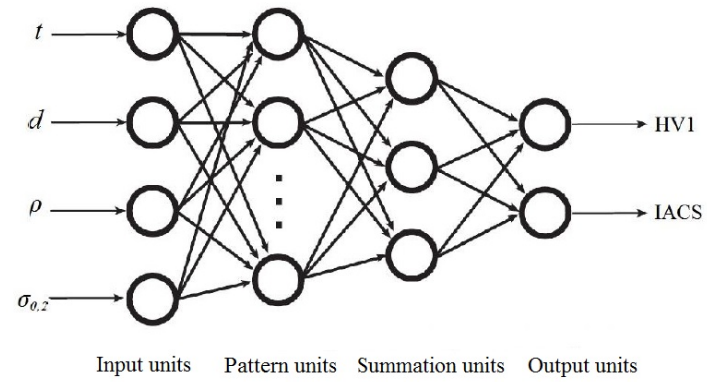

Fig. 1. Architecture of the GRNN model [14].

Application of a modified Williamson-Hall method, after calculation of the values D and ε, can be used for determine dislocation density (ρ_d) of the observed material by the equation [15]:

$$\beta\left(d^*\right) = \frac{1}{D} + \alpha\left(d^* C_{hkl}^{-\frac{1}{2}}\right) + O\left(d^{*2}\overline{C}_{hkl}\right) \tag{2}$$

The coefficient α is the mean square value of microstrain and is given by

$$\alpha = \left(\frac{\pi A^2 b^2}{2}\right)^{\frac{1}{2}} \rho^{\frac{1}{2}} \quad (3)$$

where

$$d^* = 2sin\theta / \lambda \quad (4)$$

Particle size distribution of MA powders was obtained with device Mastersizer 2000 which covers particle size range of 20 nm to 2 mm. The applied method was laser diffraction (LD), wherein the Fraunhofer scattering was used. The compressive test was carried out at room temperature using 1185 Instron-type testing machine on cylindrical samples with the length/diameter ratio of 2, at a strain rate of 1 mm per minute. Vickers macrohardness was determined by using Buehler Hardness Tester under the load of 9.8 N. Electrical conductivity was tested on device Forester Sigma Test 2069, at a frequency of 120 kHz.

Results and discussion

One of the most important characteristics of copper alloys is their ability to excellently conduct heat and electricity. Adding alloying elements to copper matrix, in most cases, reduces the conductivity of copper, but on the other hand improves its mechanical properties. Previous studies have shown that the presence of ZrB_2 particles in copper matrix greatly affects the hardness, strength and electrical properties [16,17]. In the present paper, prediction of electrical conductivity and hardness of Cu-7 vol.% ZrB_2 was performed using a general regression neural network, since relatively small input dataset was available. Figure 2 shows the results of the GRNN model for predicting value of the electrical conductivity.

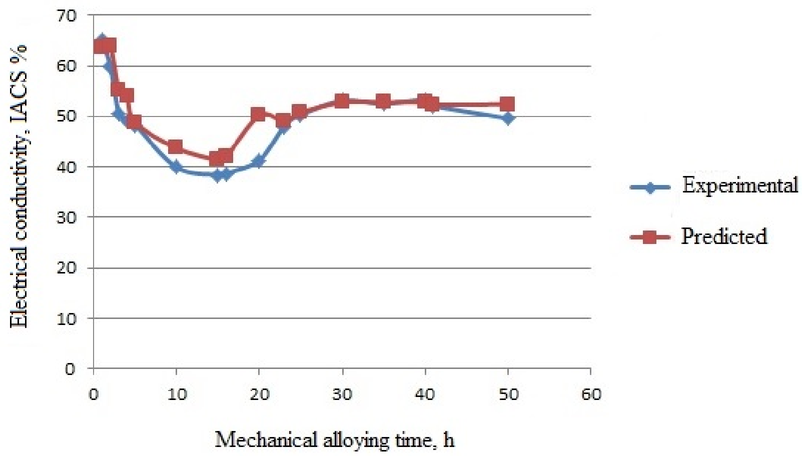

Fig. 2. The influence of milling time on electrical conductivity of Cu-7 vol.% ZrB_2 – experimental and model results.

The model curve exhibits good agreement with experimental results of the tested Cu-7 vol.% ZrB_2 composites. Curves in Fig. 2 show the influence of milling time on electrical conductivity of Cu-7 vol.% ZrB_2. It can be seen that the samples made of powders mechanically alloyed longer than 25 h have electrical conductivity above 50 IACS%, which puts them in a group of high conductive alloys. The presence of ZrB_2 particles in the metal matrix causes different types of defects in crystal structure of copper which enhance the effect of electron scattering and cause decreasing of the electrical conductivity. With higher dispersion of fine ZrB_2 particles in the metal matrix and with lower porosity, the formation of metallic clouds is easier and the conduction of electricity is better.

Strength and hardness of composites with copper matrix are dependent on the particle size and distribution of reinforcing ZrB_2 particles, presence of the agglomerates, pores and recrystallized grains. As the size and distribution of ZrB_2 particles in copper matrix depend on the time of mechanical alloying, it can be concluded that with longer time of mechanical alloying composites will have better mechanical properties. Also, with longer time of mechanical alloying powders become more rounded which leads to lower porosity of hot pressed samples. Figure 3 shows the predicted results of the hardness of compacts, and it may be noted that the model curve shows good matching with the curve of the experimental data.

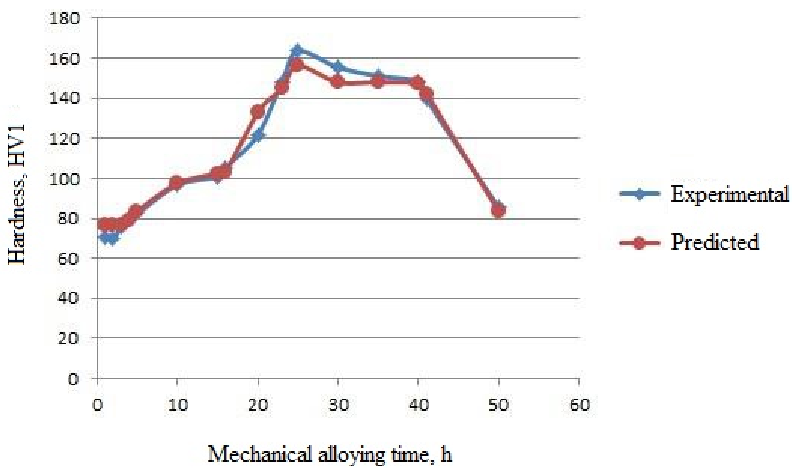

Fig. 3. The influence of milling time on the hardness of Cu-7 vol.% ZrB_2 – experimental and model results.

By comparing experimentally obtained results with the ones predicted by model it can be concluded that the use of GRNN model provides a valid prediction. Also, for more accurate network training, as well as for predictions concerning the impact of the composite composition to its mechanical and physical properties, much more input data is needed.

Conclusions

- Distribution and size of ZrB_2 particles in the copper matrix depend on the milling time and have strong influence on physical and mechanical properties of Cu-7vol.%ZrB_2 alloy.
- GRNN model can provide a valid prediction of mechanical and physical properties of composite materials.
- Experimental values of electrical conductivity and hardness of specimens have shown a consistency with predicted results.

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