



Neural network application for prediction mechanical properties of Mg-Al-Zn alloys

L.A. Dobrzański*, M. Król

Division of Material Processing Technology, Management and Computer Techniques in Materials Science, Institute of Engineering Materials and Biomaterials, Silesian University of Technology, ul. Konarskiego 18a, 44-100 Gliwice, Poland

* Corresponding author: E-mail address: leszek.dobrzanski@polsl.pl

Received in a revised form 23.09.2009

ABSTRACT

Purpose: The paper presents results of the research connected with the development of new approach based on the neural network to predict chemical composition and cooling rate for the mechanical properties of the Mg-Al-Zn cast alloys. The independent variables on the model are chemical composition of Mg-Al-Zn cast alloys and cooling rate. The dependent parameters are hardness, ultimate compressive strength and grain size.

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. Compression test were conducted at room temperature using a Zwick universal testing machine. Compression specimens were tested corresponding to each of three cooling rates. Rockwell F-scale hardness tests were carried out using a Zwick HR hardness testing machine.

Findings: The results of this investigation show that there is a good correlation between experimental and predicted dates and the neural network has a great potential in mechanical 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.

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

Reference to this paper should be given in the following way:

L.A. Dobrzański, M. Król, Neural network application for prediction mechanical properties of Mg-Al-Zn alloys, Archives of Computational Materials Science and Surface Engineering 2/4 (2010) 181-188.

ENGINEERING MATERIALS PROPERTIES

1. Introduction

A strong emphasis on environmental protection all over the world in recent years has led to an increasing interest in topics on low energy consumption and product recycling. Magnesium alloy has a density of 1.74 g/cm^3 , which is less

than the 2.7 g/cm^3 of aluminum alloy and other iron and steel materials. Magnesium metal for structural applications is processed into casting (die, sand, permanent mould and investment), extrusions, forgings, impact extrusions and flat rolled products. Castings far exceed cast and wrought products for reasons which will be discussed later and die castings account for 70% of the castings shipped; with demand for

automobile parts produced by this technology (about 85% of the die castings total) projected to reach greater than 100,000 metric tons worldwide by the turn of the century. Magnesium can be joined by riveting, or any commonly used welding methods. Magnesium can be machined faster and has the best strength-to-density ratio of any commonly used structural metals. Its use in a variety of applications, particularly in automobile components is expanding as knowledge on the interactions between forming processes, components design, component function/properties and cost increases. However, particularly for the new alloys this knowledge is as yet, incomplete. It provides the advantage of superior strength, resistance to electro-magnetic interference, fast heat conduction and shock absorption, among others. Moreover, the application of magnesium alloy products in the automobile industry will effectively improve the efficiency of fuel consumption. Many new types of magnesium alloys are being developed in the world in order to improve further the mechanical properties and processing performances of the magnesium alloys. However, conventional methods for developing new alloys need a lot of experimental work and take long time [1].

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. Efforts have been made to use this technique for predicting the hot extrusion processes of AZ31 and AZ61 magnesium alloys and for investigating the influence of Y and Zn additions on the mechanical properties of Mg-Zn-Zr-Y alloys [2-6]. However, significant prediction errors in some cases call for further improvement of the neural network model for more accurate predictions. In the present work, an improved neural network model was developed to predict mechanical properties and grain size in the design and development of new types of magnesium alloys [7].

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 Technical 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 $750 \pm 10^\circ\text{C}$, 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 250x150x25mm.

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 $\varnothing=18\text{mm}$ and length of $l=20\text{mm}$ taken from the ingot. In order to assure high repeatability and reproducibility of the thermal data, the test sample mass was 9.3g within a very closely controlled range of $\pm 0.1\text{g}$. 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.

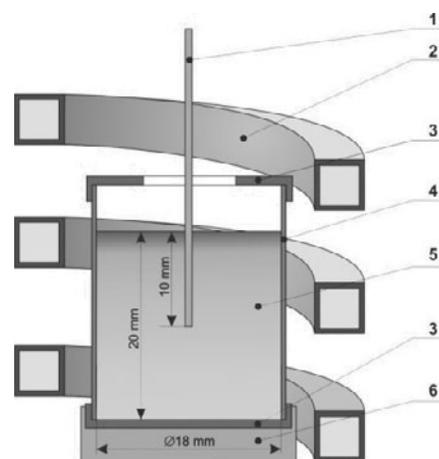


Fig. 1. Scheme of the UMSA Thermal Analysis Platform experimental set-up: 1 – low thermal mass thermocouple, 2 – heating and cooling coil, 3 – thermal insulation, 4 – steel foil, 5 – test sample, 6 – ceramic base

The thermal analysis during melting and solidification cycles was carried out using the Universal Metallurgical Simulator and Analyzer (UMSA) [16]. 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.

Samples for compression testing were machined from a centre of the thermal analyses specimen ingots. The machined samples

were polished with fine sandpaper to remove any machining marks from the surface. Compression tests were conducted at room temperature using a Zwick universal testing machine. Prior to testing, an extensometer was used to minimize frame bending strains. Compression specimens were tested corresponding to each of the three cooling rates.

Rockwell F-scale hardness tests were conducted at room temperature using a Zwick HR hardness testing machine.

2.2. Data collection and database construction

The performance of an ANN model depends upon the dataset used for its training. Therefore, for a reliable neural network model a significant amount of data as well as powerful computing resources are necessary. Amounts of data on mechanical properties of magnesium alloys at different conditions are currently available in the literature [8-10]. However, these data are rather disordered and confusing for the use of engineering practice. Moreover, in Mg-system, the experimental data in the literature are very sparse compared to Al-alloys and steels.

The gathered set of data designed for formation of a numerical model determining: UCS, HRF and GS 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.

2.3. Application of ANN for analyzing mechanical properties

ANN has two functions: learning and recalling [11-15]. 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 [4]:

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

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.

Model of neural network was used to verify correctness of experimental mechanical properties including Rockwell hardness in F scale, ultimate compressive strength (UCS, MPa) and metallographic characterisation (grain size, μm). The feed forward neural networks have been applied for calculations – Multi Layers were applied for calculations – Multi Layerceptron (MLP). The number of nodes in input was defined as eight, 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, Si, Cu, Fe and Mg.

Number of nodes in output layer was defined as three – hardness, ultimate compressive strength and grain size (Fig. 2). One-of-N conversion type was applied for nominal variable, and minimax conversion for other variables. One-of-N conversion type using neurons number answering one nominal variable is an equal number of values achieved by this variable. In order to represent selected variable, appropriate neuron is activated and the rest of them stays inactive.

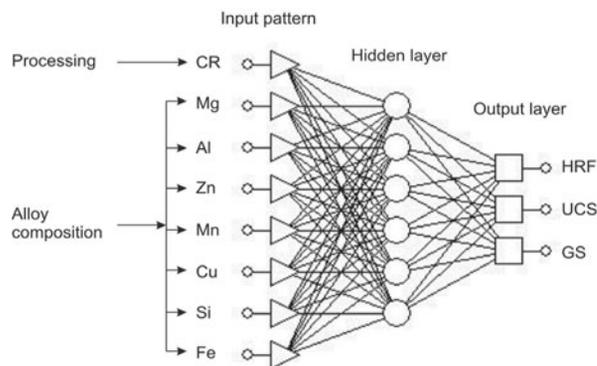


Fig. 2. Schematic diagram of the ANN model for prediction of properties of magnesium alloys.

Data set was divided into three subsets: training, validating and testing ones. 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 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. Neural network training was carried with errors back propagation method and conjugate gradient algorithm.

The neural network with one hidden layer and numbers of neurons in this layer as 6 was assumed to be optimal. The highest value of Pearson’s correlation coefficient and the lowest value of standard deviation were achieved for MLP neural network that was trained by error back propagation method in 50 epochs and conjugate gradient algorithm in 59 epochs.

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

Mechanical properties	Average of tested population	Absolute mean error	Standard error deviation	Standard deviation quotient	Pearson correlation coefficient
Hardness [HRF]	50.03	4.12	3.37	0.17	0.98
Ultimate compressive strength [MPa]	278.59	5.46	6.96	0.32	0.94
Grain size [μm]	118.36	6.43	7.59	1.85	0.91

The standard deviation ratio calculated for the training set is: 0.17 for hardness; 0.32 for ultimate compressive strength and 1.85 for grain size. Table 2 shows the values of errors, standard deviation ratios and Pearson correlation coefficients (R) for the calculated values of hardness ultimate compressive strength and grain size.

Figures 3-5 show the comparison of real hardness, ultimate compressive strength and grain size with data calculated by neural network. It can be noticed that very good results can be obtained for the prediction of the ultimate compressive strength and hardness and acceptable results can be predicted for the grain size.

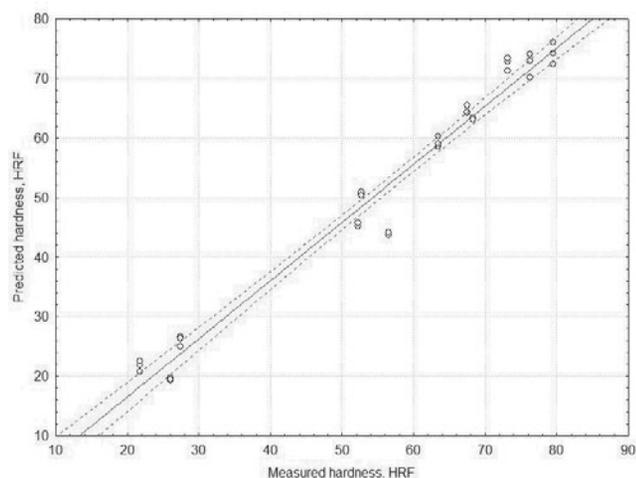


Fig. 3. Predicted hardness (HRF) for magnesium alloys by the ANN model with different processing parameter values vs. experimental data

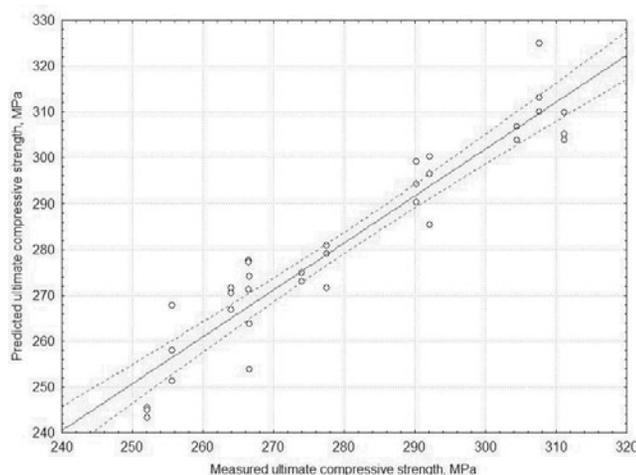


Fig. 4. Predicted ultimate compressive strength [MPa] for magnesium alloys by the ANN model with different processing parameter values vs. experimental data

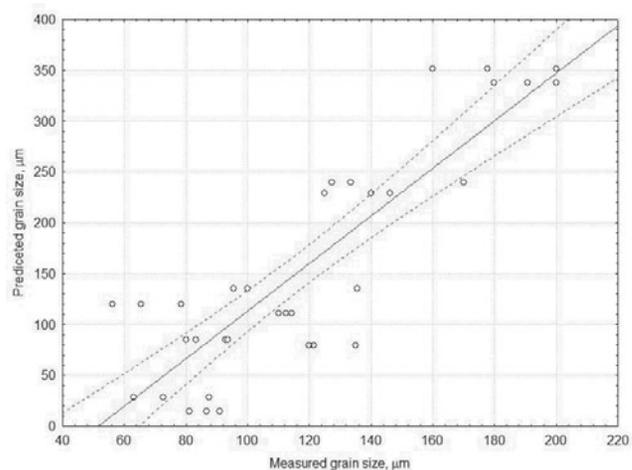


Fig. 5. Predicted grain size [μm] for magnesium alloys by the ANN model with different processing parameter values vs. experimental data

Figures 6 and 13 are some research results by the ANN model as well as experimental work.

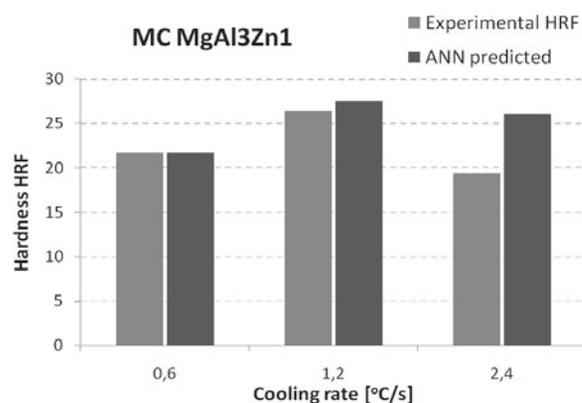


Fig. 6. The predicted and experimental values of the hardness of MC MgAl₃Zn₁ alloys for different cooling rates

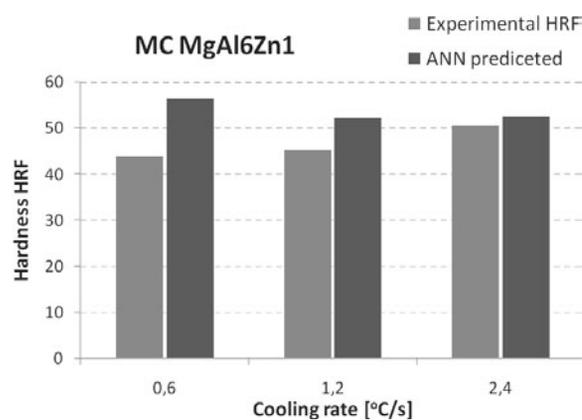


Fig. 7. The predicted and experimental values of the hardness of MC MgAl₆Zn₁ alloys for different cooling rates

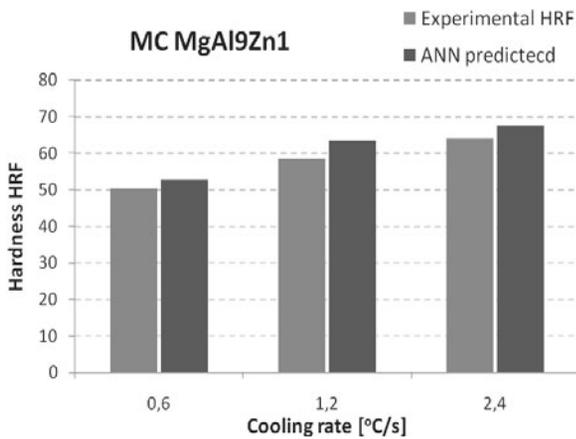


Fig. 8. The predicted and experimental values of the hardness of MC MgAl9Zn1 alloys for different cooling rates

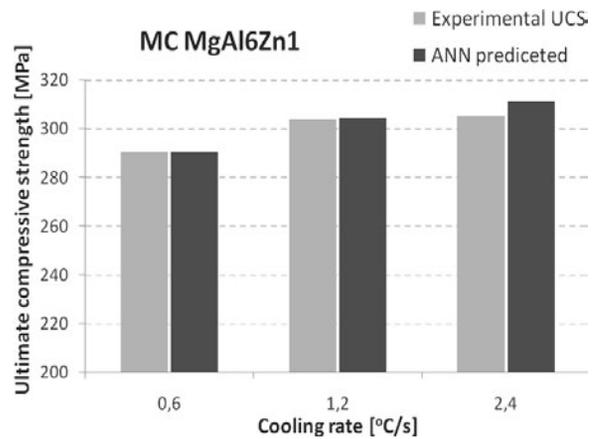


Fig. 11. The predicted and experimental values of the ultimate compressive strength of MC MgAl6Zn1 alloys for different cooling rates

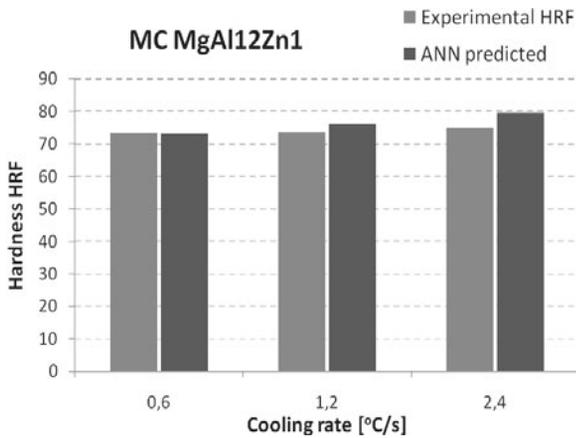


Fig. 9. The predicted and experimental values of the hardness of MC MgAl12Zn1 alloys for different cooling rates

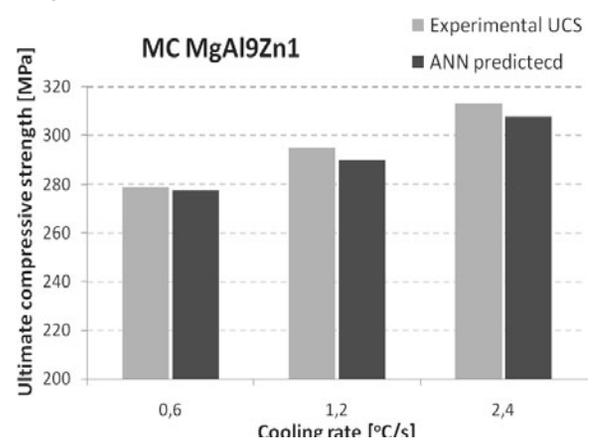


Fig. 12. The predicted and experimental values of the ultimate compressive strength of MC MgAl9Zn1 alloys for different cooling rates

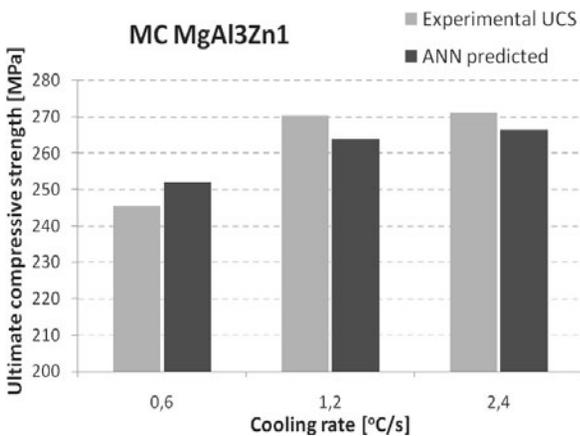


Fig. 10. The predicted and experimental values of the ultimate compressive strength of MC MgAl3Zn1 alloys for different cooling rates

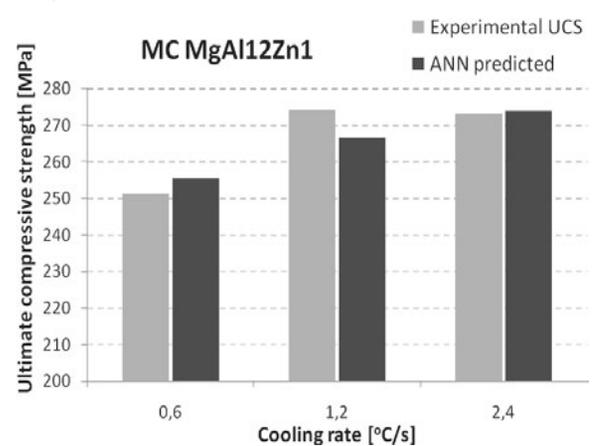


Fig. 13. The predicted and experimental values of the ultimate compressive strength of MC MgAl12Zn1 alloys for different cooling rates

It can be noticed from Figures 6-13 that the predicted mechanical properties and grain size 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.

Mechanical properties of the magnesium alloys are strongly depended on cooling rate and aluminum content (Fig 14), the hardness grows with increment of aluminum content and slightly with increment of cooling rate. In the opposite way it is with ultimate compressive strength. UCS grows with increment of cooling rate and slightly with increment of aluminum content (Fig 15). Measuring errors occurred during testing did not exceed 5%.

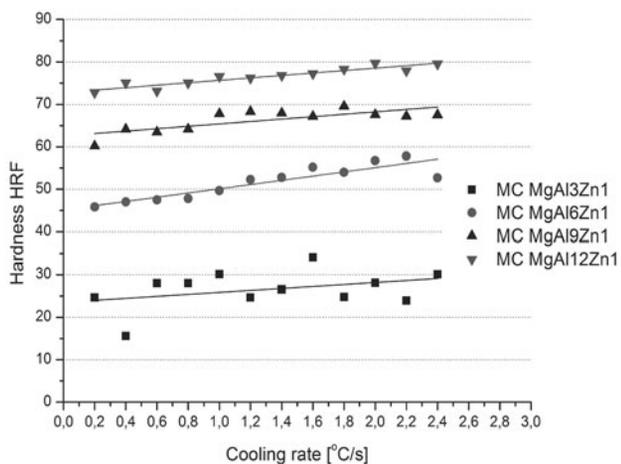


Fig. 14. Influence of cooling rate on the hardness of Mg-Al-Zn alloys

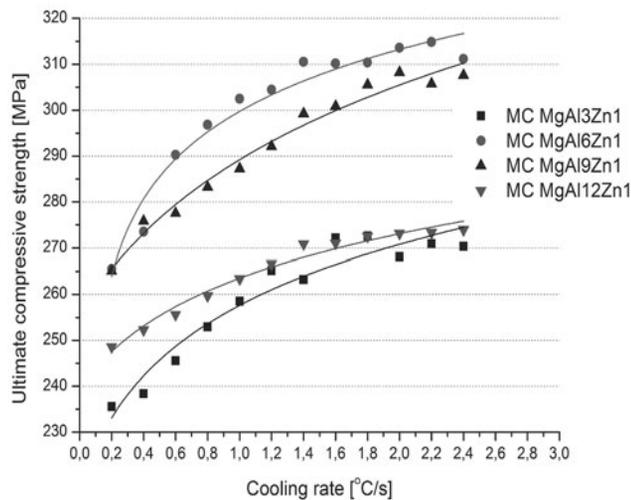


Fig. 15. The predicted influence of cooling rate on the ultimate compressive strength of Mg-Al-Zn alloys

On the basis of the worked out models of neural networks, the diagrams of the influence of the cooling rate and aluminium content were done on the hardness, ultimate compressive strength and grain size of the analyzed magnesium cast alloys (Fig. 16-18).

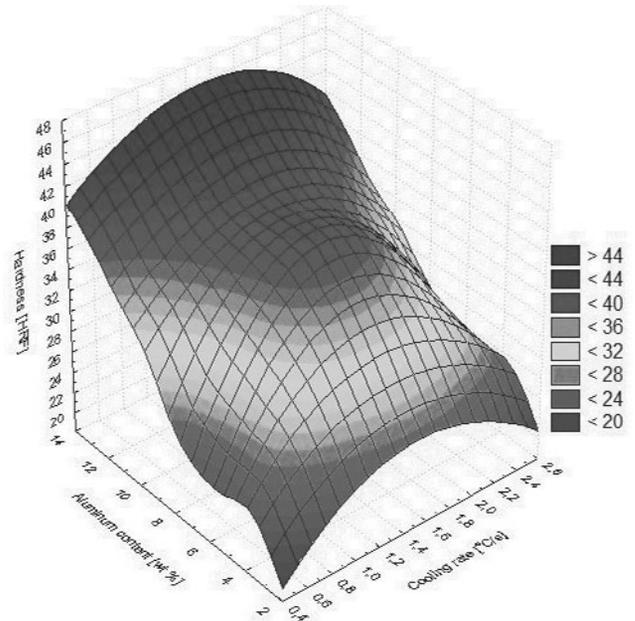


Fig 16. Simulation of the cooling rate and aluminium content on hardness of the cast magnesium alloys

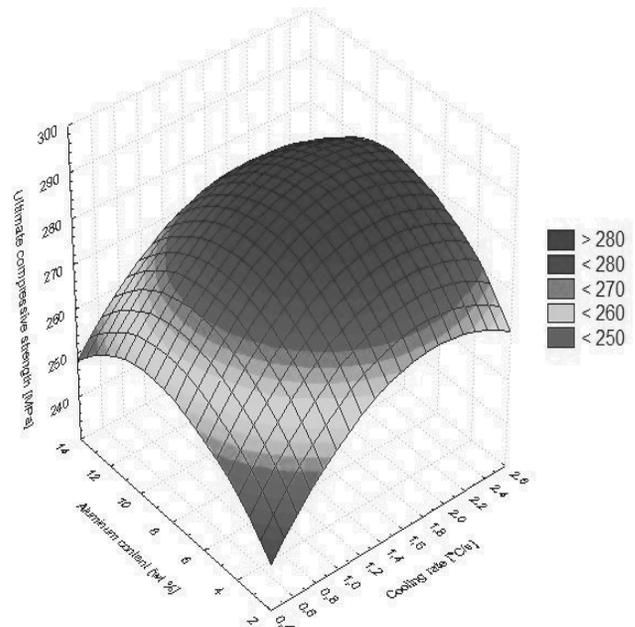


Fig. 17. Simulation of the cooling rate and aluminium content on ultimate compressive strength of the cast magnesium alloys

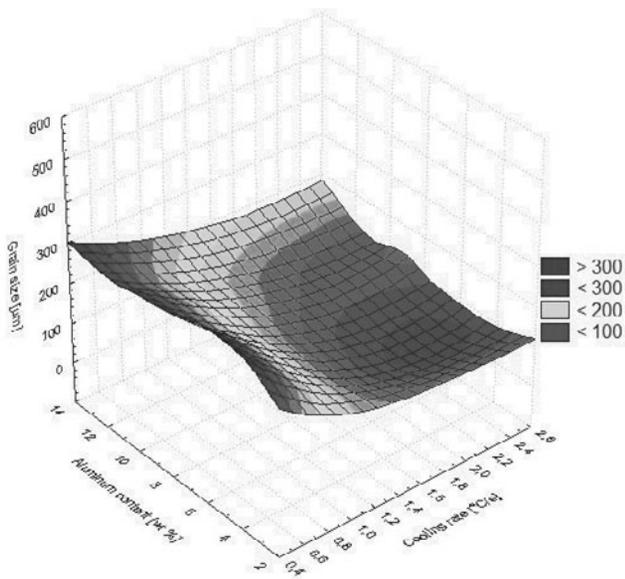


Fig. 18. Simulation of the cooling rate and aluminium content on grain size of the cast magnesium alloys

4. Conclusions

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

Acknowledgements

The authors would like to thank Dr. M. Kasprzak for his valuable contributions to the UMSA Technology Platform's configuration.

Additional information

Selected issues related to this paper were presented at the 18th International Scientific Conference on Achievements in Mechanical and Materials Engineering AMME'2010.

The paper is published also in the Journal of Achievements in Materials and Manufacturing Engineering.

References

- [1] K.U. Kainer, Magnesium – alloys and technologies, Wiley-VCH Verlag GmbH & Co. KG aA, Weinheim, 2003, 33-341.
- [2] T. Malinova, Z.X. Guo, Artificial neural network modelling of hydrogen storage properties of Mg-based alloys, *Materials Science and Engineering* 365/1-2 (2004) 219-227.
- [3] J. Sungmoon, G. Jamshid, Neural network constitutive for rate-dependent materials, *Computers and Structures* 84 (2006) 955-963.
- [4] S.H. Hsiang, J.L. Kuo, Applying ANN to predict the forming load and mechanical property of magnesium alloy under hot extrusion, *The International Journal of Advanced Manufacturing Technology* 26 (2005) 970-977.
- [5] S.H. Hsiang, J.L. Kuo, F.Y. Yang, Using artificial neural networks to investigate the influence of temperature on hot extrusion of AZ61 magnesium alloy, *Journal of Intelligent Manufacturing* 17/2 (2006) 191-201.
- [6] H.D. Liu, A.T. Tang, F.S. Pan, A model on the correlation between composition and mechanical properties of Mg-Al-Zn alloys by using artificial neural network, *Materials Science Forum* 488-489 (2005) 793-796.
- [7] A.T. Tang, B. Liu, F.S. Pan, J. Zhang, J. Peng, J.F. Wang, An improved neural network model for prediction of mechanical properties of magnesium alloys, *Science in China Series E: Technological Sciences* 52/1 (2009) 155-160.
- [8] L.A. Dobrzański, M. Król, T. Tański, R. Maniara, Effect of cooling rate on the solidification behaviour of magnesium alloys, *Archives of Computational Materials Science and Surface Engineering* 1/1 (2009) 21-24.
- [9] L.A. Dobrzański, M. Król, Thermal and mechanical characteristics of cast Mg-Al-Zn alloy, *Archives of Foundry Engineering* 1/10 (2010) 27-30.
- [10] L.A. Dobrzański, T. Tański, J. Domagała, M. Król, Sz. Malara, A. Klimpel, Structure and properties of the Mg alloys in as-cast state and after heat and laser treatment, *Journal of Achievements in Materials Science And Engineering* 31/2 (2008) 123-147.
- [11] L.A. Dobrzański, S. Malara, J. Trzaska, Project of computer programme for designing the steel with the assumed CCT diagram, *Journal of Achievements in Materials and Manufacturing Engineering* 20 (2007) 351-354.
- [12] W. Sitek, J. Trzaska, L.A. Dobrzański, Evaluation of chemical composition effect on materials properties using AI methods, *Journal of Achievements in Materials and Manufacturing Engineering* 20 (2007) 379-382.
- [13] J. Trzaska, L.A. Dobrzański, A. Jagiełło, Computer programme for prediction steel parameters after heat treatment, *Journal of Achievements in Materials and Manufacturing Engineering* 24/2 (2007) 171-174.
- [14] L.A. Dobrzański, T. Tański, J. Trzaska, L. Čížek, Modelling of hardness prediction of magnesium alloys using artificial neural networks applications, *Journal of Achievements in Materials and Manufacturing Engineering* 26/2 (2008) 187-190.

[15] L.A. Dobrzański, S. Malara, J. Trzaska, Project of neural network for steel grade selection with the assumed CCT diagram, *Journal of Achievements in Materials and Manufacturing Engineering* 27/2 (2008) 155-158.

[16] Method and Apparatus for Universal Metallurgical Simulation and Analysis – United States Patent, Patent No.: US 7,354,491 B2, Date of Patent: Apr. 8.