ARCHIVES
of
FOUNDRY ENGINEERING

Published quarterly as the organ of the Foundry Commission of the Polish Academy of Sciences

ISSN (1897-3310)
Volume 15
Special Issue
2/2015

59 – 64

14/2

The Integration of Knowledge about the Manufacturing Process of ADI with the Use of Artificial Intelligence Methods

B. Mrzygłód *, I. Olejarczyk-Wożeńska, K. Regulski
AGH – University of Science and Technology, Al. Mickiewicza 30, 30-059 Krakow
*Corresponding author. E-mail address: mrzyglod@agh.edu.pl

Received 14.05.2015; accepted in revised form 01.06.2015

Abstract

The authors of this article highlight the need to integrate knowledge about the design process of products made from ADI contained in thematic publications. Integration and centralization of the results can be the basis for the planning and execution of subsequent experiments, covering areas previously unexplored. The integrated knowledge can also give rise to the production of new knowledge by discovering relationships and dependencies that are not visible in single experiments. Attempts were made to construct inference algorithms and systems based on artificial intelligence methods. This article presents the results of the use of artificial neural networks and one of the methods in the area of data mining called regression trees to develop models of the ADI manufacturing process.

Keywords: ADI, Data extraction, Artificial neural networks, CAPCAST system

1. Introduction

The subject discussed in this article concerns the possibility of extension of one of the modules of the CAPCASTexpert system (Computer Aided Process CAST), which for several years is being developed in the Department of Applied Informatics and Modelling [1-5]. The presented module is responsible for the integration of knowledge about the design and fabrication of products from the Austempered Ductile Iron (ADI), made available to the public via a large number of articles in specialized journals (Fig. 1).

Publications, which most often result from costly experiments, are an invaluable source of knowledge for their readers and for researchers, and the integration and centralization of the results can be the basis for the planning and execution of subsequent experiments, covering areas previously unexplored. Integrated knowledge about the results of experiments can also serve as a basis to generate new knowledge through the discovery of relationships and dependencies that are not visible in single experiments.

Literature in this area includes a series of presentations of the results of experiments carried out in various centres around the world. The research conducted prior to such publications is a highly time consuming process, usually requiring considerable financial outlays. The authors draw attention to the need to develop an information system that will facilitate selective access to particular portions of this knowledge, allowing its automatic processing. The cost of developing such a system is certainly lower than the cost of repeated experiments.

2. Characteristics of collected experimental data

In the authors' area of interest is knowledge published on the manufacturing process of ADI. ADI is a variation of ductile iron produced in the process of properly conducted heat treatment. The heat treatment consists of two stages, which comprise austenitizing and austempering. The heat treatment parameters, including parameters of both austenitizing (T_A - temperature, t_A - time) and austempering (T_i - temperature and t_i - time of isothermal holding), are selected depending on properties which the ADI should possess, e.g. high ductility and moderate strength and hardness, or vice versa - low ductility but high hardness and strength. The combination of properties that are to be obtained must be optimal from the point of view of later operating conditions of the item produced [6-10].

A review of the technical journals was made and an analysis of articles concerning this area of knowledge was carried out in terms of the selection of production parameters of ADI to achieve the required properties of the final material. A logical scheme of the presented results of experiments, observed in the majority of analyzed articles, can be expressed in the form of the following implication:

chemical compositions and dimensions and heat treatment parameters → PROPERTIES

in which the premises are: chemical composition of the starting material, the dimensions of the heat treated item, and the heat treatment parameters, while the resultant variables are values of the selected product properties.

Using the adopted scheme, from the articles analyzed the experimental data were extracted. An array of attributes was developed for some specific variables, which are premises, and which include:

— *chemical composition*: C, Si, Mn, Mg, Cu, Ni, Mo, S, P, B, V, Cr, Ti, Sn, Nb, Al;
— *dimensions:* (usually these are the dimensions of samples in accordance with standards adopted in the experiment);
— *heat treatment parameters*: austenitizing temperature (T_A), austenitizing time (t_A), temperature of isothermal transformation (T_i), time of transformation (t_i) and cooling medium;

and for the variables which are conclusions and include: tensile strength (Rm); elongation (A); reduction of area (Z); hardness (HRC); impact strength (KC); yield stress (Re).

Table 1.
Part of the table developed

	chemical composition												austempred		isothermal transformation				
Lp.	C	Si	Mn	Mg	Cu	Ni	Mo	S	P	B	V	Cr	TA, °C	tA, s	Ti, °C	ti, s	tensile strength, MPa	elongation, %	hardness, HRC
26	3,21	2,57	0,28	0,024	0	0,098	0,015	0,01	0,061	0	0	0,036	830	3600	350	7200	947	9,8	32,2
27	3,21	2,57	0,28	0,024	0	0,098	0,015	0,01	0,061	0	0	0,036	830	3600	350	14400	912	5,8	25,3
28	3,21	2,57	0,28	0,024	0	0,098	0,015	0,01	0,061	0	0	0,036	830	3600	300	900	1348	2,8	36,7
29	3,21	2,57	0,28	0,024	0	0,098	0,015	0,01	0,061	0	0	0,036	830	3600	300	1800	1282	4,1	33,3
30	3,21	2,57	0,28	0,024	0	0,098	0,015	0,01	0,061	0	0	0,036	830	3600	300	3600	1329	2,7	33,6
31	3,21	2,57	0,28	0,024	0	0,098	0,015	0,01	0,061	0	0	0,036	830	3600	300	7200	1021	4,7	32,2
32	3,21	2,57	0,28	0,024	0	0,098	0,015	0,01	0,061	0	0	0,036	830	3600	300	14400	973	4	29,3
33	3,4	2,41	0,15	0,064	0	0	0	0,017	0,015	0	0	0	927	7200	260	7200	1528	1,9	
34	3,4	2,41	0,15	0,064	0	0	0	0,007	0,015	0	0	0	927	7200	273	7200	1522	3,1	
35	3,4	2,41	0,15	0,064	0	0	0	0,007	0,015	0	0	0	927	7200	288	7200	1470	3,4	
36	3,4	2,41	0,15	0,064	0	0	0	0,007	0,015	0	0	0	927	7200	316	7200	1326	4	
37	3,4	2,41	0,15	0,064	0	0	0	0,007	0,015	0	0	0	927	7200	357	7200	1105	9,6	
38	3,4	2,41	0,15	0,064	0	0	0	0,007	0,015	0	0	0	927	7200	371	7200	1062	10,5	
39	3,45	2,48	0,4	0,15	0	1,5	0,3	0,012	0,013	0	0	0	927	7200	260	7200	1600	3	43
40	3,45	2,48	0,4	0,15	0	1,5	0,3	0,012	0,013	0	0	0	927	7200	288	7200	1510	4,8	39,5
41	3,45	2,48	0,4	0,15	0	1,5	0,3	0,012	0,013	0	0	0	927	7200	302	7200	1400	7	36
42	3,45	2,48	0,4	0,15	0	1,5	0,3	0,012	0,013	0	0	0	927	7200	316	7200	1370	8	35,5
43	3,45	2,48	0,4	0,15	0	1,5	0,3	0,012	0,013	0	0	0	927	7200	330	7200	1230	11	28
44	3,45	2,48	0,4	0,15	0	1,5	0,3	0,012	0,013	0	0	0	927	7200	343	7200	1200	12,5	28,5
45	3,45	2,48	0,4	0,15	0	1,5	0,3	0,012	0,013	0	0	0	927	7200	357	7200	1060	13,8	27
46	3,45	2,48	0,4	0,15	0	1,5	0,3	0,012	0,013	0	0	0	927	7200	371	7200	1040	15	26,5
47	3,45	2,48	0,4	0,15	0	1,5	0,3	0,012	0,013	0	0	0	927	7200	385	7200	1090	20	23
48	3,45	2,48	0,4	0,15	0	1,5	0,3	0,012	0,013	0	0	0	927	7200	400	7200	1010	16,3	21,5
49	3,85	2,9	0,61	0,08	0	1,5	0,47	0,01	0,05	0	0	0	900	7200	370	7200	875	6,2	28
50	3,85	2,9	0,61	0,08	0	1,5	0,47	0,01	0,05	0	0	0	900	7200	320	7200	1161	3	38
51	3,85	2,9	0,61	0,08	0	1,5	0,47	0,01	0,05	0	0	0	900	7200	270	10800	1275	1,5	44

The developed test database contains at the moment 280 records; its fragment is shown in Table 1. Here it should be noted that in the described experiments certain parameters were either omitted or not provided in the publications. Therefore the table also includes areas for which no data are available. For each record included in the database, the developed database also contains information about the publication from which it was drawn. The database forms the basis for one of the modules of the CAPCAST expert system, which is intended to complement the knowledge base of the system with the rules generated from the knowledge accumulated in the literature.

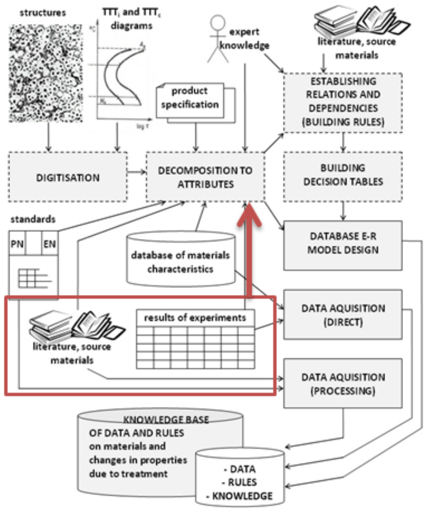


Fig. 1. Schematic decomposition of attributes and data acquisition system for the CAPCAST knowledge base [1]

Having at one's disposal the integrated knowledge relating to the production of ADI, one can try to design inference algorithms and systems enabling automatic processing of this knowledge [11]. Attempts were made to construct inference algorithms and systems based on artificial intelligence methods. This article presents the results of the use of artificial neural networks and one of the methods in the area of data mining called regression trees to develop models of a particular phenomenon.

3. The use of artificial neural networks in modelling of the ADI manufacturing process

Artificial neural networks (ANN) are mathematical structures, the operation of which is a simplified representation of the human brain [12, 13]. An artificial neural network consists of a group of interconnected cells that conduct parallel processing of information. During the learning process, basing on empirical cases, appropriately designed neural networks can reproduce the interdependencies that exist between various parameters of the examined phenomena. Using artificial neural networks, the collected experimental data on production parameters of ADI can form a basis for the development of metamodels of this process.

To accomplish this, it is necessary to establish a target for the model construction and define its basic assumptions. Consequently it has been assumed that the developed model will determine the impact of selected parameters of the heat treatment, i.e. T_i - temperature of isothermal transformation, t_i – time of isothermal transformation (these are the explanatory variables), on selected properties of the ADI, i.e. tensile strength - Rm, elongation - A hardness - HRC (these are the explained variables). The problem stated in this way requires filtering of global dataset to examine its homogeneity in respect of the starting chemical composition. The analysis should cover only the cases belonging to the cast irons included in the same group, e.g. unalloyed or alloyed Ni-Mo, Ni-Cu-Mo, Cu-Mo, Ni-Cu, Mn-Cu with similar contents of alloying elements. The adopted objective analysis also assumed the application of filter onto the austenitizing process parameters and extracting only the cases with similar ranges of values for the austenitizing temperature (T_A) and austenitizing time (t_A). Analysis of the global dataset allowed identifying the largest subset for the Ni-Mo cast iron, meeting the filtering criteria listed in Table 2.

Table 2.
The adopted filtering criteria

Ni	Mo	temp. A, °C	time A, s
1.53 ±	0.32 ±	900 ±	7200 ±

3.1. The project of artificial neural network

Of the 280 cases included in the global table, 70 cases met the preset criteria, which in further work were adopted as a base set for the analysis using ANN.

To determine the exact and optimal network architecture, the STATISTICA software and its module called *Automatic Neural Networks* were used. The generated subset was divided into training set (70%), test set (15%) and validation set (15%). Here attention deserves the fact that in the STATISTICA program the test set is a set used for ongoing monitoring of the network learning process, while the validation set is a set whose task is to evaluate the network after the completion of the learning process. In the literature, these terms are used in an opposite meaning. In this study, the authors cite the names used in accordance with the program.

Several dozens of architectures with different numbers of hidden neurons and various functions of activation (linear, sigmoidal, tangesoidal and exponential) were tested. Of all the networks generated by the program, eventually one network of the MLP2-7-3 type, characterized by top quality parameters, was selected (Fig. 2). The quality of the network is evaluated using the coefficient of linear correlation between the actual values and the theoretical values calculated by the model and comprised in the range of [0.1]. The closer to 1 is the quality of the network, the closer are the network responses to the values expected. The quality of validation is generally lower than the quality of training, because in this case, the network is tested on a dataset that was not previously analyzed. The parameters of quality and the value of other characteristics that define the developed network are shown in Table 3. The employed network learning algorithm was based on the BFGs Broyden-Fletcher-Goldfarb-Shanno method [12]. The number reported in the description of the applied learning algorithm (Table 3) indicates in which epoch training of the network has been completed. In the case of MLP2-7-3 network, the end of the training process took place in the 289 epoch. The applied function of error is the sum of squared deviations between the value set and the output of the network (indicated in Table 3 as SOS).

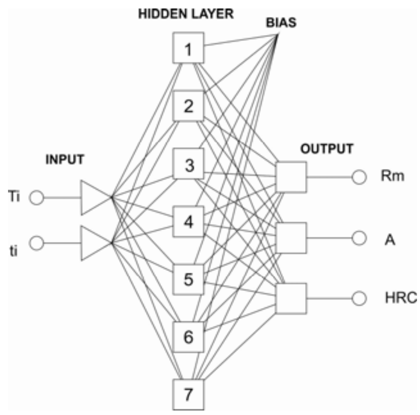


Fig. 2. The structure of the MLP network used for prediction

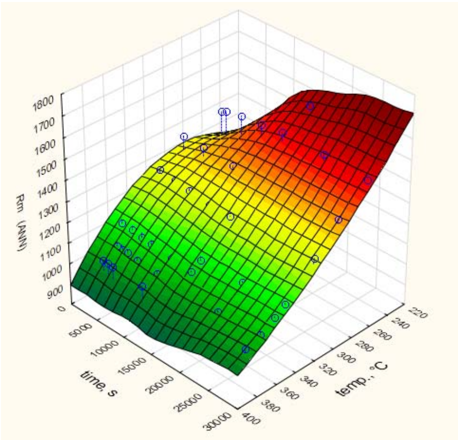
Table 3.
Summary of the network learning process

Network name	MLP 2-7-3
Quality (learning)	0,968649
Quality (testing)	0,964943
Quality (validation)	0,962866
Learning algorithm	BFGS 289
Function of error	SOS
Activation (hidden)	Logistic (Sigmoidal)
Activation (output)	Logistic (Sigmoidal)

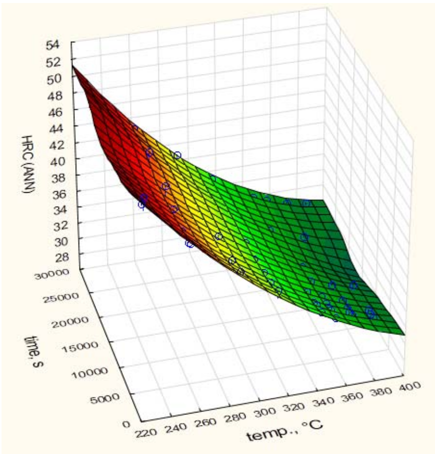
3.2. Analysis of the results of modelling using the network developed

Figure 3 presents models of relationships generated by the network for selected properties of cast iron, such as Rm, HRC, A, plotted as a function of the time and temperature of isothermal holding. For comparison, Figure 4 shows the same relationships but plotted from the experimental data.

a)



b)



c)

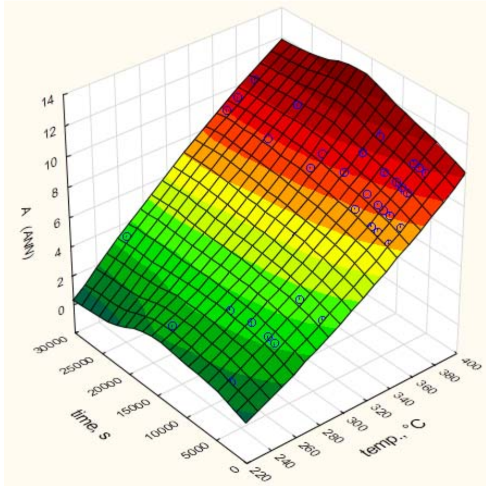
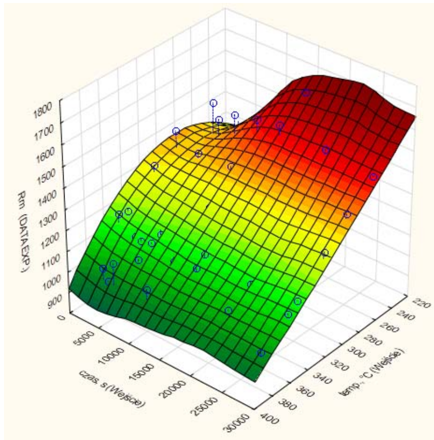
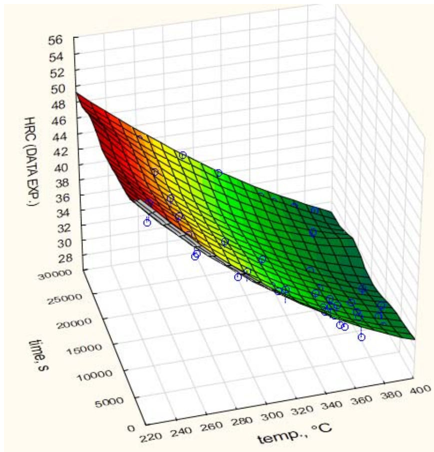


Fig. 3. Models of relationships generated by the neural network for selected cast iron properties: a) Rm, b) HRC c) A plotted as a function of the time and temperature of isothermal holding

a)



b)



c)

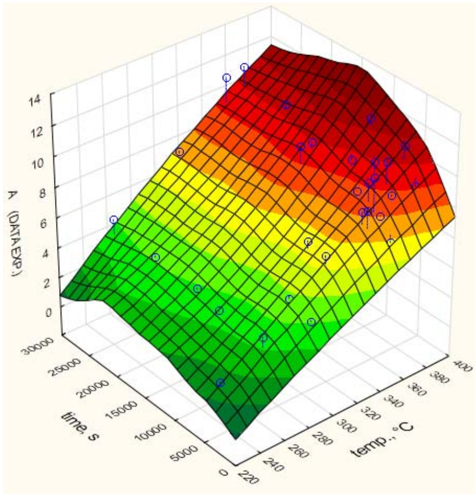


Fig. 4. Models of relationships generated from the actual data for selected cast iron properties: a) Rm, b) HRC, c) A plotted as a function of the time and temperature of isothermal holding

The results should be regarded as preliminary, indicating the possibility of using AAN to build a model of the ADI manufacturing process based on integrated data derived from various scientific publications. The development of this approach and refining of the model can be implemented in several ways:

- primarily by complementing the source database with significantly larger number of the training data obtained from further publications or from properly designed experiment;
- optimization of network parameters;
- possibly also by building a neural network for a different configuration of dependent and independent variables based on the training datasets filtered from a global set according to criteria other than those specified in this work.

4. Use of data mining methods

Artificial neural networks allow modelling the properties of designed materials, including ranges of variations in the independent variables such as the temperature and time of the austenitizing treatment, for which no experimental data are available. The weakness of models based on neural networks is, however, their characteristic feature, due to which the knowledge about the examined phenomena generated from training data is hidden in the weights assigned to the inputs to neurons. For a human this form of the knowledge recording is quite confusing and unverifiable.

The study of relationships in a training dataset can also be carried by other machine learning techniques known as regression trees. Regression trees based on CART (Classification and Regression Trees) algorithm allow for an iterative analysis of the dataset. Each of the independent variables is successively taken into account. For each of the variables is determined its validity corresponding to the readiness to participate in the division of the set into partitions. As a result, the training sample is divided according to variables and specific points of division for tests based on the criterion of the smallest square deviations. Finally a tree is obtained, which is a graphical representation of decision rules constructed on the basis of the volatility of independent variables [14, 15].

For this dataset, three regression trees were constructed, one for each dependent variable (Rm, HRC, A). Examination of the validity of predictors has showed that for the mechanical properties definitely more responsible is the austenitizing temperature than time, which is confirmed by scatterplots for these pairs of variables (Fig. 4a).

The advantage of regression trees in combination with linear regression models is the lack of specific assumptions about the volatility of variables, their expected value and variance. There is no need to examine the autocorrelation of residues or assumptions about normality.

Models obtained by induction of trees allow capturing both linear and non-linear correlations and avoid the need to study only the quantitative predictors.

The decision tree for the dependence shown in Figure 4a has a graphic form of regression tree shown in Figure 5 and may give rise to the creation of its representation in the form of rules such as for example:

R1: *to obtain the highest strength (with average of 1512MPa), the austenitizing temperature should be less than 275deg.C and the austenitizing time should be longer than 4950ms;*

R2: *the lowest strength values with an average value = 1027MPa were recorded for the highest austenitizing temperature above 377deg.C.*

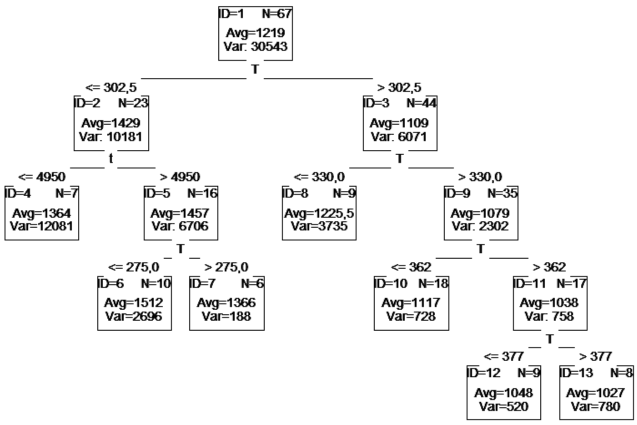


Fig. 5. Regression tree for the dependent variable R_m

The constructed regression tree allows the assessment of quantitative dependencies between the explanatory variables (predictors) and the dependent variable. Each generated leaf represents the path of inference, and thus allows creating a rule. A sample tree shown in Figure 5 allows formulating the seven rules for different areas of variations in the tensile strength.

5. Conclusions

The work presented included the implementation of metamodels predicting the value of individual mechanical properties with the help of automated artificial neural networks (ANN) and regression trees (CART).

The benefits afforded by the use of tools in the field of artificial intelligence, machine learning in particular, have been demonstrated. The integration of knowledge in the form of experimental data and patterns obtained with the help of intelligent algorithms allows: (1) an approximation of the unknown values of mechanical parameters of the tested materials based on experimental data, and (2) the formalization of rules which are an algorithmic record of the acquired knowledge.

The main differences between the presented tools are: (1) inability to offer interpretation of metamodel obtained with the help of neural networks; (2) inability to formulate rules of inference for ANN; (3) lack of continuity in the area offorecasting with the aid of decision trees (CART); (4) inability to create a single model for the three dependent variables in the case of CART regression trees.

The individual characteristics of each of the metamodels allow concluding that the full range of benefits of metamodelling the user gets only with the use of two algorithms.

To sum up it can be stated that the main objective of the article was to present and test a basic version of the concept, which is based on the integration of experimental results relating to the production of ADI, and examine the possibility of using this concept in the design of inference algorithms and systems, which will enable its automatic processing. The development and provision of such a system will in the future prevent the multiple repetition of experiments which have already been carried out and can be a source of inspiration for:

— finding new areas of research;
— scanning those portions of knowledge that can be used to solve a particular problem;
— the creation of new knowledge (discovering relations and dependencies that are not visible in single experiments, but can be revealed during comparison of a large number of studies);

Acknowledgements

Financial assistance of the NCN Project No. 2013/11/N/ST8/00326 is hereby gratefully acknowledged.

References

[1] Mrzygłód, B. & Regulski, K. (2011). Model of knowledge representation about materials in the form of a relational database for CAPCAST system. *Archives of Foundry Engineering*. 11(3), 81-86.

[2] Mrzygłód, B. & Ścira, K. (2012). Module to generate rules for the knowledge base in a CAPCAST expert system. *Archives of Foundry Engineering*. 12(2), 167-170.

[3] Olejarczyk-Wożeńska, I., Adrian, A., Adrian, H. & Mrzygłód, B. (2012). Parametric representation of TTT diagrams of ADI cast iron. *Archives of Metallurgy and Materials*. 57(2), 613-617.

[4] Mrzygłód, B., Adrian, A., Regulski, K., Olejarczyk-Wożeńska, I., Kluska-Nawarecka, S. (2013). The exploitation of TTTi diagrams in the CAPCAST system. *Transactions Of Foundry Research Institute*. 53(4), 45-56.

[5] Mrzygłód, B., Kluska-Nawarecka, S., Kowalski, A. & Wilk-Kołodziejczyk, D. (2013). Application of TTT diagrams low-alloy ductile iron to assist the manufacturing process of cast iron. Transactions Of Foundry Research Institute, 53(4), 85-111.

[6] Zahiri, S.H. & Davies C.H.J., (2003). Simultaneous prediction of austemperability and processing window for austempered ductile iron. *Materials Science and Technology*. *19*, 1761-1770.

[7] Dymski, S. (1999). Formation the structure and mechanical properties of ductile cast iron during isothermal bainitic transformation. Thesis No. 95. Bydgoszcz: Publishing Department *ATR*. (in Polish).

[8] Putatunda, S.K. (2001). Development of austempered ductile iron (ADI) with simultaneous high yield strength and fracture toughness by a novel two-step austempering process. *Materials Science and Engineering*. *A315*, 70-80.

[9] Putatunda, S.K. (2001). Influence of austempering temperature toughness of low magnese austempered ductile iron (ADI), *Materials and Manufacturing Processes*. 16(2).

[10] Janowak, J.F. & Morton, P.A. (1984). A guide to mechanical properties possible by austempering 1,5% Ni-0,3% Mo ductile iron, *AFS Transactiion.* 5(92), 489-498.

[11] Kochański, A., Kozłowski, J., Kłębczyk, M., Perzyński, P. (2010). Modeling properties of ductile iron ADI using literature data developed using the methodology of data preparation. *Polish metallurgy in years 2006-2010*. Krakow: WN Akapit. (in Polish).

[12] Tadeusiewicz, R. (1993). Neural networks. Warszawa: AOF.

[13] Lula, P., Paliwoda-Pękosz, G., Tadeusiewicz, R., (2007), Artificial intelligence methods and their applications in economics and management. Krakow: *Publishing University of Economics.*

[14] Regulski, K., Rojek, G., Skóra, M., Kusiak, J. (2012). Data exploration approach in control of metal forming manufacturing chain: example of fasteners production, Metal Forming 2012: proceedings of the 14th international conference on Metal Forming: September 16–19, 2012, Krakow, Poland, ed. Jan Kusiak, Janusz Majta, Danuta Szeliga, Steel Research International; spec. ed., 1319-1322.

[15] Regulski, K., Szeliga, D. & Kusiak, J., (2014). Data Exploration Approach Versus Sensitivity Analysis for Optimization of Metal Forming Processes. *Key Engineering Materials*. 611–612, 1390-1395.