Multi-scale Approach for Strength Properties Estimation in Functional Materials

I.M. Gitman[1,*], **A.V. Klyuev**[2], **M.B. Gitman**[2], **and V.Yu. Stolbov**[2]

[1] University of Sheffield, Department of Mechanical Engineering, Sheffield, UK
[2] Perm National Research Polytechnic University, Perm, Russia

Received XXXX, revised XXXX, accepted XXXX
Published online XXXX

Key words functional materials, strength properties, microstructure parameters, fuzzy sets
MSC (2010) 00-xx

A new methodology to obtain metallic functional materials with predefined sets of strength properties has been developed. It has been shown that in order to accurately estimate set of material properties at the macro-level, information from the micro-level needs to be taken into account. As a result a two-level estimation model, based on the theory of fuzzy sets, has been proposed. To demonstrate the developed methodology, a reinforcing steel has been analysed. Using microstructural information, derived from an available set of experimentally obtained digital images of material microsections under different heat treatment conditions, macroscopic strength properties of reinforcing steel have been determined.

1 Introduction

In recent years, metallic functional materials [4], with predefined set of performance characteristics such as strength, electrical conductivity, thermal stability, etc., are attracting increasingly growing interest. These effective characteristics can be obtained by using new material manufacturing technologies and/or further mechanical treatment, leading to changes in material microstructure, and thus, desired macroscopic properties.

The main aim of this paper is to develop an effective methodology to estimate materials performance characteristics, e.g. macroscopic properties, based on cognitive analysis of its microstructural parameters through the scrutiny of materials microsections digital images. The main advantage of this methodology is that it does not require the development of complex material models or elaborate empirical relations, linking effective mechanical properties with microscopic grain-phase structure of metals.

Several different approaches to form materials (metals) with predefined mechanical properties can be distinguished in the literature. One of these is the methodology based on the multi-factors framework of designing an experiment [7]. Successfully used to define technological manufacturing processes, allowing to form materials with predefined effective characteristics [1],[15], this methodology, however, has a number of disadvantages. The necessity to perform a large number of costly experiments together with the arguments to define the rationale behind the most significant factors, influencing the forming exploitation properties of the material, are the most notable drawbacks.

Another methodology is based on the development of new constitutive relations, taking into account micro (or meso) mechanical properties of materials in order to describe elasto-plastic or thermo-elastic macroscopic materials behaviour [11],[20]. Note, among others, multi-scale models with evolution constitutive relations of different levels of observation [19]. This approach assumes analyses of different material behaviour in different loading conditions, which, again, results in the large number of experiments (and / or computational experiments).

The third approach offers the formulation of empirical relations between material mechanical properties and its microstructure, e.g. Hall-Petch [16],[8] law, linking the strength of some crystal materials and the parameters of their grains. Further work, refining this law, is based on the increase of the micro parameters number to improve the accuracy of the model (see [6] where an empirical relation is developed to estimate mechanical properties of steel as a result of three-parametrical microstructural analysis). These relationships are especially useful for particular types of steels and structures, where estimation of materials macro-characteristics can be done fairly quickly and accurately. However, in our view, the proposed methodology [6] requires a serious justification when generalised to other classes of materials.

* Corresponding author E-mail: i.gitman@sheffield.ac.uk, Phone: +44 114 222 7728, Fax: +44 114 222 7890

The methodology, proposed in this paper, does not require a specific format of approximation function, (e.g. constitutive relation) and the methodology of approximating the results (e.g. least square method); instead it allows to estimate parameters of interest by formulating fuzzy relationships between microscopic characteristics of the metals grain-phase structure and macroscopic effective performance characteristics. Assuming that materials properties are determined by its internal microscopic structure, it will then be possible, by controlling this microstructure, to obtain materials with required combinations of properties. It is thus essential to develop tools to analyse the material microstructure based on microsections images and images obtained with atomic force microscopy, scanning probe microscopy, X-ray topography or other methods [13]. This analysis is particularly relevant, since it leads to the development of novel methodologies, which can facilitate the development of manufacturing strategies and tools for predicting aforementioned performance characteristics of functional materials [4].

2 Methodology

In this Section the general formulation of the methodology to obtain predefined properties of a functional material (here metallic functional material) will be formulated. This methodology will be later split in a series of steps. This theoretical methodology will later be illustrated on a practical example.

2.1 Mathematical formulation of the general problem of manufacturing material with predefined properties

In the framework of a general mathematical methodology to guide the manufacturing process of the metallic functional material with predefined set of properties, it is required to identify particular material manufacturing technologies, initial characteristics of a primary un-treated part and its further mechanical treatments, referred here as $\mathbf{X}$, resulting in pre-defined set of effective performance characteristics such as strength, ductility, heat resistance, etc., denoted here as $\mathbf{Z}$. Dimensions of these sets $\mathbf{X}$ and $\mathbf{Z}$ depend on the number of technological parameters and the number of specified performance characteristics of functional metal or alloy. From various experimental data, it can be assumed that a unique relationship can be formed between elements of these sets

$$z = \mathbf{F}(x),\ x \in \mathbf{X},\ z \in \mathbf{Z} \tag{1}$$

Here x and z are specific values of the functional material initial parameters and values of performance characteristics correspondingly; e.g. a particular mechanical treatment results in the unique change in performance characteristics. The operator $\mathbf{F}$ can take a form of a particular functional (vector-function, differential function etc.), depending on the form of sets $\mathbf{X}$ and $\mathbf{Z}$.

When manufacturing a functional material, the aim is to define such initial characteristics and manufacturing technologies (x^*), which would ensure the best possible match with predefined values of effective performance characteristics (z^*). Mathematically, the following optimization problem can be formulated:

$$\begin{aligned} &\text{define such parameters } x^* \in \mathbf{X}, \text{ that minimize} \\ &\parallel z - z^* \parallel \Rightarrow \min \\ &\text{subject to equality (1)} \end{aligned} \tag{2}$$

Noted that the problem (2), depending on the form of operator $\mathbf{F}$, can be attributed either to the problem of optimal control [2] or to the problem of parametric optimization [10]. The construction of the operator $\mathbf{F}$ is, undebatably, the main issue in solving problem (2). Typically these operators are constructed for some particular cases, e.g. the form of the operator connecting the materials yield surface with parameters of its thermomechanical treatment is presented in [17]. However, for the case of multiple characteristics, especially considered simultaneously, this problem is particularly complex, and currently there exist no specific analytical solutions or even generic approaches to solve it. Typically every materials mechanical property on the macroscopic level is analysed separately by modeling particular thermomechanical process, this inevitably complicates the solution of the general multi-characteristics problem (2).

As a step forward in analysing the general formulation of the problem (2), a new approach is proposed below, consisting in decomposition of the initial formulation into several interrelated sub-stages.

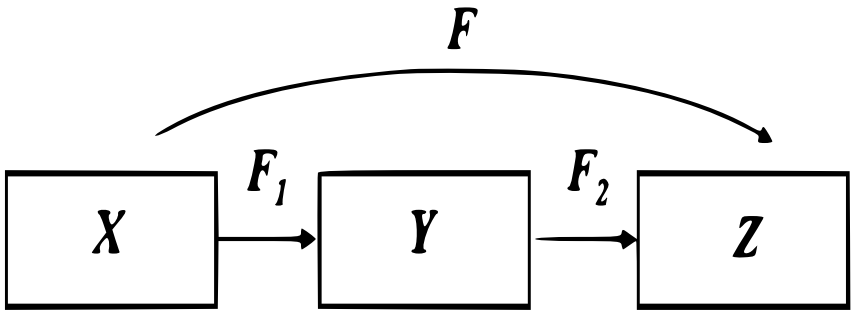

Fig. 1 Decomposition of the problem.

2.2 Problem decomposition. Two-level model

Initially, a hypothesis is introduced that the set of required mechanical characteristics of the material is uniquely determined by its microstructure. For the case of metals and alloys, considered in this paper, the microstructure is defined by the grain-phase structure of the material. Let us denote by $\mathbf{Y}$ the set of parameters describing the materials microstructure. Then the relation (1) takes the following form:

$$z = \mathbf{F}(y(x)),\ x \in \mathbf{X},\ y \in \mathbf{Y},\ z \in \mathbf{Z} \tag{3}$$

where y are specific values of parameters of the grain-phase structure of material.

Now the problem of obtaining predefined properties of functional material can be divided into two stages, shown in Figure 1.

In Figure 1, the operator $\mathbf{F_1}$ establishes the relations between the *manufacturing process* parameters and *the grain-phase microstructural* parameters of the functional material; and the operator$\mathbf{F_2}$ connects the *microstructural parameter*s with the resulting set of *performance characteristics*.

Now relation (1) can be transformed to the following form:

$$z = \mathbf{F}(x) = \mathbf{F_2}(\mathbf{F_1}(x)) = \mathbf{F_2}(y) \tag{4}$$

Here $y = \mathbf{F_1}(x)$, and operator $\mathbf{F} = \mathbf{F_2}\mathbf{F_1}$.

Thus, the problem of obtaining the predefined properties of the functional material is reformulated as a combination of two problems:

- recovering a grain-phase microstructure of the material as a result of a manufacturing process via $\mathbf{F_1}$; and
- an estimation of materials macroscopic performance properties, depending on parameters of the material microstructure via $\mathbf{F_2}$.

The first problem, i.e. the particular form of the operator $\mathbf{F_1}$, will not be considered in this paper. The only contribution of this first part is the identification of parameters of resulting grain-phase micro-structure. It is assumed that technologies for obtaining the required functional material are known and thus, as a result, its grain-phase structure, represented by digital images of microsections of this material under various technological processes, are given.

It is also assumed that a sufficient number of experimental data has been collected, which allows the possibility to establish relations between parameters of the material microstructure and technological processes.

Of particular interest here is the second problem, where an estimation of mechanical macroscopic properties is performed, based on the predefined set of parameters of the grain-phase materials microstructure. Thus the general problem reduces to the solution of the second part only:

$$z = \mathbf{F_2}(y) \tag{5}$$

2.3 Analysis of parameters of functional materials microstructure

The analysis of microstructural properties can be further split in two stages:

- identification of all possible parameters of obtained grain-phase structure (i.e. all possible components of the vector y) takes place; and

- the determination of the number of significant components of the vector y (further denoted as $\tilde{y}$), characterizing this microstructure from the point of the set of macro-characteristics of the material.

Below the logical sequence of these stages will be discussed, starting with the second stage.

Following the proposed hypothesis that the macroscopic properties of a material unambiguously follow from its microstructure, it is necessary to determine which microstructural parameters, and their minimum number, are uniquely determined by the required set of macro-characteristics of the functional material. In other words, it is required to find such $\tilde{y} \in \mathbf{Y}$ where:

$$\exists \mathbf{F_2}, \text{ such that } \parallel \tilde{z} - \mathbf{F_2}(\tilde{y}) \parallel < \varepsilon \tag{6}$$

where $\tilde{z}$ contains available experimental data on required set of macro characteristics, and ε is the required accuracy.

To ensure the completeness of $\tilde{y}$, it is necessary to determine the maximum possible number of microstructural parameters. This can be determined by the identification of these parameters from the available set of microsections in the analysed material.

Typically, in order to analyse a microstructure, parameters of interest are related to grains structures, e.g. grain area, perimeter of boundaries, lengths (mean and deviation) of small and large grain axes, aspect ratio, elongation, compactness, etc. Automation of image segmentation procedure allows obtaining these parameters in a direct way, i.e. avoiding manual processing.

It should also be noted that thermomechanical properties of the material depend not only on parameters of the grain structure, but also on the phase composition, as well as the presence of dislocation substructures within the grain. In the case of intense plastic deformations, a stable fragmented substructure can be formed, stabilized by particles of secondary carbides [12]. Attention should also be given to the wall-effect and influence of triple junctions [16]. Note that the automation of identification of the aforementioned features from images could significantly improve the prediction of material properties.

In this paper, an automated system [18], allowing to estimate, with the user specified accuracy, parameters of grain-phase structure from a digital image of microsections, was used to determine phase classification and segmentation of grains. Note that automating the microstructural parameters identification leads to significant increase in the number of these parameters, potentially impacting macro-characteristics of the material.

Having determined the parameters of the microstructure $\tilde{y}$, the problem of macro-properties estimation in functional material can be approached, i.e. the next step is the determination of the operator $\mathbf{F_2}$ in the general problem (4).

2.4 Estimation of macro-properties as a function microstructural parameters

Analysing the microstructure of metal or alloys, the main parameters of the grain-phase structure can be distinguished, including phase state parameters, e.g. volume fraction of phases, parameters of the grain structure, e.g. the mean grain size, the grain size variation coefficient, the degree of grain anisotropy, the volume fraction of grains, etc. Following the analysis of aforementioned parameters, it is thus required to estimate materials performance characteristics (here strength), i.e. define the form of the operator $\mathbf{F_2}$ in

$$\tilde{z} = \mathbf{F_2}(\tilde{y}) \tag{7}$$

At this stage, an unambiguous conformity between parameters of the grain-phase structure and parameters characterizing the performance characteristics of functional material cannot be guaranteed, thus in order to define the operator $\mathbf{F_2}$, fuzzy relations S^i [14],[21] between parameters can be built.

Assuming the number of available experiments (microsections and measurements of performance characteristics corresponding to each of them) is n, then

$$S^i = A^i \times B^i, \; i = 1..n \tag{8}$$

where A^i is a special fuzzy set containing parameters of the grain-phase micro-structure for the i-th experiment; B^i is a special fuzzy set containing macroscopic performance characteristics for the i-th experiment; $\times$ represents Cartesian product of fuzzy sets [21]. Thus, for each i-th experiment, the relation of S^i between fuzzy sets A^i and B^i is defined.

The mathematical objects A^i and B^i introduced above are structurally represented as a multiple of couples, formed by an element (carrier) and a membership function quantifying the grade of membership of this element to the particular mathematical object. Note that the membership function may vary from 0 (fully "non-belong") and 1 (fully "belong"). A similar structure can be found in fuzzy sets [21]. However, unlike conventional fuzzy sets, elements of which belong to the same physical space and are of same type with the same dimensions, elements of sets A^i and B^i can have a different nature

and, as a result, different dimensions. To underline these differences between sets A^i and B^i from the conventional fuzzy sets, they are defined as *special* fussy sets. Further details will be discussed below in the worked example.

Note that (8) defines fuzzy relations that can be represented in a matrix form [21], where l, m-th term $s_{(l,m)}$, defined for the element (a_l, b_m) is determined by the rules of vector product for fuzzy sets [21]; here $l = 1..d$ and $m = 1..w$, i.e. d is the total number of couples (elements with corresponding membership functions) in the fuzzy set A^i, and w is the total number of couples in the fuzzy set B^i defined as follows:

$$d = k \times n; w = r \times n \tag{9}$$

Here r is the number of parameters characterizing the required set of macroscopic performance properties of the functional material in each experiment, k is the total number of selected parameters of the grain-phase microstructure in each experiment, and n is the number of experiments. Note here, that although desired, it is not strictly necessary to have all microstructural parameters measured in all experiments. The methodology is still robust in the absence of some elements. The user should assume zero for the missing component. However, in order to improve accuracy as many parameters as possible should be collected.

The relation between arbitrary sets A^i (containing parameters of the grain-phase micro-structure) and B^i (containing known parameters characterizing the macroscopic performance characteristics), or, in other words, the form of the operator $\mathbf{F_2}$, can be determined in the following way:

$$\mathbf{F_2} = \cup_{i=1}^{l} S^i \tag{10}$$

here the operator $\cup_{i=1}^{l} S^i$ refers to the standard fuzzy union of membership matrices: $f_2^i = max(s_i)$ [14]. This leads to the set $\tilde{B}$ (set of unknown macroscopic parameters) be being determined as

$$\tilde{B} = \tilde{A} \circ \mathbf{F_2} \tag{11}$$

where $\tilde{A}$ refers to the set of microscopic parameters, corresponding to the set of unknown macrostructural characteristics, and $\circ$ is the sign of *maximin* product (e.g. an ordinary product of matrices [21], where *min* is substituted for the multiplication operation, and *max* is used instead of the addition operation).

It should be noted that, as a result of (11), $\tilde{B}$ will be obtained as a fuzzy set. If the requirement is to obtain $\tilde{B}$ in the form of an ordinary set (i.e. any performance characteristic must be represented as a uniquely determined scalar quantity), it will be necessary to define the ordinary representative of the fuzzy element [21] for each characteristic. For example, if an element of the fuzzy set is a discrete value, then the determination of an ordinary representative $\tilde{b}_j^*$ of this fuzzy element can be carried out as the determination of the mean [3] for discrete random variables.

$$\tilde{b}_j^* = \sum_{j=1}^{r} \left(\frac{m(\tilde{b}_j)}{\sum_{i=1}^{r} m(\tilde{b}_i)} \tilde{b}_j \right) \tag{12}$$

Here $\tilde{b}_j$ is the j-th element of a fuzzy set $\tilde{B}$, $m(\tilde{b}_j)$ is a membership function of the j-th element and r is the number of element couples in the fuzzy set $\tilde{B}$.

Following the determination of the operator $\mathbf{F_2}$, the problem of identifying such microstructure that ensures a predefined set of macroscopic materials characteristics, i.e. the solution of the optimization problem (1-2), can be approached.

3 An example of estimation of strength properties of steel subjected to heat treatment

As an illustration of the above methodology, the manufacturing of reinforcing steel with predefined strength characteristics, obtained through heat treatment (see for details the work of the Nanosteel R&D at the Magnitogorsk State Technical University [5], [9]), was considered. In order to obtain the qualitative and quantitative characteristics of the forming structure, the GLEEBLE 3500 research complex was used with Meiji Techno optical microscope using Thixomet PRO computer image analysis system and scanning electron microscope JSM 6490 LV. In analysed heat treatment modes, 3 phases are formed (see [9]): ferritic-carbide mixture (FCM), martensite (M) and bainite (B), volume fractions of which determine the strength of a material. In addition to the phase composition, the performance characteristics of analysed steel are strongly influenced by the parameters of the grain structure. The shape and size of grains can vary significantly (see [9]), which undoubtedly affects the strength of steel.

The main parameters of the grain-phase structure were identified as: volume fractions of phases - FCM, B, M; as well as the average grain size, coefficient of grain size variation, degree of grain anisotropy and volume proportion of grains.

Thus, the total number of microstructure parameters in this case is $k = 7$. The parameters of the grain-phase structure were calculated using the automated system [18].

The Vickers hardness (HV_{30}) and impact strength (KC) were selected as macroscopic performance characteristics of the functional material (reinforcing steel). The measurement of Vickers hardness were taken at 30 kg load using the third generation Emco Test M4C075G3 universal hardness tester with high-resolution camera and automatic measurements using Brinell, Rockwell, Vickers methods. Thus, the number of performance characteristics in this case is $r = 2$.

Results of the experimental study, i.e. parameters of the grain-phase structures and performance characteristics of steel for 7 samples ($n = 7$), obtained under different heat treatment modes (here cooling rates), are presented in Table 1.

Table 1 Microscopic parameters and macroscopic characteristics.

Experiments	Cooling rate, °C/s	Phase composition, % FCM/B/M	Grain structure parameters: Mean grain size, μm	Grain size variation coefficient	Anisotropy degree	Volume fraction of grains	Material hardness HV_{30}	Impact strength KC, J/cm^2
1	10	100/0/0	0.10	0.11	0.98	0.87	400	54.3
2	20	60/10/30	0.10	0.07	1.14	0.26	412	55.7
3	25	80/10/10	0.16	0.06	1.09	0.44	436	58.5
4	30	70/20/10	0.26	0.17	1.18	0.98	469	64.0
5	40	50/30/20	0.25	0.03	1.25	0.37	554*	55.7*
6	50	40/30/30	0.21	0.06	1.1	0.79	617	50.1
7	60	10/0/90	0.13	0.07	1.08	0.91	800	44.6

As it can be seen, the number of micro-structural grain-phase parameters for 7 experiments, following equation (9), is $d = 49$, leading to the vector A^i having dimensions 49×1, and the vector B^i having dimensions 1×14 (as the number of macroscopic properties after 7 experiments is $w = 14$). We will return to this full description at the end of this Section, and now for a clearer and more visual illustration of the above methodology, a much simplified example will be considered first.

In this simplified case (see Table 2) only three experiments (cooling rates 20, 30 and 40 °C/s, i.e. experiments 2, 4 and 5) were analysed with only measured microscopic mean grain size and grain size variation coefficients. Also, for simplicity, only the macroscopic material hardness was chosen to represent the macroscopic characteristic. It is assumed that for the tests 2 and 4 all information is known, and for the final 5^{th} test microstructural information was collected, but one macrostructural characteristic is unknown and to be found.

Table 2 Microscopic parameters and macroscopic characteristics (reduced test).

Mean grain size	Grain size variation coefficient	Material hardness HV_{30}
0.10	0.07	412
0.26	0.17	469
0.25	0.03	unknown

As a first step matrices A^i with microstructural parameters and B^i with macroscopic characteristics were constructed. The membership functions of an arbitrary element c_j in fuzzy sets A or B can be found from the following relation:

$$m(c_j) = 1 - |\frac{(c_j - \bar{c}_j)}{\max(c_j, \bar{c}_j)}| \tag{13}$$

where $\bar{c}_j$ is a value of corresponding element with the membership function equal to 1. Following equation (13), elements of matrices A^i can be constructed as

$$\begin{aligned} A^2 &= [1.0/0.1\ 0.39/0.26\ 0.4/0.25\ 1.0/0.07\ 0.41/0.17\ 0.43/0.03] \\ A^4 &= [0.39/0.1\ 1.0/0.26\ 0.96/0.25\ 0.41/0.07\ 1.0/0.17\ 0.18/0.03] \\ A^5 &= [0.4/0.1\ 0.96/0.26\ 1.0/0.25\ 0.43/0.07\ 0.18/0.17\ 1.0/0.03] \end{aligned} \tag{14}$$

Here superscript denotes the experiment under the consideration experiments (i.e. experiments 2, 4 and 5 for cooling rates 20, 30 and 40 °C/s). Note that elements of the matrix A^i contain the couple of the membership function, following by the

value of the actual microstructural parameter itself (denoted as "membership function/parameter value). Similarly, matrices B^i, corresponding to the known macrostructural characteristics, can be constructed as

$$\begin{aligned} B^2 &= [1.0/412\ 0.88/469] \\ B^4 &= [0.88/412\ 1.0/469] \end{aligned} \tag{15}$$

In the next step, following equations (8) and (10), an operator $\mathbf{F_2}$ can be built as follows:

$$\mathbf{F_2} = \begin{bmatrix} 1.0 & 0.88 \\ 0.88 & 1.0 \\ 0.88 & 0.96 \\ 1.0 & 0.88 \\ 0.88 & 1.0 \\ 0.43 & 0.43 \end{bmatrix} \tag{16}$$

For simplicity of the presentation, the actual formalism of the operator $\mathbf{F_2}$ has not been kept. Below the schematic presentation is given to guide the reader through elements of this operator:

$$\mathbf{F_2} = \begin{array}{c} \\ A^i \\ \downarrow \end{array} \begin{array}{c} \begin{array}{cc} B^i & \rightarrow \end{array} \\ \begin{bmatrix} 1.0 & \boxed{0.88} \\ 0.88 & 1.0 \\ 0.88 & 0.96 \\ \boxed{1.0} & 0.88 \\ 0.88 & 1.0 \\ 0.43 & \boxed{0.43} \end{bmatrix} \end{array} \begin{array}{l} \\ \\ 0.88/(0.1;412) \\ \\ 1.0/(0.07;469) \\ \\ 0.43/(0.03;412) \end{array}$$

Here elements are represented as membership functions with corresponding couples of microscopic parameters and macroscopic characteristics, following equations (8) and (10). Finally, following equation (11), the unknown macroscopic characteristics, missing in Table 2, can be found:

$$B^5 = A^5 \circ \mathbf{F_2} = [0.88/412\ 0.96/469] \tag{17}$$

If it is required to obtain $\tilde{B}$ in the form of an ordinary value (i.e. as a uniquely determined scalar quantity, representing fuzzy set), following equation (12), unknown macroscopic material hardness can be determined as $\tilde{b}_3^* = 441.8$. Comparing the estimated number with the experimentally obtained $HV_{30}^e = 554$ (see Vickers hardness with a star in table 1, corresponding to the 5^th experiment) the error of the proposed methodology is

$$\delta_{HV} = |\frac{HV_{30}^r - HV_{30}^e}{HV_{30}^e}| \times 100\% = 20\% \tag{18}$$

A relatively large 20% error can be observed here. In order to improve the accuracy, more parameters need to be taken into consideration, as will be discussed further.

As the next test, the full set of data (presented in Table 1) has been analysed. To demonstrate the proposed methodology, now samples No. 1, 2, 3, 4, 6, 7 (six samples in total) are taken as the initial data, and sample No. 5 as the test sample. Macroscopic characteristics of the 5^th test sample are assumed unknown and are denoted with stars $(*)$.

Recall that in the new, complete, case the vector A^i has dimensions 49×1 (as the number of micro-structural grain-phase parameters for 7 experiments is $d = 49$) and the vector B^i has dimensions 1×14 (as the number of macroscopic properties after 7 experiments is $w = 14$). However as it was assumed that macroscopic material hardness and impact strength in the fifth experiment are unknown, the dimension of the vector B^i is 1×12.

As a result, see equation (8), matrixes S^i $(i = 1, 2, 3, 4, 6, 7)$ and thus operator $\mathbf{F_2}$, has dimensions 49×12 (due to the complexity of the presentation the full forms of the operator $\mathbf{F_2}$ and matrices A^i and B^i, with $i = 1, 2, 3, 4, 6, 7$, are not presented here).

Following equations (8), (10), (11) and (13) a fuzzy set, containing unknown macroscopic characteristics for the fifth experiment, B^5 has been found; and eventually, following equation (12), an ordinary representative of the fuzzy set B^5

for each separate characteristic (Vickers hardness (HV_{30}) and impact strength (KC)), following relation (12) has been obtained as

$$HV_{30}^r = 525\ KC^r = 54.6 \tag{19}$$

Note that, experimental measurements (see elements with a star in Table 1) were taken as

$$HV_{30}^e = 554\ KC^e = 55.7 \tag{20}$$

Thus errors of the proposed methodology can be estimated as

$$\begin{aligned} \delta_{HV} &= |\frac{HV_{30}^r - HV_{30}^e}{HV_{30}^e}| \times 100\% = 5\%; \\ \delta_{KC} &= |\frac{KC^r - KC^e}{KC^e}| \times 100\% = 2\% \end{aligned} \tag{21}$$

The justification of a *sufficient* number of experiments and parameters, to obtain a required accuracy of predictive estimation of macroscopic materials properties, can be of further study. However analyzing the obtained results, it can be concluded that even with a relatively small number of experiments and parameters, the accuracy of estimation is rather high. An increase in the number of experimental data will lead to a further increase in the accuracy of the predicted results.

4 Conclusion

A new methodology has been formulated that allows, using the analysis of the grain-phase micro-structural parameters of the functional material, to estimate its macroscopic performance characteristics. A hypothesis has been formulated on the unique correspondence between macroscopic properties of the material and its microstructure. Following this hypothesis, it is sufficient to determine a certain minimum number of corresponding microstructural parameters, which will uniquely determine the required set of macro-characteristics of the functional material. A particular novelty of the proposed methodology is the application of fuzzy sets theory while establishing relations between predefined strength characteristics and parameters of the phase state and grain structure, obtained from the image of microsections of the analysed material.

Acknowledgements The reported study was funded by the Ministry of Education and Science of the Russian Federation (the unique identifier RFMEFI58617X0055) and by the EC Horizon 2020 is MSCA-RISE-2016 FRAMED Fracture across Scales and Materials, Processes and Disciplines.

References

[1] Y. Adler, E. Markova, and Y. Granovsky, The design of experiment to find optimal conditions a programmed introduction to the design of experiments (Mir Publishers, 1975), [in Russian].
[2] V. Alekseyev, V. Tikhomirov, and S. Fomin, Optimal control (Nauka, 1979), [in Russian].
[3] V. Ashikhmin, M. Gitman, O. Naimark, V. Stolbov, P. Trusov, and P. Frick, Introduction into mathematical modeling (Logos, 2015), [in Russian].
[4] S. Banerjee and A. K. Tyagi, Functional materials: preparation, processing and applications (Elsevier, 2011).
[5] M. Baryshnikov, D. Dolgiy, K. Kuranov, and M. Zaitseva, Thermal and mechanical treatment of high-carbon steel rebar, Steel in Translation **42(2)**, 177–179 (2012).
[6] V. Bolshakov, Y. Dubrov, and O. Kasjan, Microstructure as a predominant parameter in predicting mechanical characteristics of steel, Reports of the National Academy of Sciences of Ukraine **6** (2010), [in Russian].
[7] R. Fisher, The Design of Experiments (liver and Boyd, 1951).
[8] H. Gao, B. Ji, I. Jger, E. Arzt, and P. Fratzl, Materials become insensitive to flaws at nanoscale: Lessons from nature, Proceedings of the National Academy of Sciences of the United States of America **100 (10)**, 5597–5600 (2003).
[9] M. B. Gitman, A. V. Klyuev, V. Y. Stolbov, and I. M. Gitman, Complex estimation of strength properties of functional materials on the basis of the analysis of grain-phase structure parameters, Strength of Materials **49(5)**, 710–717 (2017).
[10] D. Himmelblau, Applied nonlinear programming (McGraw-Hill, 1972).
[11] A. Ilyushin, Plasticity, foundations of the general mathematical theory (Academy of Sciences of the USSR, 1963), [in Russian].
[12] E. Kozlov, N. Koneva, and N. Popova, Grain structure, geometrically necessary dislocations and second-phase particles in polycrystals of micro- and mesolevel, Physical Mesomechanics **12 (5-6)**, 280–292 (2009).
[13] V. Malakhov, Diagnosis of functional materials, Industrial Laboratory. Material Diagnostics **77(2)**, 310 – 318 (2011), [in Russian].
[14] K. Peeva and Y. Kyosev, Fuzzy Relational Calculus: Theory, Applications and Software (World Scientific, 2005).
[15] P. Ray, R. Ganguly, and A. Panda, Influence of heat treatment parameters on structure and mechanical properties of an hsla-100 steel, Steel Research (Germany) **73(8)**, 347–355 (2002).

[16] V. Rybin, Large plastic deformations and fracture of metals (Metallurgiya, 1986).
[17] V. M. Schastlivtsev, T. I. Tabatchikova, I. L. Yakovleva, S. Y. Klyueva, A. A. Kruglova, E. I. Khlusova, and V. V. Orlov, Microstructure and properties of low-carbon weld steel after thermomechanical strengthening, The Physics of Metals and Metallography **113 (5)**, 480–488 (2012).
[18] S. Sharybin, V. Stolbov, M. Gitman, and M. Baryshnikov, Developing of an intellectual system of complex microstructures analysis and classification on thin metal sections, Neurocomputers: development, application **12**, 50–56 (2014), [in Russian].
[19] P. V. Trusov and A. I. Shveykin, Multilevel crystal plasticity models of single- and polycrystals. direct models., Physical Mesomechanics **16(2)**, 99–124 (2013).
[20] V.G.Bazhenov, Mathematical modeling and methods of indentifying strain and strength characteristics of materials, Physical Mesomechanics **10(5-6)**, 302–314 (2007).
[21] L. Zadeh, From computing with numbers to computing with words from manipulation of measurements to manipulation of perceptions, International Journal of Applied Math and Computer Science **12 (3)**, 307–324 (2002).