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Application of the artificial neural networks for prediction of magnetic saturation of metallic amorphous alloys

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ABSTRACT

Purpose: The aim of the work is to employ the artificial neural networks for prediction of magnetic saturation of the amorphous alloys with the iron and cobalt matrix.

Design/methodology/approach: It has been assumed that the artificial neural networks can be used to assign the relationship between the chemical compositions of amorphous alloys, temperature of heat treatment and magnetic saturation. In order to determine the relationship it has been necessary to work out a suitable calculation model. It has been proved that employment of genetic algorithm to selection of input neurons can be very useful tool to improve artificial neural network calculation results. The attempt to use the artificial neural networks for predicting the effect of the chemical composition and temperature of heat treatment on the magnetic saturation BS succeeded, as the level of the obtained results was acceptable.

Findings: Artificial neural networks, can be applied for predicting the effect of the chemical composition and temperature of heat treatment on the magnetic saturation.

Research limitations/implications: Worked out model should be used for prediction of magnetic saturation only in particular groups of amorphous alloys, mostly because of the discontinuous character of input data.

Practical implications: The results of research make it possible to calculate with a certain admissible error the magnetic saturation Bs value basing on combinations of concentrations of the particular elements and heat treatment temperature.

Originality/value: In this paper it has been presented an original trial of prediction of the required magnetic properties of the iron and cobalt amorphous alloys.

Keywords: Computational material science; Artificial neural networks; Amorphous materials

METHODOLOGY OF RESEARCH, ANALYSIS AND MODELLING

1. Introduction

Magnetic materials are classified according to their magnetic susceptibility that is capability of a substance to change its magnetization under the influence of the external magnetic field, as soft magnetic, which are characteristic of a narrow hysteresis loop, high magnetic saturation even at the inconsiderable magnetic field intensity and high initial permeability, and as hard ones, characteristic of a broad hysteresis loop, high residual magnetism and coercion, which results in their capability to permanent magnetization [1].

Discovery of the soft magnetic materials with the amorphous structure that turned out to be a foretoken of the even more modern nanocrystalline materials was the hope to reduce enormous losses connected with magnetostriction effect [2, 3]

Amorphous materials called more often the metallic glasses, characteristic of the nonexistense of the structural order of further range, are fabricated using the "melt spinning" method. This method consists in the immediate directing of the stable molten metal stream onto the external surface of the spinning metal drum with the horizontal axis and a few to several dozen centimetres wide. An alloy characteristic of its propensity to vitrification, composed most often from the transition metal (Fe, Co, Ni) and metalloid (B, C, P, Nb, Si), spills on the drum surface and solidifies as a strip at the rate of 10^5 - 10^6 K/s [4, 5].

Yoshizawa with associates from the Japan Hitachi Metals concern proved in 1988 that the magnetic metallic glasses may be used as a parent substance for the nanocrystalline magnetics. They were fabricated during the heat treatment to which the FeSiB metallic glass strip was subjected with additives of Cu and Ni making it easier to obtain the very fine nanocrystalline structure. The fine-crystalline particles with the nanometric sizes nucleate in the amorphous material at the suitable heat treatment conditions, depending mostly on time and temperature. These particles, along with the amorphous structure that is not subject to crystallization form the structure which is very advantageous from the soft magnetic materials point of view [6, 7].

The metal amorphous materials and the nanocrystalline materials fabricated from them by heat treatment are used mostly in the electronic and electrical industries. The amorphous and nanocrystalline soft magnetic materials are characteristic of the high permeability connected with the high saturation magnetic induction beyond the conventional materials limit. Therefore, they are used as material for the transformers cores design. In addition, the nanocrystalline materials demonstrate low magnetic losses, low magnetostriction and provide the possibility to control the hysteresis (B-H) loop width; therefore, they are the right material for the converter transformers, reactors, noise filters, pulse transformers, current transformers, magnetic switching devices, high frequency magnetic amplifiers, magnetic measurement sensors, recording heads, sensors, flexible screens, etc. [8-11].

Relationships between the chemical composition and heat treatment parameters, and magnetic properties, feature the key information in optimisation of the manufacturing process and chemical composition in a strive to obtain the desired properties for any commercial applications.

Partial analysis carried out using approximation made it possible to evaluate approximately the effect of the annealing temperature on the magnetic properties of the amorphous strips. Regrettably, due to the not that representative nature of the analyzed data, only alloys with the same or very close chemical composition may be subjected to an attempt to evaluate the sought values [12].

Employment of the artificial neural networks for prediction of the effect of the chemical composition and also heat treatment conditions on the magnetic properties of the amorphous strips features the alternative for the classical investigation methods and makes it possible to predict the magnetic properties. The goal of this work was an attempt to develop the artificial neural network model for predicting the properties of the magnetic amorphous alloys in the form of thin strips, based on their chemical composition and heat treatment parameters. It has been proved in many papers that artificial neural networks have great potential in prediction and modeling properties of different kinds of materials [13-15].

2. Material and experimental methodology

The data set was developed basing on literature data including chemical compositions, heat treatment parameters and magnetic properties of the amorphous alloys of the relevant set of the representative experimental data.

The MLP 25-6-1 network type was proposed characteristic on the average absolute error at the level of 0.093, average quotient deviation of 0.377, and the average correlation coefficient of 0.931, one should state that employing the artificial neural networks makes it possible – based on the data set encompassing the chemical composition and heat treatment parameters – to calculate with a certain admissible error the magnetic saturation B_s value [16]. Correctness of the obtained results is dependant to a great extent on the correct preparation of the representative experimental data set, on applying some simplifications, and even neglecting some data.

Limiting of the input data to alloys subjected to heat treatment for 60 minutes was proposed to improve the neural network quality, moreover, the number of input neurons was reduced also using the genetic algorithm. The genetic algorithm used in this case is the optimisation strategy which can carry out effective search in binary strings. These binary strings represent the so called masks in case of optimisation of the input data set for the neural network. Genetic algorithm generates randomly a population of such strings and carries out next the process analogous to the natural selection taking place in nature during evolution. The goal of this modelling is selection of the better strings (masks culling the input data) which correspond to the networks performing best. Each mask determines, based on the specified parameters, which input variables should be used in the neural network design, and which should be omitted.

Parameters of the genetic algorithm (presented in Table 1) used, like sampling, population size, unit penalty, mutation coefficient, number of generations, smoothing coefficient, and the cross-breeding coefficient were selected taking the effect of these quantities into account on the designed network quality assessment coefficients' values.

3. Calculation of magnetic saturation

The artificial neural networks implemented in StatSoft Statistica Neural Network PL 4.0 F were used to determine the relationship between the chemical compositions of alloys and heat treatment parameters. Initially in the structure of the analyzed networks 25 input neurons were established, 23 out of which referred to the alloying elements occurring in the investigated alloys, like: Fe, Co, Al, Au, B, C, Cr, Cu, Ga, Ge, Hf, Mn, Mo, Nb, Ni, P, Pd, Pt, Si, Ta, Ti, V, Zr, and two referring to the heat treatment parameters: annealing temperature and time. As a result of using genetic algorithm, data set was limited to 15 input neurons referring to selected elements and annealing temperature. The ranges of atomic concentrations of elements and heat treatment parameters consisted in the isothermal annealing in the argon atmosphere are presented in Table 2.

The input data was divided into three sets: training (62 cases), validation (31 cases), testing (31 cases). The training set was used for development of the neural network model, the validating set was used for checking the model during

Table 1.

Sampling	Population size	Unitary penalty	Mutation coefficient	Number of generations	Smoothing coefficient	Cross-breeding coefficient
1	100	0	1	1000	0.5	1

Table2.

Ranges of atomic concentrations of elements of the analysed amorphous alloys

Danga	Mass fractions of elements, %							Annealing							
Kange -	Fe	Co	Al	В	Cu	Hf	Mo	Nb	Ni	Р	Si	Та	Ti	Zr	temperature [°C]
Min	0	0	0	0	0	0	0	0	0	0	0	0	0	0	100
Max	92	80	8	22	1	9.8	4	8	40	16	17	8	7	10	730

Table 3.

	Quality assessment coefficients of the MLP 15-5-1 neural netw	ork
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Assessment coefficient	Training	Validating	Testing
Average absolute error [T]	0.032	0.041	0.033
Quotient of standard deviations	0.134	0.153	0.146
Pearson correlation coefficient	0.991	0.988	0.989

establishing the values of weights, and the testing set was used for verifying the model when the network training was completed. Allocation of data to the particular subsets was done randomly. The following quantities determined for the testing set were used as the basic coefficients for evaluation of the neural network model performance: average network prediction error, standard deviation of the network prediction error, quotient of the standard deviations of the prediction errors and of the standard deviation of the resulting variable, Pearson correlation coefficient. For data analysis four neural networks models were used: multilayer perceptron MLP, linear neural networks, radial basis functions neural network RBF, generalized regression neural networks GRNN, also the following learning methods: back propagation method, conjugate gradient, quasi-Newton, fast propagation.

Selection of the number of hidden layers, number of nodes in these layers, values of weights, threshold values, training method and parameters, that is parameters of the architecture of the designed network was made taking into account effect of these quantities on values of the quality assessment coefficients of the designed network.

The analysis of the quality coefficients in the magnetic saturation calculated for training, validating, test and verifying sets has proven that smallest error occurs in the network with five neurons in the hidden layer. Figure 1 presents part of the analysis on example of average absolute error for different number of neurons in hidden layer. The approximate values of the mentioned coefficients for particular data sets indicate the ability of the network to generalize the knowledge acquired in the training process. The mean error value, ratio of standard deviations and the correlation coefficient for the magnetic saturation have been compared in Table 3 and Figure 2 presents analysis of the unit errors structure.

Selection of the optimum MLP 15-5-1 network was made based on this analysis; the network was trained with the error back propagation method for 446 epochs and using the conjugate gradients for 503 epochs, and again back propagation method for 300 epochs. The selected network is characteristic of the relatively lowest average absolute error and of the highest correlation coefficient, at the simultaneously low amplitude between the sets: training, validation, and the test one.





Fig. 1. Analysis of average absolute error for different number of neurons in hidden layer

Fig. 2. Analysis of the unit errors of MLP 15-5-1 network

The developed model of the artificial neural network was subjected to verification consisting in comparing the consistence of the magnetic saturation with the experimental results (Figure 3). Wrong mapping of



Fig. 3. Comparison of the experimental and calculated B_s values for MLP 15-5-1 network sets: training, validating, testing

the diagram for the calculated data compared with the experimental values will be the consequence of the incorrect determining of the sought magnetic saturation B_{s} .

4. Summary

The neural networks model developed from experimental data can be used to predict a value of magnetic saturation. The overall prediction error is about 3.5% for a predicted value of magnetic saturation as compared with the measured value of the thin films. A mathematical relationship between inputs and output of the proposed network model has been determined by neural network and sensitivity analysis. An analytical equation for the magnetic properties as depending on input parameters has been obtained and it is also comparable with the experimental data. However, worked out model should be used for prediction of magnetic saturation only in particular groups of amorphous alloys, mostly because of the discontinuous character of input data. It is necessary to considerable increase the training set for the further investigations.

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