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Modelling of mechanical properties of Al-Si-Cu cast alloys using the neural network

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Analysis and modelling

ABSTRACT

Purpose: The paper presents some results of the research connected with the development of new approach based on the neural network to predict the chemical composition and cooling rate to the mechanical properties of Al–Si–Cu cast alloys. The independent variables in the model are chemical composition of Al–Si–Cu cast alloys and cooling rate. The dependent parameters are hardness, microhardess, yield strength and apparent elastic limit.
Design/methodology/approach: The experimental alloy used for training of neural network was prepared at the University of Windsor (Canada) in the Light Metals Casting Laboratory, in a 10 kg capacity ceramic crucible. Thermal analysis tests were conducted using the UMSA Technology Platform. 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 rate. Rockwell F–scale hardness tests were conducted at room temperature using a Zwick HR hardness testing machine. Vickers microhardness tests were conducted using a DUH 202 microhardness 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 behavior modeling of Al–Si–Cu castings.
Practical implications: The worked out model can be applied in computer system of Al–Si–Cu casting alloys selection and designing for Al-Si-Cu casting parts.
Originality/value: Original value of the work is applied the artificial intelligence as a tools for designing the required mechanical properties of Al-Si-Cu castings.
Keywords: Artificial intelligence methods; Numerical techniques; Mechanical properties

1. Introduction

Cast aluminum alloys are important construction materials, which are used in various fields of technology. Because of their low density, relatively low melting point, good heat and electrical conduction, low thermal expansion coefficient, good castability and low casting shrinkage, they are mainly used in car manufacturing as: piston castings, cylinder head castings, engine blocks, structural supporting reinforcements and elements absorbing crash impact. Aluminum alloys are also widely used in production of household goods, as well as in telecommunication and information technology [1-3].

The main characteristic of neural networks is the ability to generalize knowledge for new data not provided during learning process. It is not necessary for neural networks to gather data and have access to entire database containing knowledge on predicted issue. They also show tolerance to discontinuity, random disturbances or shortage in learning set. Such characteristics allow their application where there are problems with data

transformation, analysis, sorting and classification along with prediction or controlling on their basis of a certain process. Research carried out by Prof. L. A. Dobrzanski's team [4-10] has shown that the neural network models are a useful tool to predict materials engineering phenomena. They have facilitated formation of numerical models describing phases kinetic transformations in working steel. Results obtained from neural networks turned out more precise than the ones obtained from empirical calculations.

This article presents the application of neural networks for calculation of yield strength (YS), apparent elastic limit (EL), hardness (HRF) and matrix microhardness (μHV0,025) in relationship to chemical composition and cooling rate.

2. Materials and experimental procedure

2.1. Materials for training Neural Networks

Formation of a numerical model that allows calculation of the characteristical temperature, microstructural features and mechanical properties depending on chemical composition and cooling rate has been determined by working out a suitable set of experimental data.

The set of representative data including: mass concentration of elements, cooling rate, EL, YS, HRF and μHV0,025 has been elaborated through own research, and the results from specialist publications [3, 11-16]. The range of concentration of alloy elements and cooling rates has been presented in Table 1.

Table 1.
Range of mass concentration of elements and cooling rates (CR) in investigated Al-Si-Cu hypoeutectic alloys

Range	Mass concentration of elements, wt %							CR, °C /s
	Si	Fe	Cu	Mn	Mg	Zn	Ti	
min	5	0,08	0,006	0	0,02	0	5	0,03
max	11,9	1,35	4,64	0,6	1,28	2,9	11,9	2,5
%Sr+%Ni+%Sn+%Pb+%Na%Ca≤0,3								

The gathered set of data designed for formation of a numerical model determining: EL, YS, HRF and μHV0,025 in relation of the chemical composition and cooling rate has been divided into two subsets: the learning set and the validation set. The data have been divided in proportion of 75% for the learning set and 25% for the validation set. The division into two sets has been made random.

In order to control the learning correctness of neural networks, data obtained from a metallurgical experiment have been used. The results of the experiment have been used to make a test-verification set. The data used in the process of learning and testing have been normalized by means of the minimax function that transforms the domains of variables to range ⟨0, 1⟩.

2.2. Materials for testing Neural Networks

The data obtained from the metallurgical experiment have been used for testing neural networks. For the sake of research in the metallurgical laboratory of the University of Windsor there had been made six Al-Si-Cu experimental hypoeutectic alloys cooled with three different cooling rates.

The alloys of chemical content shown in Table 2 were casted in an electrical resistance furnace with a ceramic melting crucible. The process of melting took place in the nitrogen protective atmosphere. Directly before casting of ingots, melted metal was degassed for 20 minutes in order to eliminate from the alloy hydrogen atoms as one of the learning vectors which influenced the liquidus and solidus temperatures and was undesirable in the investigated alloys. The melting and soaking temperature of the alloy was 850 ºC. Ingots of 45 mm in diameter and 50 mm in height were cast into thin-walled cups made of hot-work tool steel. The ingot mass was 330 g ±10 g.

Table 2.
Chemical content of alloys used for neural networks testing

Alloy label	Mass concentration of elements, wt %,						
	Si	Fe	Cu	Mn	Mg	Zn	Ti
7-1	7,17	0,14	0,99	0,11	0,27	0,05	0,08
7-2	6,98	0,17	1,91	0,01	0,26	0,43	0,09
7-4	7,45	0,34	3,60	0,25	0,28	0,05	0,13
9-1	9,09	0,72	1,05	0,36	0,27	0,14	0,07
9-2	9,03	0,19	2,25	0,01	0,19	0,45	0,10
9-4	9,27	0,17	4,64	0,01	0,28	0,05	0,09
%Sr+%Ni+%Sn+%Pb+%Na%Ca≤0,95							

2.3. Compression, hardness and microhardness testing

Samples for compression testing were machined from a center 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. Vickers microhardness tests were conducted using a DUH 202 microhardness testing machine. Load of indenter was set at 25 g.

2.4. Evaluate of the Neural Networks

Variety of neural networks used in the experiment makes it necessary to apply number indicators, which allow the evaluation of the learning process. The following indicators have been regarded as the essential ones: mean network error, standard deviation quotient for errors and data, standard deviation for the error and the Pearson correlation coefficient (R).

The mean network error has been calculated according to the following:

$$E = \frac{1}{N}\sum_{i=1}^{n}\left(\left|X_{mi} - X_{pi}\right|\right) \quad (1)$$

Where:
E – mean network error,
N– number of data in test set,
X_{mi} – i-times value,
X_{pi} – i-times value by neural network.

Standard deviation quotient for errors and data has been adopted as a quality quotient of a numerical model made by neural networks. The numerical model of relationship between the mechanical properties in relation to chemical concentration and cooling rate calculated by neural networks can be accepted as a correct one provided that the output values given by the network contain smaller errors than a simple calculation of unknown output value.

The simplest method for calculation of output value is still assumption of an average value of output values for it learning and testing sets. In that case, mean error is equal of standard deviation for output value in the learning set, whereas standard deviation quotient equals one. The smaller network error is, the smaller values for the standard deviation quotient become, finally reaching zero for the "ideal" forecast [4–7].

3. Results and discussion

This paper presents the technique of determination of mechanical properties depending on the cooling rate and chemical composition with the application of neural networks. To solve this problem the computer system was designed.

The calculation of EL, YS, HRF and µHV0,025 was possible thanks to the application of the radial basis functions neural network with net k-mean and k-nearest neighbour learning algorithms with the search option of the optimal ones in input parameters. The designed neural network consists of six inputs (Si, Cu, Mg, Fe, Mg, Mn, CR) and four outputs (HRF, µHV, EL, YS). The standard deviation ratio calculated for the training set is: 0.628 for microhardness; 0,343 for hardness, 0,32 for elastic limit and 0,28 for yield strength. Table 3 shows the values of errors, standard deviation ratios and Pearson correlation coefficients (R) for the calculated values of microhardness, hardness, elastic limit and yield strength .

Table 3.
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
µHV0,025	84,241	5,066	2,94	0,628	0,94
HRF	76,915	3,227	1,18	0,342	0,97
EL, MPa	138,79	12,54	1,37	0,32	0,96
YS, MPa	203,46	9,05	3,44	0,28	0,97

Figures 1 and 2 show the comparison of real hardness and apparent elastic limit with data calculated by neural network. The biggest error in the calculation of mechanical properties occurs for the determination of microhardness. In 30% of cases the difference between the real microhardness and the microhardess calculated by the neural networks exceeds ±10 µHV 0,025. However, this error can be acceptable when taking into account the range of measurement of the calculated microhardness and while comparing the error to the experimentally measurable error value.

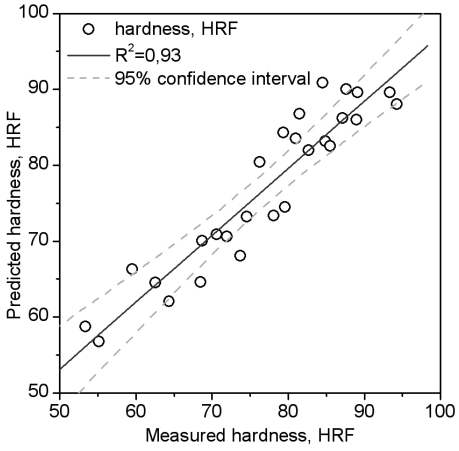

Fig. 1. Comparison of experimental determination hardness with hardness calculated by applied neural network

The designed computer system enables the calculation of mechanical properties in relation to chemical composition and cooling rate. It was possible to perform simulation of the influence of cooling rate on: HRF, µHV, EL, YS for the experimental AC AlSi7Cu alloy. The chemical composition of the tested alloy is presented in Table 4. The calculation results are presented in Figure 3.

Table 4.
Chemical content of alloys used for prediction of the cooling rate influence on the phases transformation temperature, microstructure feature and mechanical properties

AC AlSi7Cu	Mass concentration of elements, wt %,						
	Si	Fe	Cu	Mn	Mg	Zn	Ti
	7,00	0,15	1,00	0,10	0,2	0,05	0,08

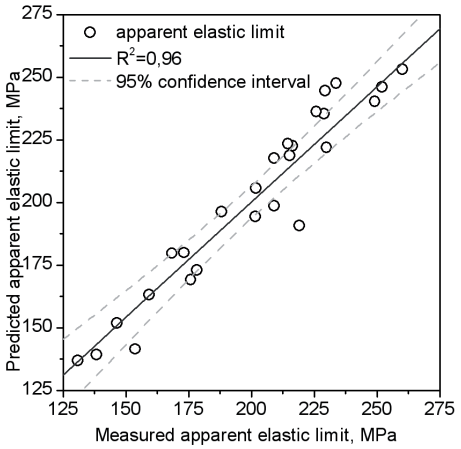

Fig. 2. Comparison of experimental determination EL with EL calculated by applied neural network

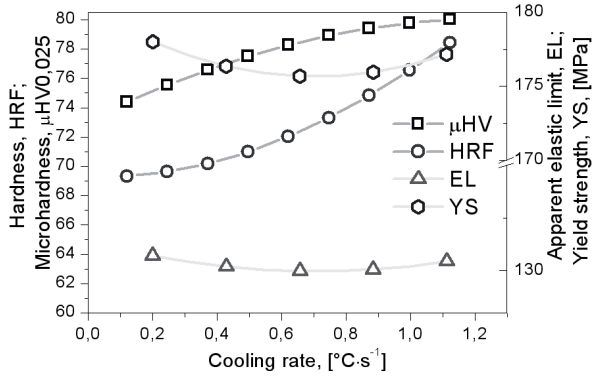

Fig. 3. Influence of cooling rate on the mechanical properties of AC Al Si7Cu4 casting alloy

4. Conclusion

The neural network approach appears to be a very powerful tool in materials engineering. The results show that the prediction of the mechanical properties of the considered Al–Si–Cu alloys are in a good compatibility with the experimental data. Obtained results show that the model based on the ANN can predict with good accuracy such microhardness, hardness, yield strength, apparent elastic limit. The network was trained on the data obtained in the laboratory tests, and next validated using the data from the industrial measurements. The accuracy of values evaluated by the ANN model is much higher than that obtained from calculations using the classical, experimental models.

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