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METHODOLOGY FOR THE CONSTRUCTION OF A RULE-BASED KNOWLEDGE BASE ENABLING THE SELECTION OF APPROPRIATE BRONZE HEAT TREATMENT PARAMETERS USING ROUGH SETS

METODYKA BUDOWY REGUŁOWEJ BAZY WIEDZY UMOŻLIWIAJĄCEJ DOBÓR ODPOWIEDNICH PARAMETRÓW OBRÓBKI CIEPLNEJ BRĄZÓW Z ZASTOSOWANIEM ZBIORÓW PRZYBLIŻONYCH

Decisions regarding appropriate methods for the heat treatment of bronzes affect the final properties obtained in these materials. This study gives an example of the construction of a knowledge base with application of the rough set theory. Using relevant inference mechanisms, knowledge stored in the rule-based database allows the selection of appropriate heat treatment parameters to achieve the required properties of bronze. The paper presents the methodology and the results of exploratory research. It also discloses the methodology used in the creation of a knowledge base.

Keywords: application of information technology to the foundry industry, heat treatment, classification algorithms, rough sets, data mining

Decyzje dotyczące odpowiedniej metody obróbki cieplnej brązów mają wpływ na uzyskanie końcowych własności tych materiałów. W pracy przedstawiono przykład budowy bazy wiedzy z zastosowaniem teorii zbiorów przybliżonych. Wiedza zgromadzona w bazie reguł umożliwia za pomocą mechanizmów wnioskowania dobór odpowiednich parametrów obróbki w celu uzyskania pożądanych własności brązu.

1. Introduction

In determination of the properties of new materials, experiment and materials research play the most important role. On this basis, using samples, one can collect data on the material properties. An obstacle here is usually the limited number of samples as well as the limited budget expenditures for studies and research. Thus, in most cases, the researcher can take only a few measurements, on the basis of which he is expected to draw conclusions about the properties of the material. Extrapolation of the results to draw general conclusions for new materials entails the use of statistical tools, which help to avoid a methodological mistake.

In a situation when the researcher can use a larger number of the measurements, such conclusions may also comprise the methods of treatment prepared in several scenarios. Each new parameter of the treatment considerably increases the possible space of results, hence the number of measurements necessary for statistical analysis increases exponentially.

Experimental studies for new types of bronze conducted at the Foundry Research Institute in Cracow allowed collecting 82 samples from 7 melts undergoing different modification [1]. The collected data were subjected to statistical analysis and exploratory analysis. Based on the results of these analyses, it was possible to create a knowledge base in the form of rules of inference about the heat treatment scenarios ensuring the expected mechanical properties. This paper presents the methodology and the results of these studies as well as a methodology serving the creation of a knowledge base.

2. Description and analysis of the experimental data

The analysed data were derived from studies of the effect of heat treatment on the properties of CuAl10Fe3Mn2 alloy. Altogether 84 samples were available. Two samples were removed from the analysis. In one case, the reason was the lack of measurements, in another case, the experimenter indicated the measurements clearly deviating from other data included in the group. Finally, the analysis consisted of 82 records.

The following designations were used: L- as-cast condition; P – quenching at 950°C (using microjet and water as a cooling medium); S1 – tempering at 350°C for 6h and cooling in air; S2 – tempering at 700°C for 6h and cooling in air. The data were systematised and collected in one table, a fragment of which is shown in TABLE 1 below.

After the initial choice of features based on the knowledge of researchers, it was decided to select the following variables: Inoculant {L, M, N, P, S, T, R}, where L – unmodified alloy; Quenching {absent, P}, where P: Quenching at 950°C as above; Tempering {absent, S1, S2}, where S1, S2 as above.

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TABLE 1

Fragment of a collective table showing the results of materials testing

Sample No.	Inoculant	Hardening	Ageing	R_m	$R_{p0,2}$	A_5	Heat treatment
53	S	P	S	826	800	1	PS1
56	S	P	S2	719	411	7	PS2
57	S	P	S2	732	406	9	PS2
58	S	P	S2	758	480	10	PS2
62	T	P	absent	668	548	2	P
63	T	P	absent	757	550	2	P
64	T	P	absent	749	528	2	P

It was decided to create an auxiliary variable describing the course of heat treatment: HT {L, P, PS1, PS2}, where L – as-cast condition, P – sample subjected to quenching, PS1 – sample subjected to quenching and tempering at 350°C, PS2 – sample subjected to quenching and solutionising at 700°C.

An exploratory analysis allowed discovering the correlations that occur in a set of experimental data describing the process of heat treatment to build a model enabling approximation of the unknown variables (tensile strength – R_m; yield strength – $R_{p0.2}$ and elongation – A_5, respectively) for the area of results not included in the measurements. Previous studies of the authors in this field enabled the creation of approximation models using fuzzy logic and decision trees [1-3].

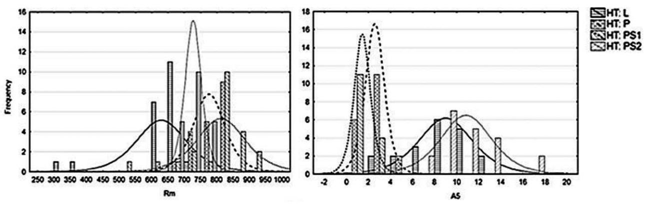

Fig. 1. Categorised histograms for the variables R_m and A5

A relationship between the variables and individual heat treatment scenarios was studied (Fig. 1). In this way it was determined that quenching increases the tensile strength and yield strength, but reduces elongation. The analysis has also shown that tempering S1 reduces the elongation, while tempering S2 causes an opposite effect – the elongation increases compared to samples which are not undergoing this type of treatment.

It is easy to note that in the case of melt T – alloy modified with mischmetal – the decrease has involved all three parameters, i.e. the tensile strength, yield strength and elongation. These were not, however, statistically significant differences, and therefore it was decided to disregard in further analysis the inoculant as a variable.

It has been shown that treatments P (quenching) and PS1 are indistinguishable with respect to mechanical properties. In other words, the samples that undergo tempering or quenching with tempering at 350°C achieve similar mechanical properties (Fig. 2). In subsequent steps of the studies, it was decided to combine these classes into one class P, and therefore the variable HT could assume further only the values of {L, P, PS2}.

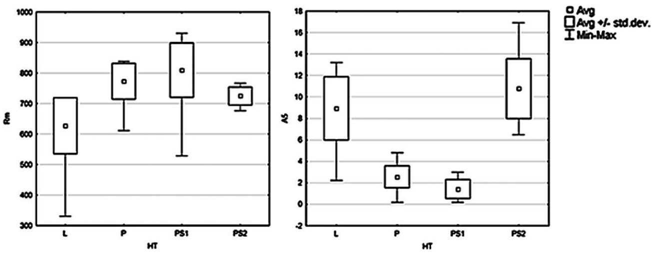

Fig. 2. Categorised box plot diagram for the variables R_m and A5

Using ANOVA analysis, cross tabulation was performed for the variables R_m, $R_{p0.2}$ and A5, obtaining mean and standard deviations in the group of heat treatment scenarios (HT). The results are presented in Table 2.

Fig. 3 shows distributions categorised for particular groups of heat treatment according to each variable. One can observe characteristic differences for the as-cast condition, for quenching, and for quenching with tempering. Depending on the priority established for selected mechanical properties, it is also possible to determine on this basis the weight for each criterion. In the presented results, the priority has not been specified for any of the properties, each was treated with equal importance.

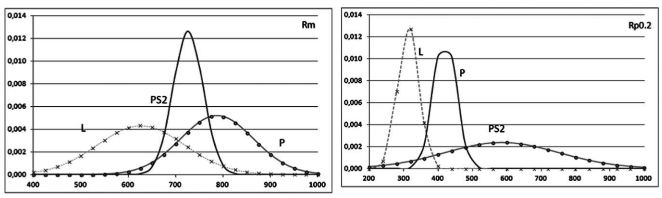

Fig. 3. Distribution of classes for the variable HT used in the discretisation of variables

TABLE 2

Cross tabulation for the variable HT

	R_m	R_m standard deviation	$R_{p0.2}$	$R_{p0.2}$ standard deviation	A5	A5 standard deviation
L	627.0952	92.25124	313.9048	30.7195	8.94000	2.933545
P	786.8864	76.83695	585.7568	166.8436	2.84054	2.956674
PS2	725.9412	31.55644	420.0588	32.1023	10.61765	2.834439
Total	733.3293	99.63775	472.0800	167.9378	6.27568	4.541794

Using thus established groups, the places of cuts in the extent of variables were determined. The cuts allow the discretisation to be performed in such a way as to make the variability gain the greatest discriminative strength. Discretisation in this case becomes necessary due to the relatively small number of measurements, not allowing for the construction of a continuous model but only for the solution of classification problem. In [4], the authors present the methodology for the construction of fuzzy models that also allow specifying the sets of strong discrimination to optimise the classification. In this approach, it was decided to use an analytical technique, allowing the results to be compared with the classification using decision trees.

3. Application of rough set theory

The rough sets theory is based on the notion of approximate information system:

$$S \equiv \ < XAV\rho > \tag{1}$$

where: X – object set, A – attribute set, V – set of attribute values, $\rho\rho$ – function defined on the Cartesian product:

$$\rho{:}X{\times}A{\to}P(V) \tag{2}$$

which assigns for couple $(x, a), x \subseteq X, a \subseteq A$ a subrange P(V) containing the unknown exact value of an attribute a. Also the equivalent formula is being applied:

$$\rho\,(x{,}a) \subset V_a \tag{3}$$

where V_aVa – set of values which can take an attribute a describing the object x.

In our case, X is a set of samples (observations); A is a set of attributes: tensile strength – R_m; yield strength – $R_{p0.2}$, elongation – A_5, and variant of heat treatment HT; V – is a range of values described in former chapter and ρ is the sought classification function.

As can be seen, defined model of an approximate information system is adapted to the situation where the knowledge of the individual sites is incomplete – defines the attributes of the approximations (to the nearest interval). Rough sets were a number of interesting applications (e.g. [7,8,9]), but in the Foundry characterized by far-reaching specifics, existing solutions [3,5,6], as well as presented in this study proposal, have novel character.

The reduct in a rough sets theory means a minimal subset of attributes which is sufficient to discern between objects with different decision values. Based on the calculated reduct it is possible to calculate decision rules. A rule generated by a reduct is able to recognize at least one object. Application of rough sets allows for the induction of 14 rules with RSES program [9]. These rules are shown in Fig. 4. They represent logical implications allowing the inference about the heat treatment. On the left side there are premises of the rule, while on the right side there is a conclusion stating the choice of the variable HT, that is, the heat treatment scenario, and also the support number for each rule validating its reliability.

```
(Rm="(643.0,692.0)")&(Rp0.2="(-Inf,356.0)")=>(HT=L[11]) 11
(Rm="(-Inf,643.0)")&(A5="(7.5,Inf)")=>(HT=L[5]) 5
(Rm="(-Inf,643.0)")&(A5="(2.15,7.5)")=>(HT=L[2]) 2
(Rm="(694.5,702.5)")&(A5="(7.5,Inf)")=>(HT=L[2]) 2
(Rm="(694.5,702.5)")&(Rp0.2="(-Inf,356.0)")=>(HT=L[1]) 1
(Rm="(-Inf,643.0)")&(Rp0.2="(356.0,484.5)")=>(HT=L[1]) 1
(Rm="(694.5,702.5)")&(Rp0.2="(356.0,484.5)")=>(HT=L[1]) 1
(Rp0.2="(484.5,Inf)")=>(HT=P[28]) 28
(A5="(-Inf,2.15)")=>(HT=P[19]) 19
(Rm="(702.5,Inf)")&(Rp0.2="(-Inf,356.0)")=>(HT=P[3]) 3
(Rm="(702.5,Inf)")&(A5="(7.5,Inf)")=>(HT=PS2[14]) 14
(Rm="(643.0,692.0)")&(Rp0.2="(356.0,484.5)")=>(HT=PS2[4]) 4
(Rm="(692.0,694.5)")=>(HT=PS2[1]) 1
(Rm="(702.5,Inf)")&(Rp0.2="(356.0,484.5)")&(A5="(2.15,7.5)")=>(HT=PS2[1]) 1
```

Fig. 4. Rough set rules

The quality of classification using the above rules is shown in Fig. 5 along with the classification matrix. The reader can see, that system is able to predict all cases correctly according to actual observations. Hence it follows that using the specified 14 rules we are able to carry out an error-free classification.

Results of experiments by train&test method: gkndwkkr_v1D

	Predicted						
Actual		L	P	PS2	No. of obj.	Accuracy	Coverage
	L	20	0	0	21	1	0.952
	P	0	34	0	41	1	0.829
	PS2	0	0	20	20	1	1
	True positive rate	1	1	1			

Total number of tested objects: 82
Total accuracy: 1
Total coverage: 0.902

Fig. 5. Rough set rules confusion matrix

4. Summary

The disclosed methods of data mining supported by algorithms of the induction of rules based on the theory of rough sets or decision trees allow for the construction of a knowledge base as a set of rules that enable inference about the possible scenarios of the course of heat treatment. Based on the obtained rules, an error-free classification of appropriate variant of heat treatment parameters to achieve the required properties of bronze can be made. The problem of classification, although known in the industrial issues [10,11], is sensitive to the type, number and characteristics of the learning data. It should be noted, however, that testing proceeded in the space of results based on the stored measurement data. To ensure higher reliability of the obtained results, the proposed methodology should be applied to a larger number of experiments. The disclosed algorithm of induction of inference rules with rough sets theory has, however, the advantage that they are well scalable and provide the ability to automatically generate rules.

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