Data mining tools in identifying the components of the microstructure of compacted graphite iron based on the content of alloying elements

Dorota Wilk-Kolodziejczyk¹ · Krzysztof Regulski¹ · Grzegorz Gumienny³ · Barbara Kacprzyk³ ·
Stanisława Kluska-Nawarecka² · Krzysztof Jaskowiec²

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Abstract

The application of data mining techniques in the design of modern foundry materials allows achieving higher product quality indicators. Designing of a new product always requires thorough knowledge of the effect of alloying elements on the microstructure and hence also on the properties of the examined material. The conducted experimental studies allow for a qualitative assessment of the indicated relationships, but it is the use of intelligent computational techniques that enables building an approximation model of the microstructure and, owing to this, make predictions with high precision. The developed model of prediction supports the technology-related decisions as early as at the stage of casting design and is considered the first step in selecting the type of material used.

Keywords Compacted graphite iron · Data mining · Support vector machine · Decision trees · Artificial neural networks

1 Introduction

Materials Engineering is the field of science characterized by an interdisciplinary nature. It uses the knowledge of basic sciences (physics, chemistry, biology) to improve engineering materials. Many modern solutions and designs can be created only with the use of new materials. Owing to the development of materials engineering, we now have materials that allow for the construction of machines working under most extreme conditions. The functional

properties of the objects and devices that are currently in use depend on the properties of materials from which they have been made, while the properties of materials depend on the structure which is formed in the manufacturing process.

With models predicting the microstructure, it becomes possible to improve and automate the process of designing new materials with desired properties. It is essential to define the rules, laws, and relationships existing in the specified area, and then the data mining tools can support the experimental research process. Alloying additives forming part of the material composition influence shaping of the compacted graphite iron structure. However, the relationships are not of a linear nature and, as will be shown later, the traditional methods of regression do not work.

Where statistical tools fail to do their work, models developed in the field of artificial intelligence can prove to be applicable. Very popular in recent years, data mining techniques [1, 2] and machine learning [3] are based on similar principles. To create models and carry out their calibration (training), historical empirical data is used. Based on this data, models are constructed and their task is to capture the data that occur in the relationships between various variables [4–6]. These relationships are used to create prediction models (where the dependent variable is of a quantitative type) or classification models (where the dependent variable is discrete or categorical). The common

✉ Dorota Wilk-Kolodziejczyk
dwilk@agh.edu.pl

Krzysztof Regulski
regulski@agh.edu.pl

Grzegorz Gumienny
grzegorz.gumienny@p.lodz.pl

Stanisława Kluska-Nawarecka
stanislaw.kluska@iod.krakow.pl

Krzysztof Jaskowiec
krzysztof.jaskowiec@iod.krakow.pl

¹ AGH University of Science and Technology, Krakow, Poland

² Foundry Research Institute, Krakow, Zakopiańska 73, Poland

³ Lodz University of Technology, Lodz, Poland

goal of these methods is to provide the possibility of determining the unknown value of the dependent variable based on the values taken by the explanatory variables [7]. In the case under discussion, it is the determination of the content of phase constituents in the microstructure, based on the percent values of the chemical composition and wall thickness. There are very few publications on the influence of alloying elements on the microstructure and properties of compacted graphite iron [8] and [9].

Compacted graphite iron (CGI) occupies a special place as the casting material. This is due to a specific form of graphite and large contact surface with the matrix. The result is the tendency of this cast iron to direct ferritization and a complex of the most interesting properties. Compared to gray iron, CGI has higher mechanical properties and improved ductility. The microstructure of the matrix is less sensitive to the thickness of the casting wall. Compared to ductile iron, the cast iron with compacted graphite has a lower coefficient of thermal expansion, higher thermal conductivity, greater resistance to dynamic changes in temperature, higher vibration damping capacity, and better castability. All these advantages predestine this material for a variety of applications. The first utilitarian use of this cast iron covered brake discs for high-speed railway stock. Currently, this material is mainly used for the construction of blocks of internal combustion engines, exhaust manifolds, and the like cast automotive parts. The interesting complex of properties obtained in this type of cast iron is the object of intensive research and numerous publications [10–17]. By changing the chemical composition, it becomes possible to modify in a wide range the cast iron microstructure, and consequently its properties. There is a fairly large group of publications describing the possibility of obtaining ausferrite in the cast iron with compacted or vermicular graphite and obtain AVI (Vermicular Austempered Iron) or CAVI (Carbide Vermicular Austempered Iron) [18–21]. Ausferrite is a mixture of bainitic ferrite and austenite supersaturated with carbon. The amount of retained austenite in ADI can be up to 40%. It is a desirable component of the microstructure, undergoing under the effect of stress a twinning-induced martensitic transformation with the resulting strengthening. To produce ausferrite, the casting has to be subjected to a heat treatment, which consists in isothermal quenching and holding within the temperature range of austenite $\rightarrow$ bainite transformation. There is also an alternative method of obtaining ausferrite involving a modification of the cast iron chemical composition, using for this purpose molybdenum, copper or nickel added in appropriate proportions.

The use of models of artificial intelligence in microstructure prediction is the subject relatively popular. There are various embodiments of the neural networks to approximate the cement structure [22] and [23], and well-known is also

Fig. 1 Schematic layout of mold components for the vermicularizing treatment of cast iron by Inmold process; 1—downgate, 2—reaction chamber, 3 – mixing chamber, 4—control chamber, 5—pilot casting, 6—overflow

the use of support vector machine (SVM) in classification of the structure of aluminum alloys (AA3002) [24] or zinc alloys (Zircaloy-2) [25]. Quite widespread is the use of cellular automata in the simulation of microstructure evolution [26] and [27].

2 Research methodology

The test metal was melted in an electric induction medium frequency furnace with crucible of 30 kg capacity. The vermicularizing treatment was made by Inmold process. The charge for the furnace consisted of special-purpose pig iron with sulfur concentration of 0.01%; the charge also contained FeSi75 ferrosilicon, FeMn75 ferromanganese and technically pure Mo, Cu, Ni and Cr. The cast iron at a temperature of about 1480 °C was poured to a sand mold shown in Fig. 1.

The gating system incorporates the spherically shaped reaction chamber (2) with $\phi 85$ mm diameter. In this chamber, the Lamet 5504 magnesium master alloy made by Elkem Norway is placed. The composition of the master alloy is shown in Table 1. Behind the reaction chamber, there is the mixing chamber (3), ensuring a very thorough dissolution of the master alloy, and control chamber (4) where the cast iron cooling and solidification process is recorded. The test casting (5) has a stepped configuration

Table 1 The chemical composition of master alloy

Chemical composition, wt%					
Si	Mg	Ca	La	Al	Fe
44–48	5–6	0.4–0.6	0.25–0.40	0.8–1.2	rest

Table 2 The chemical composition of CGI tested

Chemical Composition %	Cr	0–2.81
	Ni	0–21.04
	Cu	0–3.80
	Mo	0–2.44
	Mg	0.015–0.023
	Mn	0.03–1.31
	Si	2.28–2.71
	C	2.91–3.82

with the wall thickness of 3, 6, 12 and 24 mm. The range of the chemical composition of the tested cast iron is shown in Table 2. In the literature, the chamber is most often rectangular. However, in the paper [28], the effect of the shape of the reaction chamber on the graphite shape in the cast iron obtained by Inmold technology was investigated. The chambers have rectangular, cylindrical, and spherical shape. It was shown that the highest graphite coefficient was in cast iron obtained in the mould where the reaction chamber was spherical.

The wide range of the chemical composition used in the tests enabled obtaining the microstructure of a ferritic-pearlitic, pearlitic, austenitic, martensitic, and ausferritic type. Samples for metallographic examinations were cut out from the central part of the stepped casting. Metallographic examinations were carried out at a magnification of 500x under an Eclipse MA200 Nikon optical microscope. The surface content of carbides was examined using an NIS-Elements BR image analyzer. Hardness of the cast iron was measured with an HPO-2400 durometer under the following conditions: ball diameter $\phi = 2.5$ mm, load $F = 1840$ N.

3 Data analysis

There are many dependent variables in the studied problem (the individual components of the matrix) and one (wall thickness) or more (chemical composition) explanatory variables. It is a system very difficult for analysis by the methods of regression, which allow using only one dependent variable.

Table 3 A map of correlations

	Ferrite	Pearlite	Carbides	Martensite	Ausferrite	Austenite
Mn	0.25	0.38	− 0.02	0.075	− 0.46	0.07
Cr	− 0.16	0.28	0.74	− 0.11	− 0.28	− 0.10
Cu	− 0.26	− 0.06	− 0.14	− 0.19	0.36	− 0.18
Ni	− 0.17	− 0.36	− 0.24	0.40	− 0.26	0.93
Mo	− 0.36	− 0.63	− 0.07	− 0.25	0.915	− 0.24
Thickness	0.20	− 0.03	− 0.22	0.01	0.02	− 0.01

3.1 Regression and MARSplines

Studies of the relationships between variables were performed using Pearson's linear correlation coefficient. Correlations for the wall thickness were too weak to make building of regression models possible, and therefore it was necessary to introduce data on the chemical composition to the model developed (Tables 3 and 4).

The correlation coefficients seem promising and by selecting the strongest correlations, respective scatter plots can be made (Fig. 2).

In each of the cases described, the relationships are well visible, but configurations of individual points indicate a strongly non-linear character of these relationships.

A MARSplines model (spline regression) based on all the variables was developed.

Multivariate Adaptive Regression Splines (MARSplines), being a generalized form of regression model, aim to create a model for the prediction of dependent variable based on the volatility of explanatory variables [29–33]. For the analysis of MARSplines, it is not necessary to have a priori knowledge about the form of the relationship between variables. The relationship is determined from the data using basis functions. MARSplines is a multiple linear regression composed of segments. The boundaries of segments are determined from the data and define areas subject to individual linear equations [34] and [35].

Using MARSplines, very poor results of the fit were achieved. The only variable that has been defined as statistically significant was the Mo content. The only notable model was the model for pearlite with 42% fit and for ausferrite with 90% fit ($R^2 = 0.9$).

Let us now examine the model for ausferrite.

$$\text{ausferrite} = 84, 28 - 60, 2 * \max(0; 1, 4 - Mo) \quad (1)$$

Analyzing the scatter plot, it is clear that this fit is false as a result of the selection of cases. If the model was built on the basis of samples containing molybdenum (removing the cases in which the content of $Mo = 0$), the chart would be as shown in Fig. 3.

The fit is in this case unsatisfactory. By examining the data set, one can specify the cases for individual factors (explanatory variables), in which the content is different

Table 4 A map of correlations

	Ferrite	Pearlite	Carbides	Martensite	Ausferrite	Austenite
Mean (observed)	8.21	34.57	8.09	7.19	35.27	6.59
Standard deviation (observed)	14.47	35.57	13.42	23.35	43.93	22.76
Mean (predicted)	8.21	34.57	8.09	7.19	35.27	6.59
Standard deviation (predicted)	5.55	23.41	1.34	6.00	41.68	5.61
Coefficient of determination R^2	0.15	0.43	0.01	0.07	0.90	0.06

Fig. 2 Scatter plots for Mo: ferrite; Mo: pearlite; Cr—carbides; Ni—martensite; Mo—ausferrite; Ni—austenite

Fig. 3 A molybdenum : ausferrite scatter plot for cases containing molybdenum

from zero. Analyzing in this way the influence of individual alloying elements on the components of microstructure (Fig. 4), the following conclusions are drawn:

- Cr: an increase in its content favors the formation of carbides,

Fig. 4 The effect of various alloying elements on microstructure

- Ni: present in small concentrations it supports the formation of ferrite and pearlite, whereas in the range of 5–9% it promotes the formation of martensite; in higher concentrations it behaves as an austenite-forming element,
- Mo: it allows for the formation of ausferrite.
- Cu: it is the strongest pearlite-forming additive.

The quality of predictive models can be assessed in each case by the coefficient of determination R^2 . It determines the extent to which the model is fit to the empirical data, that is, the degree to which it is capable of explaining the variability of the dependent variable.

3.2 Artificial neural networks

Artificial neural networks are mathematical structures consisting of layers of neurons that are simple calculation tools based on the function of activation and weights for multiplication of the input signals. The principle of operation of neural networks is based on processing a set of input signals independently by each neuron in each layer, where the decisive influence on the output signal have the weights on

Table 5 The results yielded by artificial neural networks

Error (validation)	179.2556		
Error (testing)	57.22190		
Error (training)	217.0059		
Quality (validation)	0.907	Activation (output)	Logistic
Quality (testing)	0.989	Activation (hidden)	Tanh
Quality (training)	0.974	Error function	SOS
Network name	MLP 6-11-6	Learning algorithm	BFGS 146

the inputs to each neuron. Neurons are connected together in series between the layers. Literature on artificial neural networks is very extensive, as this is the tool known and applied for many years in the data analysis. It is enough to give a few examples of the application of neural networks in metals engineering [36–40]. The essence of the training of neural network is based on the modification of weights at the inputs to the neurons. The modification is performed with the learning algorithms based on optimization of the root mean square error at the output from the network with respect to the experimental observations. The modification of weights is done iteratively, and the training iterations are

called epochs. There is a risk of overtraining the network; this happens when the model becomes too fit to empirical data and loses its ability to make generalizations in cases which have not been reflected in the training data set.

The described analysis uses the model of artificial neural network which has yielded very satisfactory results (Table 5).

Let us keep in mind that, in fact, neural networks do not provide the possibility of developing a model with more than one output variable. The technique of the network training used here is applied in sequence to several models, where each of these models has a different output variable, and then the same network architectures and weights of neurons are tested for different output variables. In the case under discussion, the fits for each component are presented in Table 6.

For analysis, the MLP 6-11-6 network has been chosen. The notation defines the network architecture: 6 input neurons (one signal for each variable); 11 neurons in the hidden layer and 6 neurons at the output specifying the content of individual phase constituents. As a function of activation, the network of a given architecture uses hyperbolic tangent function in the hidden layer and logistic function in the output layer. As a method for the error calculation, the sum of squares is used, and as a training algorithm—an optimization method based on the Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm. Thus, designed network reflects the input data with the correlation of from 0.87 for ausferrite to 0.99 for austenite and martensite, resulting for some constituents in $R^2 = 0.99$, which is a nearly perfect result.

Table 6 ANN fit for individual components

	Austenite	Ausferrite	Martensite	Carbides	Pearlite	Ferrite
Mean of squared residuals	1	376.04	0.5	8	23.48	25.27
Mean absolute error	0	7.22	0.3	2	3.08	1.91
Relative mean square error	169362563	0.63	618320.8	92073395	1919011021.96	530368731299.93
Relative mean deviation	1209	0.66	72.2	1241	6513.89	115775.56
Correlation coefficient	0.99	0.93	0.99	0.99	0.99	0.95
Coefficient of determination R^2	0.99	0.87	0.99	0.96	0.98	0.90

Italicized entries are the most important indicators

The network prediction charts are show in Fig. 5.

A typical feature of this model is that its worst prediction is for ausferrite. Obviously, the network trained on the basis of all constituents is unable to correctly predict the content of ausferrite. Presumably, the relationships valid for this particular constituent are different than for other constituents.

3.3 Support vector machine (SVM)

In non-linear models, the methods of regression become less accurate. An alternative to artificial neural networks is the method of Support Vector Machine (SVM), very fashionable in recent years. This is a binary classifier defining from the training data the widest possible boundary

between classes. In the applied strategy of cascade classifiers, this tool is also suitable for solving the problems where the dependent variable can take multiple classes of values. In the case of continuous dependent variable, the algorithm uses discretization for a fixed number of intervals. A solution to the problem of non-linearity is kernel trick - mapping of training vectors to an area of larger dimension, where one can expect them to have linear separability. The calculations are carried out using kernel functions [41] and [42]. SVM allows building models for a single dependent variable. Hence, the necessity of approximation using six different models built on the same predictors. The models and the quality of predictions are summarized in Table 7 and visualized in respective graphs (Fig. 6).

Fig. 5 Predicting the input variables for MLP 6-11-6 network

Table 7 The SVM models for individual components

Model specification	Ferrite	Pearlite	Carbides	Martensite	Ausferrite	Austenite
Number of predictors	6	6	6	6	6	6
SVM type	Regression of type 1	Regression of type 1	Regression of type 1	Regression of type 1	Regression of type 1	Regression of type 1
Kernel type	RBF	RBF	RBF	RBF	RBF	RBF
WN number	56 (41 related)	72 (60 related)	45 (28 related)	34 (24 related)	50 (31 related)	33 (19 related)
Observed mean	7.56	32.88	8.00	2.93	37.74	10.67
Predicted mean	5.82	31.27	6.00	3.09	43.22	8.19
Observed standard deviation	13.98	37.10	13.37	12.99	45.19	29.70
Predicted standard deviation	9.40	35.48	10.78	7.32	44.79	25.19
Root mean square error	65.86	189.29	74.98	135.84	421.25	63.20
Mean of the error	1.74	1.62	2.00	−0.16	−5.48	2.48
Standard deviation of the error	8.02	13.82	8.52	11.79	20.01	7.64
Mean absolute error	4.72	8.49	4.42	5.02	10.05	4.64
Ratio of standard deviations	0.57	0.37	0.64	0.91	0.44	0.26
Correlation	0.84	0.93	0.77	0.44	0.90	0.97
Coefficient of determination R^2	0.70	0.86	0.59	0.19	0.81	0.95

Italicized entries are the most important indicators

In the majority of cases, SVM gives the fit worse than neural networks. Based on the scatter plot (fit), it can be noted, however, that in the case of ausferrite, training of the model is much more efficient, despite the worse coefficient of determination R^2 .

Despite the relatively accurate results, both ANN and SVM methods have one common drawback. As a model, they actually represent a black box. Their character is difficult to interpret for a man, so their use is limited to the implementation of computer tools, and the only knowledge that can be drawn is in the form of numerical results [43]. The situation is quite different in the case of decision trees (Table 8).

3.4 CART trees

CART Trees (Classification And Regression Trees) belong to a group of algorithms of the induction of decision trees. Decision trees are a form of knowledge representation relatively easy to interpret both at the stage of knowledge acquisition (data mining) and also in the phase of its use in the decision-making process. The algorithm has already been repeatedly described in the literature [44–46]. The tree induction algorithm is iteratively dividing the training data

set into partitions, and the division goes on until all the partitions become uniform, which can be determined from the least squared deviation in the case of regression trees and the cost of resubstitution. During the construction of regression trees, the low value of the resubstitution cost is provided by the dependent variable whose value is close to or equal to the average in a given leaf. The best division of the node is the one in which there is the largest decline in the cost of resubstitution. CART tree is a graphical representation of the rules, where each node represents a test on the internal variables, each arc represents a single result of a test, each leaf represents a single class of values. Here, it should be added that in a properly built model, to one dedicated node are always assigned higher values, and to the second node, the values lower than the values in the parent node. The division is based on the variance or standard deviation. The node becomes most homogeneous in the situation when all the cases contained therein are equal to the average. In a manner similar to the classification trees, the division of the tree begins with the whole set of observations and theoretically ends when every case is assigned to a separate leaf. Generally speaking, the cost of resubstitution decreases with the increasing number of end nodes in the model.

Fig. 6 Predicting the input variables for SVM models

Regression trees are usually chosen as a method of prediction taking into consideration the advantages offered by these models, which include: (1) no need to verify the assumptions concerning the form of relationship or the normality of the distribution of variables; (2) no need for recoding and standar-

dization of input variables; (3) high utility of models as tools for the formalization of knowledge—easy interpretation.

Like in previous models, also in the CART trees, each dependent variable must be treated separately, and therefore, six independent trees are to be built for the same predictors.

Table 8 CART fit for individual components

	Austenite	Ausferrite	Martensite	Carbides	Pearlite	Ferrite
Mean of squared residuals	14.24	195.91	15.25	82.76	126.39	74.72
Mean absolute error	1.21	3.99	1.30	5.89	6.98	5.32
Relative mean square error	47.59	0.03	0.00	2.41	1.35	7.55
Relative mean deviation	2.05	0.05	0.00	1.04	0.31	0.88
Correlation coefficient	0.99	0.91	0.99	0.80	0.95	0.84
Coefficient of determination R^2	0.98	0.83	0.98	0.64	0.90	0.71

Italicized entries are the most important indicators

Fig. 7 The validity of factors predicted by CART for individual components

CART model is the best to predict austenite and martensite and the worst to predict carbides and ferrite.

CART models do not show a better fit than the models presented previously, but they have one important advantage—they allow the user to read complicated relationships between numerous predictors. They also allow keeping track of the

importance of individual factors. For example—examining the impact of casting wall thickness, the following relationships can be observed for different microstructural constituents:

- ferrite: higher content is recommended for heavy-walled castings;

Fig. 8 CART tree obtained for: **a** martensite $R^2 = 0.98$, **b** austenite $R^2 = 0.98$

- pearlite: wall thickness is of no concern;
- carbides: heavy sections in castings with a low content of Cr reduce the content of carbides;
- martensite: in castings with a low content of Ni and Mn, the wall thickness above 12 mm supports the presence of martensite;
- ausferrite: thickness has no effect on the content of ausferrite (only Mo);
- austenite: thickness has no effect on the content of austenite (only Ni).

Similarly, we can study the influence of alloying elements in mutual interactions—option in other models not available. Each of the trees will independently evaluate the validity of the predictors; a comparison of the validity is shown in Fig. 7.

The best models of trees for the martensite and austenite are illustrated by the diagrams in Fig. 8. In both cases, the coefficient of determination is $R^2 = 0.98$, which is the result slightly inferior to ANN, but superior to SVM.

Decision trees as a graphical representation of the rules can be saved in a text form. Rules allowing for prediction of the content of each phase constituent together form a knowledge base that allows for the identification of AVI microstructural constituents based on the cast iron chemical composition. Applying trees or rules, user can predict the

microstructure, even without the use of other computer tools. A sample rule derived from the tree for the martensite will have the following form (Fig. 8, left branch):

```

if ( $Ni \leq 2.05$ )
  and ( $Mn \leq 0.03$ )
  and ( $thickness \leq 18$ )
  then (martensite;  $AVG = 0.0$ ;  $VAR = 0.0$ )
if ( $Ni \leq 2.05$ )
  and ( $Mn \leq 0.03$ )
  and ( $thickness > 18$ )
  then (martensite;  $AVG = 0.57$ ;  $VAR = 1.95$ )
  
```

4 Conclusions

For data derived from the studies of AVI iron, devoted mainly to the effect of alloying elements and casting wall thickness on the matrix components (microstructure), the following models were used:

- linear regression models,
- segmental regression models with MARSplines algorithm,
- models of artificial neural networks,
- models based on the method of support vector machine (SVM),
- models using classification and regression trees—(CART).

The best results in the approximation, the user can obtain working on the hybrid models, where the best model is selected for individual components. A comparison of the related issues is shown in Table 9.

In the control of industrial processes, hybrid or heuristic models have long been used; they enjoy great popularity giving better results than uniform tools [47–52]. The integration of input data [53] or of the results of such differentiated solutions is a separate issue, where an important role will have the semantic modelling, including ontologies [54], but this is the topic for an entirely new publication.

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Table 9 CART fit for individual components

	Model	Coefficient of determination R^2
Austenite	ANN	0.99
	SVM	0.95
	CART	0.98
Ausferrite	ANN	0.87
	SVM	0.81
	CART	0.83
Martensite	ANN	0.99
	SVM	0.19
	CART	0.98
Carbides	ANN	0.96
	SVM	0.59
	CART	0.64
Pearlite	ANN	0.98
	SVM	0.86
	CART	0.90
Ferrite	ANN	0.90
	SVM	0.70
	CART	0.71

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