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Application a neural networks in crystallization process of Mg-Al-Zn alloys

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ABSTRACT

Purpose: The purpose of this paper is presents a methodology to predict crystallization temperatures during solidify of metal obtained during crystallization process using an UMSA platform, based on cooling rate and chemical composition.

Design/methodology/approach: The experimental magnesium alloy used for training of neural network was prepared in cooperation with the Faculty of Metallurgy and Materials Engineering of the Technical University of Ostrava and the CKD Motory plant, Hradec Kralove in the Czech Republic. The alloy was cooled with three different cooling rates in UMSA Technology Platform. Temperatures were registered by supersensitive K-thermocouples.

Findings: Research limitations/implications: The results of this investigation show that there is a high correlation between experimental and predicted dates and the neural networks have a great potential in crystallization process behaviour modelling of Mg-Al-Zn alloys.

Practical implications: The presented model can be applied in computer system of Mg-Al-Zn casting alloys, selection and designing for Mg-Al-Zn casting parts and makes possibility to determine a crystallization temperatures based on chemical composition.

Originality/value: Original value of the work is applied the artificial intelligence as a tools for designing the required mechanical properties for Mg-Al-Zn castings.

Keywords: Numerical techniques; Neural networks; Mechanical properties; Magnesium alloys

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METHODS OF ANALYSIS AND MODELLING

1. Introduction

An Artificial Neural Network (ANN) is an information processing paradigm that is inspired by the way biological nervous systems, such as the brain, process information. The key element of this paradigm is the novel structure of the information processing system. It is composed of a large number of highly interconnected processing elements (neurones) working in unison to solve specific problems. ANNs, like people, learn by example. An ANN is configured for a specific application, such as pattern recognition or data classification, through a learning process. Learning in biological systems involves adjustments to the

synaptic connections that exist between the neurones. This is true of ANNs as well. Neural networks, with their remarkable ability to derive meaning from complicated or imprecise data, can be used to extract patterns and detect trends that are too complex to be noticed by either humans or other computer techniques. A trained neural network can be thought of as an "expert" in the category of information it has been given to analyse. This expert can then be used to provide projections given new situations of interest and answer "what if" questions [1-3].

Neural networks take a different approach to problem solving than that of conventional computers. Conventional computers use an algorithmic approach i.e. the computer follows a set of instructions in order to solve a problem. Unless the specific steps that the computer needs to follow are known the computer cannot solve the problem. That restricts the problem solving capability of conventional computers to problems that we already understand and know how to solve. But computers would be so much more useful if they could do things that we don't exactly know how to do. Neural networks process information in a similar way the human brain does. The network is composed of a large number of highly interconnected processing elements (neurones) working in parallel to solve a specific problem. Neural networks learn by example. They cannot be programmed to perform a specific task. The examples must be selected carefully otherwise useful time is wasted or even worse the network might be functioning incorrectly. The disadvantage is that because the network finds out how to solve the problem by itself, its operation can be unpredictable [4-8].

Magnesium is the lightest of the “practical metals”. It terms of density, it is no more than 1.8 grams per cubic centimetre, compared with iron at 7.9 grams and aluminium at 2.7 grams. It is an abundant resource: its concentration is seawater is 0.13 percent, placing it just behind sodium, and it`s contained in considerable deposits of such ores as dolomite and magnesite. Magnesium is highly recyclable, requiring just 5 percent of the energy needed for original use to remelt and reuse, so the environmental burden of recycling it is low.

Magnesium has many other benefits, showing almost no dimensional change due to variations in temperature or the passage of time and absorbing vibration, making it easy to process into components quietly and without leaving rough surface behind.

At the same time , though, refining crude magnesium ore is a rather costly process, and the metal has low strength and heat resistance and corrodes easily. For these reasons, it`s been largely overlooked. People have said that in terms of research it`s about 50 years behind other metals, including aluminium, whose production began at approximately the same time.

In the 1990s, however, China built many plants using the country`s coal resources to power the so-called Pidgeon process of magnesium refining. Once it became possible to purchase inexpensive Chinese magnesium, interest in the metal skyrocketed [9, 10].

The aviation and automotive industries in particular began working on developing new magnesium alloys. If magnesium is used for vehicle structures, they can be made lighter, resulting in enhanced fuel efficiency. This metal`s capacity for enabling reduced energy used makes it a key material for tackling the environmental problems of the twenty-first century. Companies around the world are working to develop new uses for magnesium alloys.

In 2002, for example, the German automarker Volkswagen announced the 1 Litre Car, its supereconomy concept car. The use of magnesium allowed the total car weight to be just 290 kilograms-less than a third of the weight of a traditional compact passenger for 100 kilometers on just 0.89 liters of fuel. In July 2004, the US Council for Automotive Research adopted Magnesium Vision 2020 to develop new magnesium alloys and increase usage in automobiles to 10 percent by weight by 2020 compared to just 0.9 percent as of 2009 [10, 11].

Prediction of mechanical properties of engineering alloys is important for scientists and engineers which can save not only cost but also time. However, due to the complex interconnections among chemical compositions and materials properties, conventional mathematical models are sometimes very complex to be handled by the numerical technologies. In recent years, neural network models have been widely used in different metallurgical operations. In the present work, an improved neural network model was developed to predict crystallization temperatures in the design and development of new types of magnesium alloys [12].

2. Database and the artificial neural network model (ANN model)

2.1. Material

The investigations have been carried out on Mg-Al-Zn experimental magnesium alloys as-cast in cooperation with the Faculty of Metallurgy and Materials Engineering of the Technological University of Ostrava and the CKD Motory plant, Hradec Kralove in the Czech Republic. The chemical composition of the investigated materials is given in Table 1. A casting cycle of alloys has been carried out in an induction crucible furnace using a protective salt bath Flux 12 equipped with two ceramic filters at the melting temperature of 750±10ºC, suitable for the manufactured material. In order to maintain metallurgical purity of the melting metal, refining by neutral gas with the industrial name of Emgesalem Flux 12 was carried out. To improve the quality of metal surface a protective layer Alkon M62 was applied. The material was cast in dies with betonite binder because of its excellent sorption properties and shaped into plates of 250x150x25 mm.

Table 1.
Average chemical composition (wt%) of the Mg-Al-Zn alloys

Al	Zn	Mn	Cu	Si	Fe
11.894	0.55	0.22	0.0064	0.05	0.02
9.399	0.84	0.24	0.0018	0.035	0.007
5.624	0.46	0.16	0.0024	0.034	0.07
2.706	0.21	0.1	0.0018	0.032	0.005

The experiments were performed using a pre-machined cylindrical test sample with a diameter of ∅=18 mm and length of l=20 mm taken from the ingot. In order to assure high repeatability and reproducibility of the thermal data, the test sample mass was 9.3 g within a very closely controlled range of ±0.1 g. Each sample had a predrilled hole to accommodate a supersensitive K type thermocouple (with extra low thermal time constants) positioned at the centre of the test sample (Fig. 1) to collect the thermal data and control the processing temperatures.

The thermal analysis during melting and solidification cycles was carried out using the Universal Metallurgical Simulator and Analyzer (UMSA) [13]. The melting and solidification experiments for magnesium alloys were carried out using Argon as cover gas. The data for Thermal Analysis (TA) was collected using a high-speed National Instruments data acquisition system linked to a personal computer. Each TA trial was repeated three times. Calculation method to determine a crystallization temperatures were described in publication [14-18].

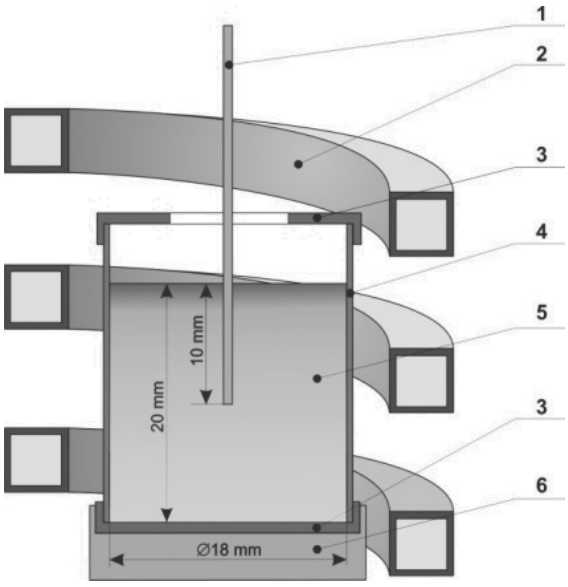

Fig. 1. Scheme of the UMSA Thermal Analysis Platform experimental set-up: 1 – low thermal mass thermocouple, 2 – heating and cooling coil, 3 – thermal insulation, 4 – steel foil, 5 – test sample, 6 – ceramic base

2.2. Data collection and database construction

The gathered set of data designed for formation of a numerical model determining: T_{DN}, T_G and T_{sol} in relation to the chemical composition and cooling rate were divided into two subsets: the learning set and the validation set. The data were divided in a proportion of 75% for the learning set and 25% for the validation set. 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-Newtona method,
- fast propagation.

2.3. Application of ANN for analyzing crystallization temperatures

ANN has two functions: learning and recalling [1-4]. It can learn from the past experience and provide new results, just like the neural networks of living creatures. In this study, the learning rule of ANN employed a back-propagation algorithm. Weight adjustment is important during the process of ANN learning. Equation 1 pertains to the equation for the purpose. After the active function is initiated, the adjusted weight converges, and the necessary result thus obtained [12]:

$$(W)_{new}=(W)_{old}+\Delta(W) \quad (1)$$

3. Results and discussions

Different pre-process parameters have important influences on the predicted results. The effort was made for improving pre-processes of the ANN model.

Data set was divided into three subsets: training, validating and testing ones. The data from the learning set has been used for the modification of the network weights, the data from the validating set, to evaluate the network during the learning process, while the remaining part of the values (the testing set) has been used for determining the network efficiency after ending completely the procedure of its creating.

The results used in the learning process and the network testing have been put to standardization. Scaling has been used in relation to the deviation from the minimal value, according to the mini-max function. The mini-max function transforms the variable domain to the range (0,1). The type of the network, the number of neurons in the hidden layer (layers), the method and learning parameters have been determined observing the influence of these quantities onto the assumed network quality coefficients.

The result of design and optimisation process is network, which is characterized by an error of value, standard deviation and Pearson's correlation coefficient. The quotient of standard deviations for errors and the data has been accepted, as the vital indicator of the model quality, made with the use of the neural network. The correctness of the network model may only be considered in case when the presented by networks forecasts are burdened with a smaller error than the simple estimation of the unknown output value.

Model of neural network was used to verify correctness of experimental crystallization temperatures including beginning of dendrite nucleation temperature T_{DN}, dendrite growth temperature T_G and solidus temperature T_{sol}. The feed forward neural networks have been applied for calculations – General Regression Neural Network (GRNN).

The number of nodes in input was defined as four, which correspond to cooling rate (0.6, 1.2 and 2.4°C/s) and alloy compositions, including the commonly used alloying elements in magnesium alloys, namely Al, Zn, Mn. Number of nodes in output layer was defined as three – dendrite nucleation temperature, dendrite growth temperature and solidus temperature (Fig. 2).

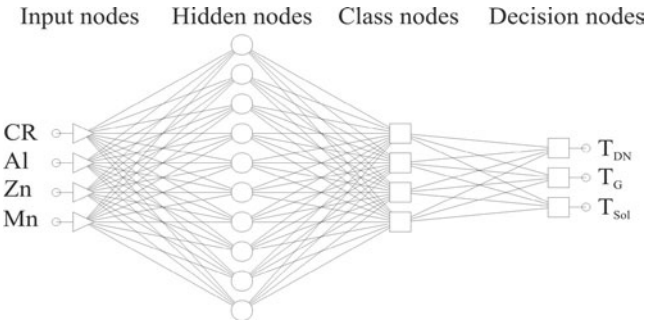

Fig. 2. Schematic diagram of the ANN model for prediction of properties of magnesium alloys

The number of hidden layers, number of nodes in these layers and the number of training epochs were determined by observing the neural forecast error for the training and validating sets. The neural network with two hidden layers and numbers of neurons in this layers as 10 and 4 were assumed to be optimal.

The standard deviation ratio calculated for the training set is: 0.16 for T_{DN}; 0.3 for T_G and 0.25 for T_{sol}. Table 2 shows the values of errors, standard deviation ratios and Pearson correlation coefficients (R) for the calculated values of crystallization temperatures.

Table 2.
Quality assessment coefficients for applied neural networks for calculate of chemical composition and mechanical properties for testing set

Mechanical properties	Average of tested population	Absolute mean error	Standard error deviation	Standard deviation quotient	Pearson correlation coefficient
T_{DN} [°C/s]	613.01	3.52	3.97	0.16	0.98
T_G [°C/s]	605.77	5.29	7.69	0.3	0.97
T_{SOL} [°C/s]	451.38	7.86	11.34	0.25	0.98

Figures 3-14 presents some research results by the ANN model as well as experimental work. It can be noticed that the predicted crystallization temperatures are consistent with the experimental data which reveal that the improved ANN model, can be used to develop new types of magnesium alloys and to optimise process parameters of magnesium alloys.

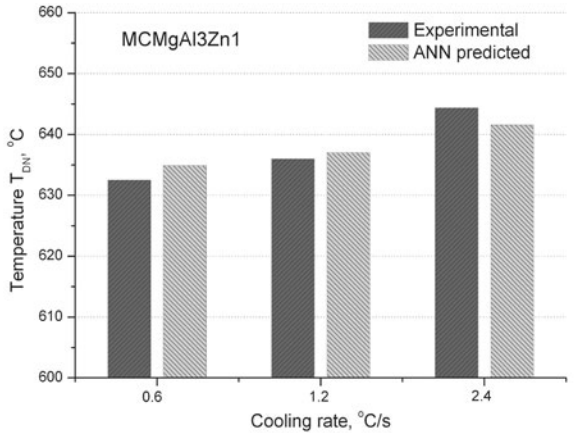

Fig. 3. The predicted and experimental values of the dendrite nucleation temperature MCMgAl3Zn1 alloy for different cooling rates

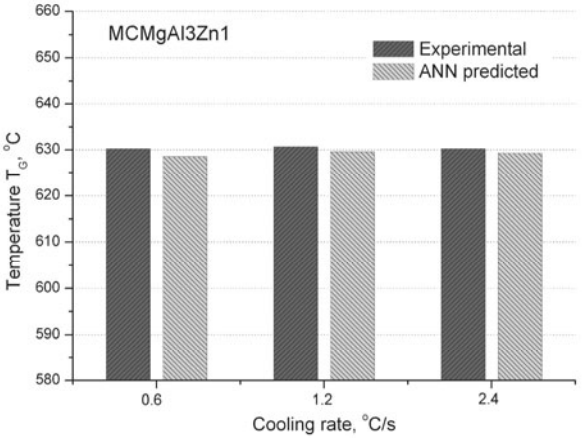

Fig. 4. The predicted and experimental values of the dendrite growth temperature of MCMgAl3Zn1 alloys for different cooling rates

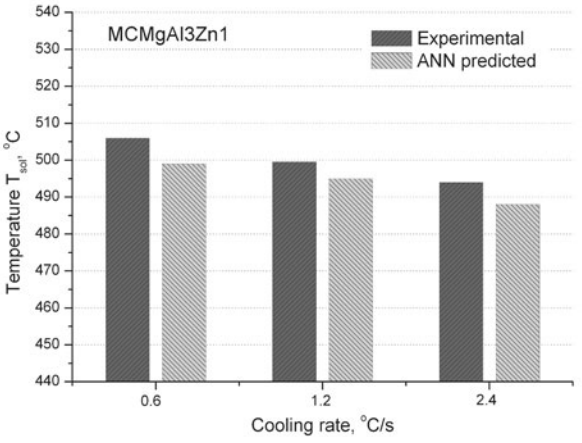

Fig. 5. The predicted and experimental values of the solidus temperature of MCMgAl3Zn1 alloys for different cooling rates

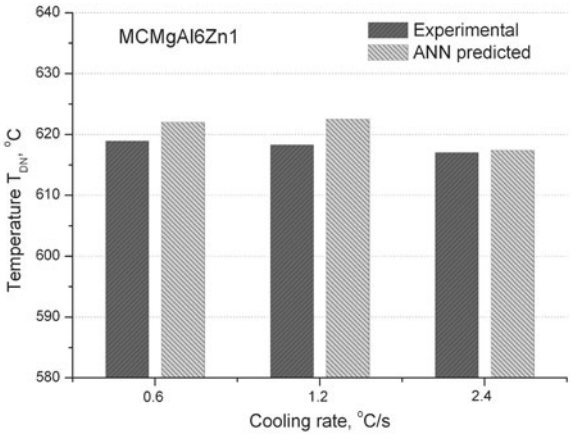

Fig. 6. The predicted and experimental values of the dendrite nucleation temperature MCMgAl6Zn1 alloy for different cooling rates

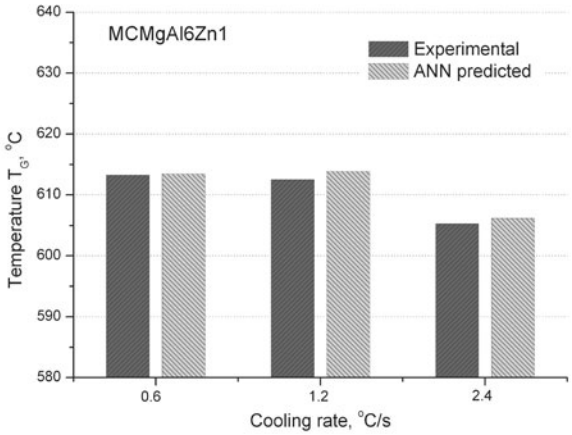

Fig. 7. The predicted and experimental values of the dendrite growth temperature of MCMgAl6Zn1 alloys for different cooling rates

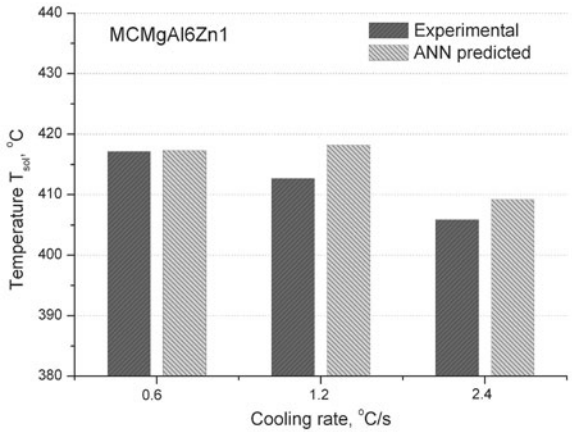

Fig. 8. The predicted and experimental values of the solidus temperature of MCMgAl6Zn1 alloys for different cooling rates

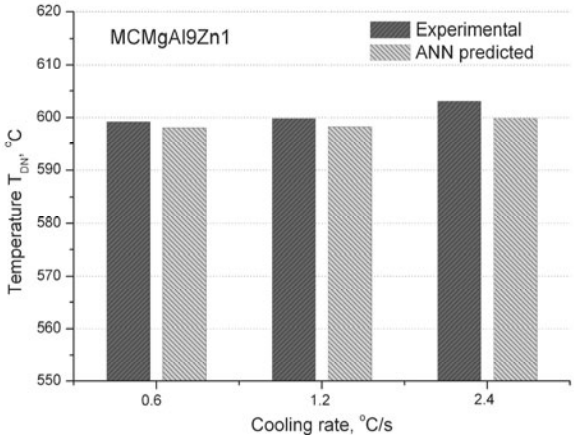

Fig. 9. The predicted and experimental values of the dendrite nucleation temperature MCMgAl9Zn1 alloy for different cooling rates

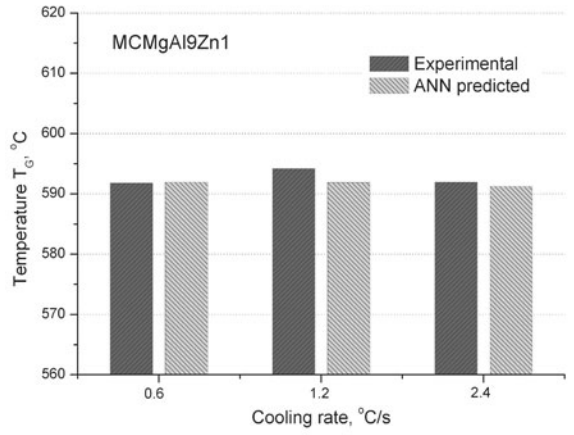

Fig. 10. The predicted and experimental values of the dendrite growth temperature of MCMgAl9Zn1 alloys for different cooling rates

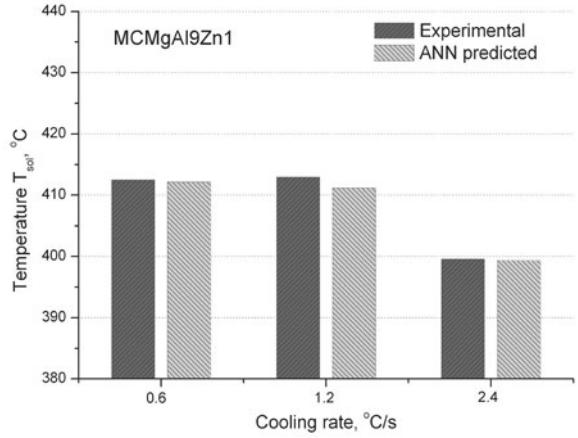

Fig. 11. The predicted and experimental values of the solidus temperature of MCMgAl9Zn1 alloys for different cooling rates

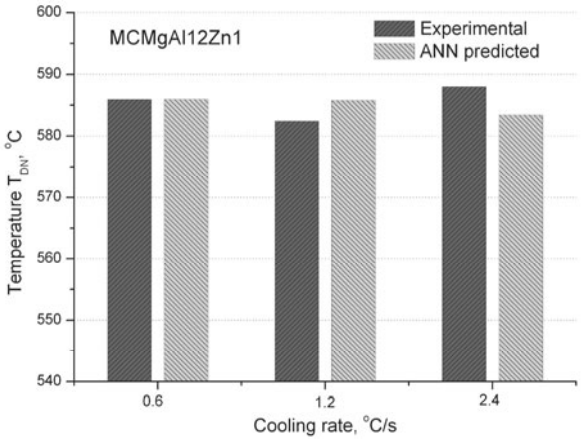

Fig. 12. The predicted and experimental values of the dendrite nucleation temperature MCMgAl12Zn1 alloy for different cooling rates

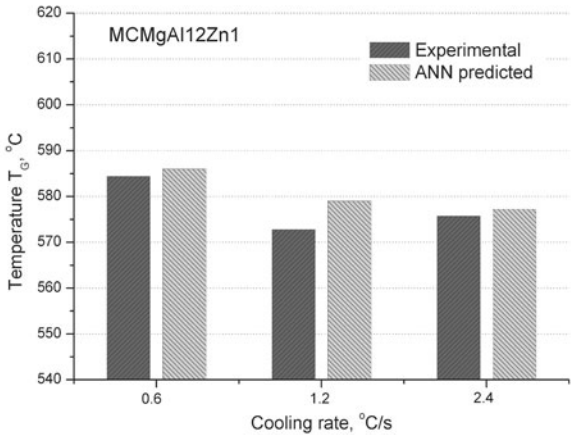

Fig. 13. The predicted and experimental values of the dendrite growth temperature of MCMgAl12Zn1 alloys for different cooling rates

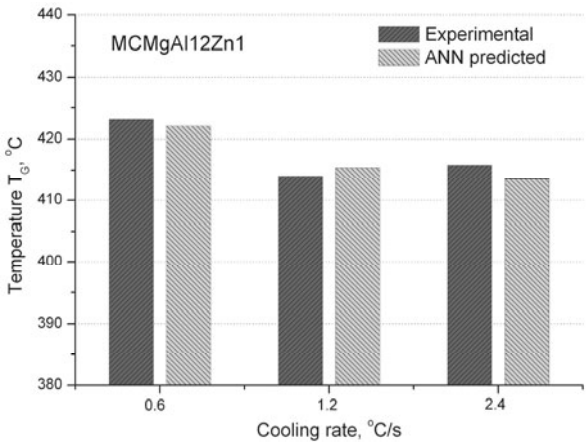

Fig. 14. The predicted and experimental values of the solidus temperature of MCMgAl12Zn1 alloys for different cooling rates

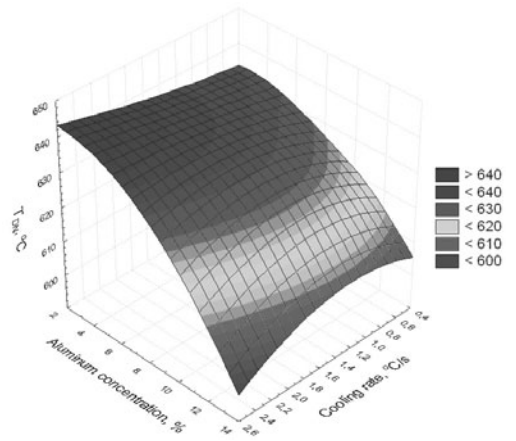

Fig. 15. Simulation of the cooling rate and aluminium concentration on beginnings of dendrite nucleation temperature

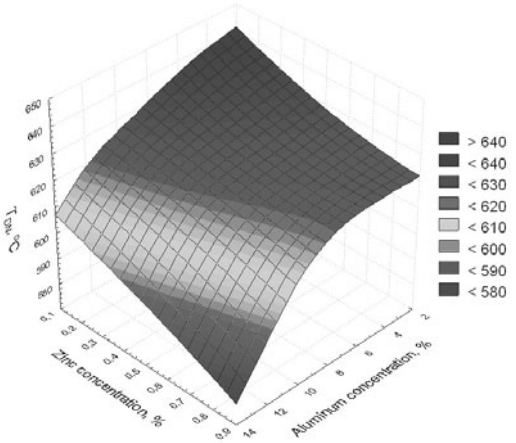

Fig. 16. Simulation of the aluminium and zinc concentration on beginnings of dendrite nucleation temperature

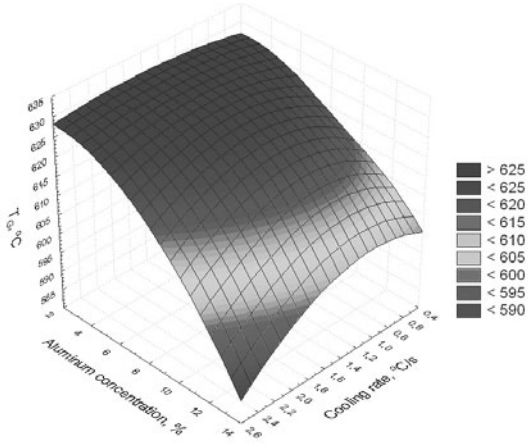

Fig. 17. Simulation of the cooling rate and aluminium concentration on dendrite growth temperature

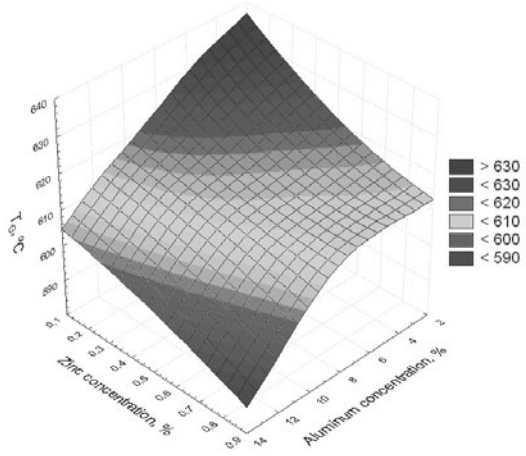

Fig. 18. Simulation of the aluminium and zinc concentration on dendrite growth temperature

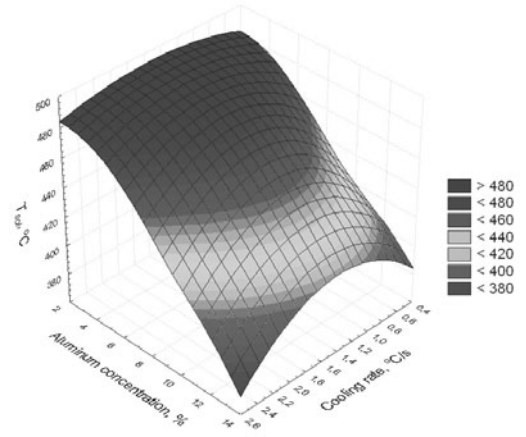

Fig. 19. Simulation of the cooling rate and aluminium concentration on solidus temperature

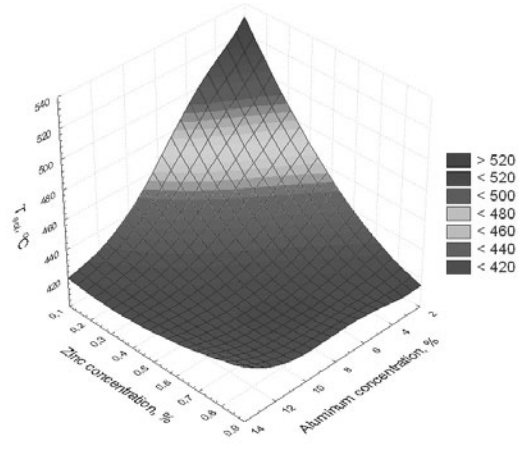

Fig. 20. Simulation of the aluminium and zinc concentration on dendrite growth temperature

On the basis of the worked out models of neural networks, the diagrams of the influence of the cooling rate and aluminium concentration, zinc and manganese concentration as well were done on the dendrite nucleation temperature, dendrite growth temperature and solidus temperature of the analyzed magnesium cast alloys (Figs. 15-20).

The presented, on the MCMgAl12Zn1, MCMgAl9Zn, MCMgAl6Zn, MCMgAl3Zn alloy example results, confirm the correlation between the results of the laboratory research of Mg alloys with the results obtained out of the neural networks.

4. Conclusions

The results can be summarized as follows:

1) The artificial neural network model (ANN model) for predicting crystallization temperatures of crystallisable magnesium alloy was improved by refining pre-processing variables and using a more reasonable structure of hidden layers;
2) The results show that the improved model could apparently decrease the prediction errors, and raise the accuracy of the prediction results;
3) The improved ANN model was used to predict the crystallization temperatures of Mg-Al-Zn alloys. The predicted results were found to be in good agreement with the experimental data.

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Additional information

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