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Application of the artificial neural networks for prediction of hardness of alloyed copper

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Analysis and modelling

ABSTRACT

Purpose: The aim of the work is to employ the artificial neural networks for prediction of hardness of the alloyed copper like CuTi, CuFe, CuCr and CuNiSi.
Design/methodology/approach: It has been assumed that the artificial neural networks can be used to assign the relationship between the chemical compositions of alloyed copper, temperature and time of solution heat treatment, degree of cold working deformation and temperature and time of ageing. 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 parameters of heat treatment and cold working deformation degree on the hardness 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, parameters of heat treatment and cold working deformation degree on the hardness.
Research limitations/implications: Worked out model should be used for prediction of hardness only in particular groups of alloyed copper, 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 hardness value basing on combinations of concentrations of the particular elements, heat treatment parameters and cold working deformation degree.
Originality/value: In this paper it has been presented an original trial of prediction of the required hardness of the alloyed copper like CuTi, CuFe, CuCr and CuNiSi.
Keywords: Computational material science; Artificial neural networks; Alloyed copper; Heat treatment; Cold plastic deformation

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1. Introduction

A widely used method of increasing the strength properties of metal alloys is the strengthening of the new phase particles separated during aging.

The precipitation process in alloyed copper like a CuCr, CuFe, CuNiSi and CuTi was examined in some detail with respect to the classical heat treatment, which consists of solutioning and aging. The kinetics of this process has been studied in detail [1-5]. It was found that the solutioning whose function is to dissolve in the matrix component of the alloy during aging emit phase, which are responsible for the effect of strengthening the alloy. These phase are Cu_4Ti-β', Ni_2Si-δ oraz Fe-α.

Attempts have also been efforts to investigate the kinetics of precipitation and recrystallization in these alloys using other, more complicated alternative version of methods involving a sequence of operations on a combination of heat treatment and cold plastic deformation [6-14], the intermediate roll in the liquid nitrogen bath [15], the aging in the atmosphere hydrogen [16,17], and heat treatment and hot plastic deformation [18,19], insert to the alloy CuTi other alloying addition [20-24], or produced using methods other than classical [25].

However, the most effective way to increase the mechanical properties of the alloys is hardening combined with the strengthening of the deformation in different variants [26]. For this reason, extensive research conducted effect of combined (alternating) heat treatment and hot plastic deformation or heat treatment and plastic cold deformation.

An analysis of published studies indicates that the experiment of combining alternating heat treatment and cold plastic deformation is long and laborious. Ability to predict properties on the basis of previous studies performed by the model-developed is the basis to work in this direction. This paper is an attempt to develop such a model. As shown in previous publications of the work undertaken in this direction have great chances of success [27-34].

The key information for optimizing the production process and the chemical composition in order to obtain the desired properties for any commercial application has a relationship between chemical composition and heat treatment parameters and the degree of cold plastic deformation and hardness. In the process of analysis of the specific properties, which are characterized by different types of copper alloy, because of the need for generalization of experimental data of residual often initially used an approximation that is used to replace some other mathematical size having approximate.

Sub-analysis performed using the approximation, to estimate the approximate degree of influence of heat treatment parameters and the degree of cold plastic deformation on the hardness of selected copper alloys.

The nature of the hardness of alloys under heat aging depends largely on whether the alloy is subjected to cold plastic deformation after solutioning. For example, industry alloy CuTi4 subjected to standard heat treatment (solutioning and aging) has a different hardness than the alloy saturated, cold-rolled and then aged. The results of hardness measurement of CuTi4 supersaturated alloy and then aged shown in Fig. 1. However, the results of hardness measurement CuTi4 supersaturated alloy, cold deformed (Z=50%) and aged shown in Fig. 2. The hardness of the alloy after solution is CuTi4 HV=125, while the deformation after solution and HV=250.

The aging of the investigated alloy over 120 minutes in the temperature range 450°C results loss in partial of coherence of the second phase precipitates and reduction of dislocation density in the matrix in the deformed cold worked alloy before aging (Z=50%) which leads to a reduction in hardness. To undeformed alloy recorded the continuous growth of hardness in range investigated. The other hand the deformed alloy, aging at 500°C over 30 minutes result in the decrease of hardness while the for undeformed alloy after 120 min. [35].

Then, with increasing aging temperature drop in hardness for the deformed alloy is, even after 30 minutes, but quite generally: the value of 265 HV to 150 HV.

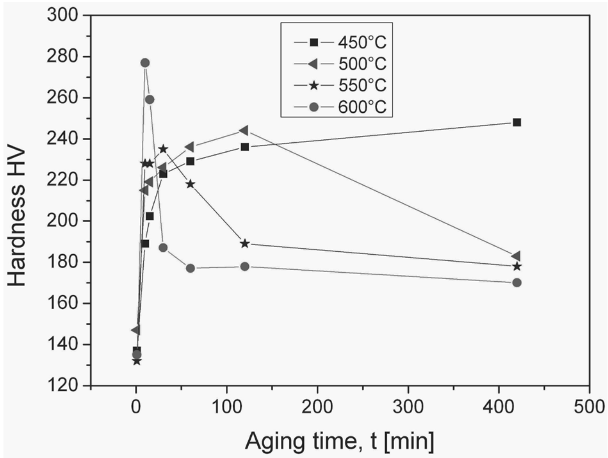

Fig. 1. Changes in hardness of the supersaturated alloy CuTi4 depending on temperature and aging time [35]

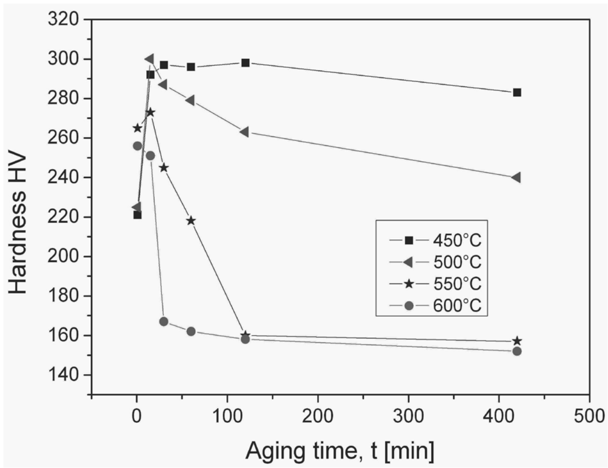

Fig. 2. Changes in hardness of supersaturated and deformed (50%) alloy CuTi4 depending on temperature and aging time [35]

The influence on hardness in CuTi alloys after the supersaturation have a titanium content what was shown in Fig. 3. Approximated by the author of this work on the basis [6,36] of simple with R^2 = 0.94

indicates that the tested range of concentrations of Ti additive effect is a linear term, which is given by:

$$y = 58{,}354x - 21{,}222 \quad (1)$$

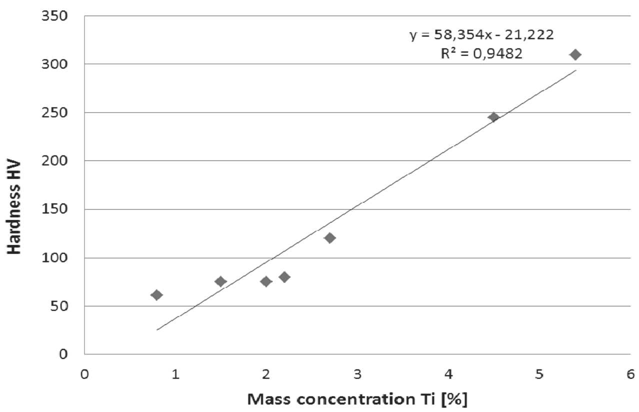

Fig. 3. Effect of the concentration of titanium in a alloyed copper CuTi for hardness after solutioning at 900°C for 120 minutes, on the basis of data from the [6,36]

The paper presents an attempt to apply artificial neural networks to predict the effects of chemical composition, supersaturation and aging parameters and the degree of cold plastic deformation on the hardness of the alloys CuTi, CuFe, CuCr and CuNiSi.

It has been shown that on the basis of the chemical composition, heat treatment and plastic deformation can use artificial neural network set, with an acceptable error, the hardness value of the selected low-alloy copper alloy.

2. Material and experimental methodology

Develop a model allowing to calculate the hardness of copper alloys using artificial neural networks, require preparation, on the basis of the literature [36-38], a corresponding set of representative experimental data. Our study began with the creation of the data sheet containing the chemical compositions of copper alloys collected at that time, degree of deformations, heat treatment parameters and their corresponding values of hardness tested.

The concentration range of atomic elements, heat treatment parameters, deformation and hardness values shown in Table 1 and Table 2 All collected data were used to develop a regression equation. Of the available data, half of the cases was used to modify the network weights in the learning process by creating a set of learners.

Spent the rest of the data to evaluate the prediction errors during learning (25% of the data - a set of validation) and to an independent determination of the correctness of the network after it has been created (25% of the data - a set of test). Split into individual collections were made at random, whereas the arithmetic mean and standard deviation for each of the sets.

Table 1.
The range of concentrations of atomic elements analyzed alloys

Range	Atomic concentration of the element, %					
	Cu	Ti	Fe	Cr	Ni	Si
min.	94.6	0	0	0	0	0
max.	99.3	5.4	2.34	1	2.08	0.89

3. Determination of hardness

If between the two variables is correlative relationship and one of the variables (y) may be considered dependent, and the other (x) as an independent, one can attempt to formulate a relationship function which represents the value of y depending on the value x of a random variable additional ε which represents random variability of the variable y is independent of x.

In order to establish between the physical quantities (the alloy composition and processing parameters) the relation of the type:

$$y = ax + b \quad (2)$$

one should find the method of least squares relationship between y and x and y. Pairs of numbers are not repeated measurements of the same size, that there is no measure of dispersion measurements. It is known, however, that the result

$$y_i - (ax_i + b) \quad (3)$$

normally distributed, so the deviation from the true relationship (1) be directed by the rules of a normal distribution. However, it isn’t known the true relationship only approximate the coefficients *a* and *b*. The number of degrees of freedom in this case equal to the number of measurements minus the number of designated coefficients, that is n-2. Thus, uncertainty in the results y_i is:

$$\sigma_y = \sqrt{\frac{1}{n-2}\sum_{i=1}^{n}(y_i - ax_i - b)^2} \quad (4)$$

Thus, uncertainties and determine the coefficients *a* and *b* is to define:

$$S_a = \sqrt{\frac{1}{n-2}\sum_{i=1}^{n}(y_i - ax_i - b)^2} \cdot \sqrt{\frac{n}{n\sum_{i=1}^{n}x_i^2 - \left(\sum_{i=1}^{n}x_i\right)^2}} \quad (5)$$

and

$$S_a = \sqrt{\frac{1}{n-2}\sum_{i=1}^{n}(y_i - ax_i - b)^2} \cdot \sqrt{\frac{\sum_{i=1}^{n}x_i^2}{n\sum_{i=1}^{n}x_i^2 - \left(\sum_{i=1}^{n}x_i\right)^2}} \quad (6)$$

Table 2.
Heat treatment temperature and duration time ranges, and hardness of the analyzed alloys

Range	Treatment parameters					Hardness, HV
	Solution treatment temperature, T [°C]	Solution treatment time, t [s]	Degree of deformation (cold work), Z [%]	Ageing temperature, T [°C]	Ageing time, t [s]	
min.	900	60	20	400	1	55.2
max.	1050	120	90	650	10140	454

To determine the degree of dependence of one quantity on the other is the correlation coefficient, denoted by R, which is defined as:

$$R = \frac{n\sum_{i=1}^{n}(x_i \cdot y_i) - \left(\sum_{i=1}^{n} x_i \cdot \sum_{i=1}^{n} y_i\right)}{\sqrt{\left(n \cdot \sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2\right) \cdot \left(n \cdot \sum_{i=1}^{n} y_i^2 - \left(\sum_{i=1}^{n} y_i\right)^2\right)}} \tag{7}$$

To develop the relationship between the chemical composition of the alloy, heat treatment parameters and the degree of cold deformations data analysis tool has been used in MS Excel and artificial neural networks using the package Statistica Neural Network UK 4.0 F StatSoft.

On the basis of data made regression fit is R^2=0.92 and standard error of 28.1. The analysis gave the following equation:

$$y = ax_1 + bx_2 + cx_3 + \ldots + nx_m + e \tag{8}$$

The calculated coefficients (x_1, x_2, …) are presented in Table 3. Based on the calculated coefficients can be concluded that the largest effect on the hardness value of the alloying elements are copper, iron, and chromium. However, nickel and silicon, according to the calculated parameters (x_5 and x_6, respectively) did not have any effect. It is puzzling and requires further detailed analysis.

Fig. 3 presents an analysis of the structure of individual error for regression analysis.

However, heat treatment parameters (temperature and time) and the draft degree not have a significant influence. In particular, it should be noted that the aging time has a minimal, almost zero influence on the hardness (x_{11}=0.001), which is contrary to the basic knowledge on the results of the heat treatment. Therefore, this issue also requires further analysis.

The Fig. 4 shows comparison of the calculated and experimental hardness value.

Due to the serious inaccuracies resulting from regression analysis it was decided to analyze the data using a neural network.

In the design phase for each network, the following parameters:

- error function - the sum of the squares,
- activation function: I layer - a linear function, the second layer-logistic function, the third layer - a linear function of saturation.

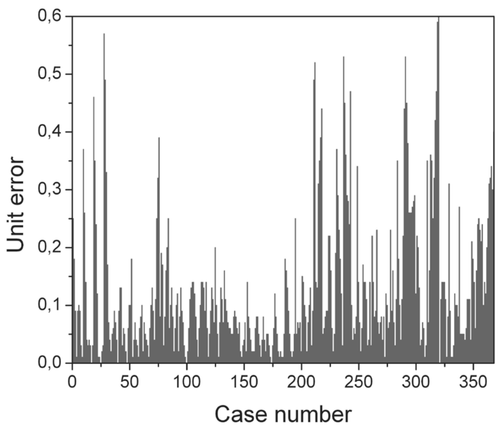

Fig. 3. Histogram of individual error for regression analysis

A set of input has been randomly divided into the following collections:

- learners (184 cases),
- validation (92 cases),
- test (92 cases).

In the structure of each of the analyzed network set 11 input neurons, and 6 correspond to the alloying element present in the tested alloys, and 5 corresponding to the parameters of the heat treatment and degree of cold deformation. The resulting output neuron shows the hardness value to be searched.

The search for an optimal neural network is initially limited to:

- radial basis functions neural network RBF,
- generalized regression neural networks GRNN,
- multilayer perceptron MLP.

Number of hidden layers, the number of nodes in these layers of weights, thresholds values, method and parameters learning, the parameters of the proposed network architecture has been made taking into account the influence of the size of the value of indicators to assess the quality of the proposed network. Modeling was carried out on the basis of 368 test cases.

Table 3.
The calculated parameters of Equation (8)

x_1	x_2	x_3	x_4	x_5	x_6	x_7	x_8	x_9	x_{10}	x_{11}
Cu	Ti	Fe	Cr	Ni	Si	stt, T [°C]	stt, t [s]	Z [%]	at, T [°C]	at, t [s]
-44.74	3.51	43.55	33.03	0	0	-0.08	0.67	0.63	0.38	0.001

Used to analyze the quality of comparison: the average absolute error, the ratio deviation and correlation coefficient. On the basis of this analysis is the choice of the optimal 11-5-1 MLP network, which trained by error back propagation through method for 50 epochs and using the conjugate gradients for 130 epochs.

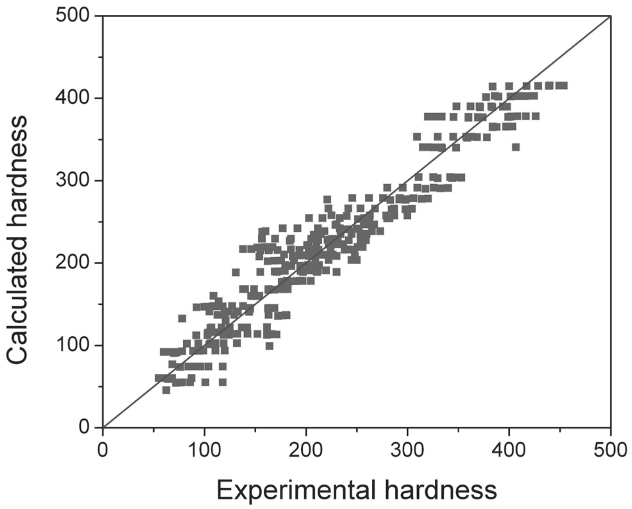

Fig. 4. Comparison of the experimental and calculated hardness values for regression

Table 4.
Quality assessment coefficients of the MLP 11-5 neural network

Assessment coefficient	Training	Validating	Testing
Average absolute error [HV]	19.14	17.02	16.15
Quotient of standard deviations	0.23	0.22	0.24
Pearson correlation coefficient	0.97	0.97	0.969

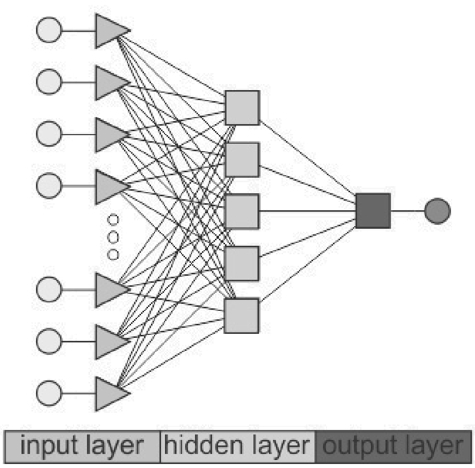

Fig. 5. Schema of MLP 11-5-1 network

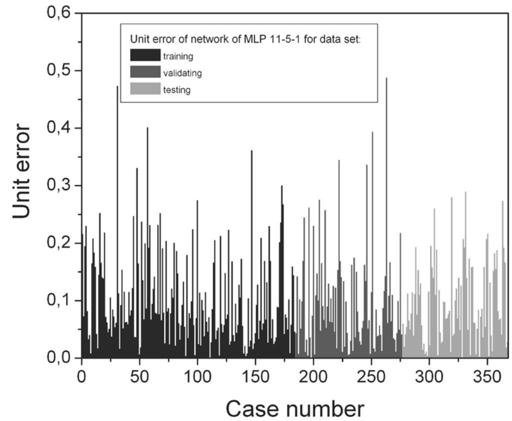

Fig. 6. Analysis of the unit errors of MLP 11-5-1 network with: bar graph, values of the unit errors

The selected network has a relatively low average absolute error and high correlation coefficient, while at the same time low amplitude between sets: learning, validation and test. In Table 4 are complete regression statistics 11-5-1 MLP selected network in Fig. 5 is the diagram, and Fig. 6 presents an analysis of the structure of individual errors.

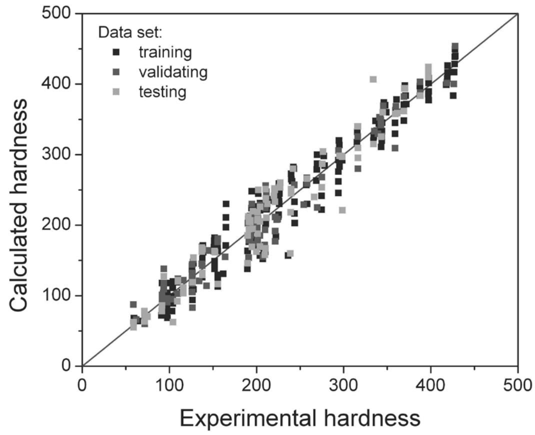

Fig. 7. Comparison of the experimental and calculated hardness values for MLP 11-5-1 network sets: training, validating, testing

Developed an artificial neural network model has been subjected to verification of compliance of comparing the hardness calculations with experimental results (Fig. 7). The consequence of an incorrect designation looking hardness values is inappropriate for the data mapping diagram calculated in comparison with the experimental values.

MLP networks are trained in supervised mode, so the required values are known patterns and weight selection should ensure the best possible fit for the network outputs of these patterns. MLP network training algorithms are the gradient methods whose use is possible and effective only if the activation function is a continuous function.

Fig. 8 presents comparison of histograms of individual error for artifical neural network (MLP-5-1) and regression analysis.

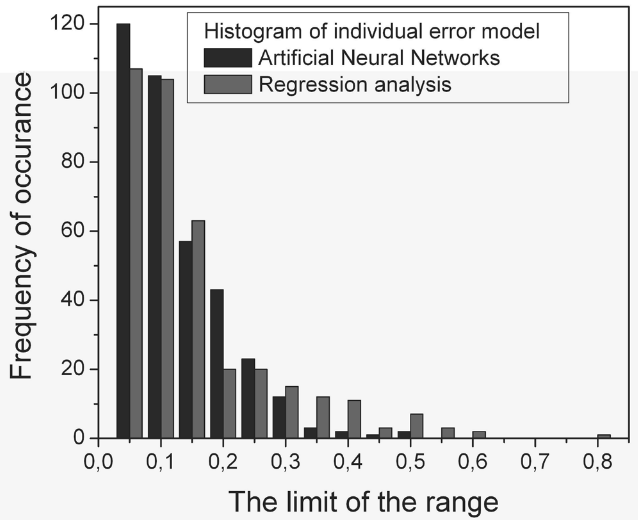

Fig. 8. Comparison of individual error histograms for artificial neural networks and regression analysis

Determination of the structure of the MLP network is usually difficult. This primarily applies to the selection of the number of neurons in the hidden layer. Modeling of more complex processes can increase the number of hidden neurons. However, this results in slow network performance and learning disabilities, especially the tendency to over-fitting to the training data.

4. Conclusions

In assessing verification the best designed 11-5-1 MLP networks characterized by average absolute error of 17.43, average deviation of the ratio - 0.23 and the average correlation coefficient - 0.97, it should be noted that the use of artificial neural networks allows the a set of data covering the chemical composition and heat treatment parameters, the calculation of the allowable error with some copper alloy hardness values. The correctness of the results is highly dependent on the proper preparation of a representative set of experimental data, the use of simplification or even miss some data. Since, as shown by the results of previous studies [27-34] in the majority of cases, good results can be achieved using a simple structure of the MLP network regardless of the analyzed area [39].

Although according to theorem Hecht-Nielsen neural network can approximate any continuous function (with any accuracy) where N neurons in the input, (2N +1) hidden neurons and one output neuron as a result of the tests it was found that the best properties is characterized by a network of MLP 11-5-1. It was also found that, in order to provide a good correlation to solve complex problems requires not only the interference in the training set, but also the structure of the network.

Analysis of the issues and the nature of the evidence that the problem is worthy of further interest and thus further research and analysis. The most appropriate suggestion that comes to mind is the recommendation to maximize the input data set, both in terms of the number of different alloys, but also a greater diversity in terms of the conditions of heat treatment.

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