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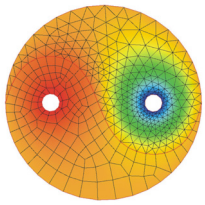

ON APPLICATION OF SHAPE COEFFICIENTS TO CREATION OF THE STATISTICALLY SIMILAR REPRESENTATIVE ELEMENT OF DP STEELS

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Abstract

The coupled finite element multiscale simulations (FE^2) require costly numerical procedures in both macro and micro scales. Exertions, leading to improvement of numerical efficiency, are focused mainly on two areas of development i.e. parallelization of numerical procedures or simplification of virtual material representation. One of the representatives of the latter area is the idea of Statistically Similar Representative Volume Element (SSRVE). It aims at the reduction of the number of finite elements in micro scale by transformation of sophisticated images of material microstructure into artificially created simple objects being characterized by similar features as their original equivalents. This paper is devoted to analysis of shape coefficients and possibilities of their application in the creation of SSRVE for DP steels. The results from sensitivity analysis of particular coefficients, obtained for different microstructure images, are presented in the paper, as well as examples of SSRVE.

Key words: DP steels, image processing, representative microstructure, Statistically Similar RVE

1. INTRODUCTION

Dual Phase steels belong to a group of advanced high strength steels (AHSS) used in the automotive industry. Two phase microstructure containing predominantly ferrite and 20-30% of martensite, is the basis of certain special properties of these steels. Required relation between volume fractions of ferrite and martensite, which is crucial for the quality of steel (Kim et al., 1981; Bag et al., 1999; Thomser et al., 2009), is obtained through special heat treatment during laminar cooling after hot rolling or during annealing after cold rolling. This is a complex process, therefore, numerical simulation is particularly needed in design of manufacturing of DP steel products. The tasks of numerical modelling are twofold. The first is simulation of metallurgical phenomena occurring in the microstructure during processing and the objective is control of processing parameters to obtain required microstructure. The second is analysis of the behaviour of the two phase microstructure during manufacturing and exploitation of products, which are mainly the car body parts. The former task is reasonably well researched. Various complexity models of phase transformation were applied to simulation of the kinetics of transformation during laminar cooling or annealing, see for example Authors earlier publications (Pietrzyk et al., 2009; Pietrzyk et al., 2010a; Pietrzyk et al. 2010b; Madej et al., 2010). In these papers both conventional models and cellular automata method are applied to simulations of phase transformations and to optimization of laminar cooling and continuous annealing processes. The latter task of the numerical modelling, which is considered in the present paper, is connected with reproduction of the

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two-phase microstructure and with an analysis of deformation of this microstructure.

Analysis of the behaviour of the two-phase microstructures during processing is usually based on the multiscale modelling concept. An intensive development of the multiscale modelling techniques has been observed after the year 2000 (Allix, 2006; Madej et al., 2008). Various hybrid methods are commonly used (Shterenlikht & Howard, 2006; Madej et al., 2010). In general, a sufficiently large section of the microstructure, which acts as a representative volume element (RVE), is used as a representation of this microstructure. This RVE is usually attached to selected points in the macroscale (nodes, Gauss integration points) and the direct micro-macro-transition procedure is created. The multilevel finite element method or the FE^2 method (Smit et al., 1998; Feyel & Chaboche, 2000) belong to this group. Techniques of creation of virtual microstructures in RVEs were developed (eg. Bernacki et al., 2007). Mesh generation methods reflecting grain and/or interface boundaries were used in FE simulations of deformation of the RVE (crystal plasticity). Authors of this paper have been for several years involved in research in this field and methods of creation of virtual microstructures based on image analysis and on cellular automata method have been developed (Cybułka et al., 2007; Rauch & Madej, 2010).

Numerical simulations based on the digital microstructures are extremely costly. Therefore, application of these methods in practice is limited, in particular when optimization of the morphology of the microstructure has to be performed. Thus, extensive search for more efficient and still reasonably accurate methods is the objective of research in several laboratories. Application of the statistically similar representative volume element is one of the interesting and promising propositions, see for example (Schroeder et al., 2011; Brands et al., 2011a; 2011b).

The objective of this paper, which is a continuation of the primary research described in Bzowski and Rauch (2011), is review of the techniques used to construct the SSRVE and presentation of the method of building of the SSRVE based on the image analysis algorithm and optimization techniques.

2. IDEA OF SSRVE

In the micro-macro modelling approach a RVE representing the underlying microstructure is attached at each Gauss point of the macroscopic solution. The constitutive law describing material behaviour in the macroscale is obtained by averaging the first Piola-Kirchoff stresses with respect to the RVE. The theoretical basis of the micro-macro modelling is well described in the scientific literature (e.g. Schroeder et al., 2011) and it is not repeated here. The focus is on development of the simple SSRVE, which will allow to decrease the computing costs and will make micro-macro modelling approach more efficient.

Considering micro-heterogeneous materials, the continuum mechanical properties at the macro scale are characterized by the morphology and by the properties of the particular constituents in the microscale. In the present paper DP microstructures composed of soft ferrite (70-80%) and hard martensite (20-30%) are considered. In the analysis we concentrate on the measures characterising the hard martensite islands only. The material models of the individual constituents are assumed to be known. The description of the microstructure is the based on statistical consideration (Beran, 1968).

An usual RVE is determined by the smallest possible sub domain, which is still able to represent the macroscopic behaviour of the material. Although these RVEs are the smallest possible by definition, they still can be too complex for the efficient calculations. Therefore, the construction of statistically similar RVEs, which are characterized by a lower complexity than the smallest possible substructure, was proposed in Schroeder et al. (2011). The basic idea is to replace a RVE with an arbitrary complex inclusion morphology by a periodic one composed of optimal unit cells, see figure 1. This idea is applied in the present work to the analysis of the DP steel microstructures.

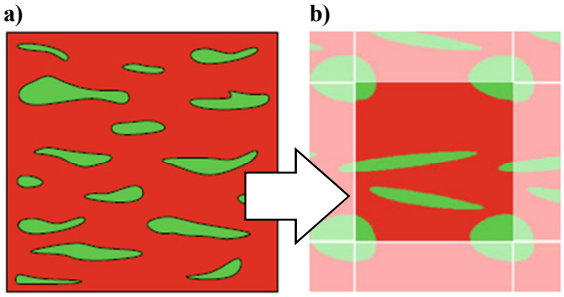

Fig. 1. *Schematic illustration of the basic concept of the SSRVE (Brands et al., 2011) – a) RVE, b) periodically arranged SSRVE.*

3. DP MICROSTRUCTURE DESCRIPTION

3.1. Shape coefficients

The parameters, describing fraction of different phases and their geometrical characteristics, form a group of the most important parameters, which, beyond statistical analysis of microstructure, is often applied. Ohser and Muecklich (2000) proposed four basic parameters. Few more parameters, which are used in the image analysis, are added and described in the present paper, as well. In consequence, the following thirteen parameters are considered. The equations (1)-(13) are written in a general form for the analysis of 3D microstructures, however, they can be easily transformed into 2D case. In the present paper the calculation of SSRVE is performed for 2D microstructures.

Volume fraction of phases:

$$\zeta_1 = \frac{V_m}{V} \tag{1}$$

where V_m is a volume fraction of martensite and V is a volume of the sample. The second coefficient is the interfacial surface to volume ratio for martensite islands:

$$\zeta_2 = \frac{S_m}{V_m} \tag{2}$$

where S_m is the interfacial surface. The next coefficient represents also relation between the interfacial surface and the volume of martensite islands, but it is given in a dimensionless form. This coefficient is represented by dimensionless parameter defined as relative difference between radiuses $(R_S - R_V)/R_V)$ calculated from the surface S_m ($R_S = \sqrt{S_m / 4\pi}$) and from the volume V_m ($R_V = \sqrt[3]{3V_m / 4\pi}$)

$$\zeta_3 = \frac{\sqrt{S_m}}{\sqrt[3]{3}\sqrt[6]{4\pi}\sqrt[3]{V_m}} - 1 \tag{3}$$

Roundness of the martensite constituents is the next basic parameter, which characterizes the DP steel microstructure. Roundness is defined as the difference between volumes of the smallest enclosing ellipsoid and the largest enclosed ellipsoid:

$$\zeta_4 = \frac{4}{3}\pi(ABC - abc) \tag{4}$$

where: A, B, C – equatorial radii of the smallest enclosing ellipsoid, a, b, c – equatorial radii of the largest enclosed ellipsoid.

Ellipsoid fit is the degree of fitting to ellipsoid with the same area and length-width-height proportions:

$$\zeta_5 = 2\frac{(x,y,z) \in v_m : \varepsilon_m(x,y,z) \le 1}{V_m} - 1 \tag{5}$$

where v_m – set of points inside the martensite inclusion, ε_m – set of points inside the ellipsoid. Ellipsoid diagonals are equal to Feret diameters calculated for particular grains transformed on the basis of Principal Component Analysis (PCA). Graphical interpretation of both coefficients describing roundness, i.e. ζ_4 and ζ_5, is presented in figure 2.

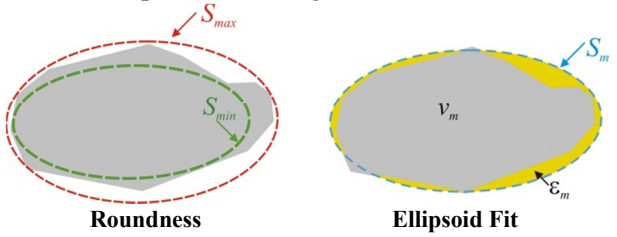

Fig. 2. *Schematic illustration of the parameters characterizing degree of roundness.*

The next parameter is the ratio between the minimum ($r_{\min}$) and maximum ($r_{\max}$) distance between contour and the centre of the island:

$$\zeta_6 = \frac{r_{\min}}{r_{\max}} \tag{6}$$

The following parameter is the border index, which is the ratio between the surface of the martensite constituent and the maximum surface of this constituent:

$$\zeta_7 = \frac{SL_m}{SL_{m\max}} \tag{7}$$

In equation (7) SL_m and $SL_{m\max}$ are the projection of the inclusion. Thus, SL_m is the perimeter of the projection of the martensite constituent and $SL_{m\max}$ is calculated as the perimeter of the smallest rectangle enclosing this projection.

The curvature of the surface of the martensite constituent is considered in the following two parameters. The specific integral of the mean curvature is:

$$\zeta_8 = \frac{1}{2V_m}\int_{S_m}\left(\min_{\beta}[\kappa] + \min_{\beta}[\kappa]\right)dS_m \tag{8}$$

where: β – the direction in the tangential plane, $\kappa = \kappa(\beta)$– curvature

The specific integral of the total curvature:

$$\zeta_9 = \frac{1}{V_m}\int_{S_m}\left(\min_{\beta}[\kappa]\min_{\beta}[\kappa]\right)dS_m \tag{9}$$

The last two parameters provide statistical information concerning the degree of the curvature of the martensite inclusion.

Additional four parameters are dedicated only for analysis of objects inside digital images and they have no equivalents in 3D case.

Malinowska coefficient:

$$\zeta_{10} = \frac{L_m}{2\sqrt{\pi S_m}} - 1 \tag{10}$$

where S_m is an area and L_m is perimeter of an analysed object.

Blair-Bliss coefficient:

$$\zeta_{11} = \frac{S_m}{\sqrt{2\pi\sum_{i=0}^{n} r_i^2}} \tag{11}$$

where S_m is an area of an analysed object, n is a number of all pixels and r_i is a distance between a pixel and object's centre of gravity.

Danielsson coefficient:

$$\zeta_{12} = \frac{S_m^3}{\left(\sum_{i=0}^{n} l_i\right)^2} \tag{12}$$

where S_m is an area of an analysed object, n is a number of all pixels and l_i is a minimal distance between a pixel and object's contour.

Haralick coefficient:

$$\zeta_{13} = \sqrt{\frac{\left(\sum_{i=0}^{n} d_i\right)^2}{n\sum_{i=0}^{n} d_i^2 - 1}} \tag{13}$$

where n is a number of pixels belonging to the object's contour and d_i is a distance between an analysed pixel and object's centre of gravity.

The graphical interpretation of mentioned shape coefficients is presented in figure 3. All these basic parameters were analysed and evaluated in the present work and those having the strongest influence on the features of the microstructure were selected, see chapter 4. Beyond this, the statistical measures of higher order are discussed briefly below, although they are of minor importance for typical martensite-ferrite microstructures of DP steels.

3.2. Statistical measures of higher order

The statistical measures, which are used for microstructure characterization in the SSRVE for micro-macro modelling of DP steels are discussed in this chapter. Following (Schroeder et al., 2011) these measures are divided into n-point probability functions, spectral density and linear-path function. A number of measures proposed by Schroeder et al. (2011), as well as those used in the image analysis technique, are listed below and those used in the present work are explained wider.

Since the parameters discussed in section 3.1 are scalar values, they are not able to cover direction-dependent information, which is required for the representation of oriented inclusion leading to an overall anisotropy. Statistical measures of higher order are needed for the construction of the SSRVE for anisotropic microstructures. Although only isotropic DP microstructures are considered in the present paper, a brief information on the higher order statistical measures is given in this section, as well.

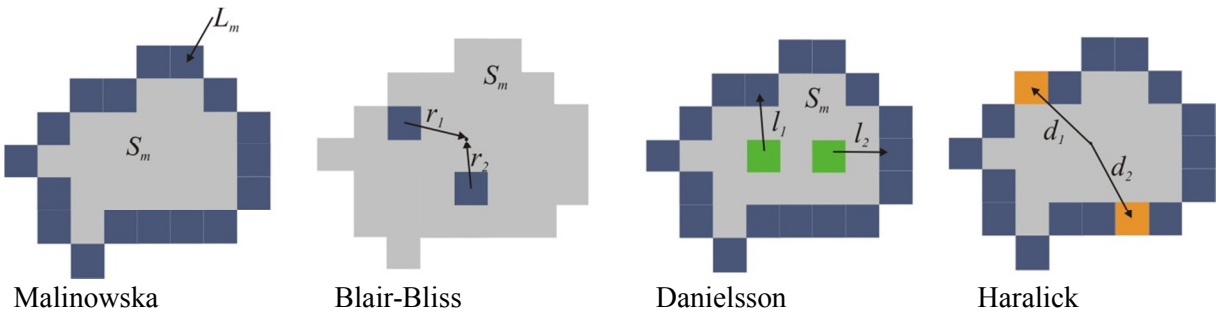

Fig. 3. *Schematic illustration of all the parameters dedicated to image analysis.*

One of these measures will be evaluated for the DP microstructures, which are analysed in chapter 5.

Schroeder et al. (2011) introduced the following higher order statistical measures for microstructures: *n*-point probability functions, spectral density and linear-path function. The latter parameter is described briefly below and is evaluated in chapter 5. This parameter describes the probability that a complete line segment $\mathbf{a} = \overrightarrow{\mathbf{a}_1\mathbf{a}_2}$ is located in the same phase, where $a_1 = \{x_1,y_1\}$ and $a_2 = \{x_2,y_2\}$ are coordinates of the ends of the line segment. Lu and Torquato (1992) gave general mathematical description of this measure for multi-phase anisotropic materials. Simplified approach, which is applicable to DP microstructures, is presented below. Let $D^{(i)}$ denote the domain occupied by the selected phase i in the particular sample. The modified indicator function is considered:

$$\chi^{(i)}\left(\overrightarrow{\mathbf{a}_1\mathbf{a}_2}\right) = \begin{cases} 1 \text{ if } \overrightarrow{\mathbf{a}_1\mathbf{a}_2} \in D^{(i)} \\ 0 \text{ otherwise} \end{cases} \tag{14}$$

Function (14) checks if a whole line segment is located in the selected phase i. The general definition of a linear-path function requires the computation of the ensemble average:

$$\zeta_{LP}^{(i)}\left(\overrightarrow{\mathbf{a}_1\mathbf{a}_2}\right) = \overline{\chi^{(i)}\left(\overrightarrow{\mathbf{a}_1\mathbf{a}_2}\right)} \tag{15}$$

Procedure of numerical evaluation of $\zeta_{LP}^{(i)}$ for a general microstructure is given by Schroeder et al. (2011). Since statistically homogeneous isotropic DP microstructures are analysed in the present paper, several simplifications are introduced to this procedure. The origin of the line segment vanishes and the only dependency is on the length (b) and orientation of the line segment. When b tends to zero, $\zeta_{LP}^{(i)}$ tends to the volume fraction of the phase $F^{(i)}$. Further simplification is due to the fact that only martensite inclusions are analysed in DP steels. Thus, in 2D binary images of statistically homogeneous microstructure with inclusions we have:

$$\chi(y) = \begin{cases} 1 \text{ if } \overrightarrow{\mathbf{a}_1(\mathbf{a}_1+\mathbf{b})} \in D \\ 0 \text{ otherwise} \end{cases} \tag{16}$$

where: $\mathbf{b} = \{x_2 - x_1, y_2 - y_1\}$ – line segment vector.

When evaluating the linear-path function for the periodic binary image of the two-phase microstructure a suitable template consisting of $N = N_x \times N_y$ pixels is defined. The pixel position in the binary image is defined by the pair (p,q). Length of the line segment vector in the binary image measured in pixels is $\mathbf{b} = \{m,k\}$. For such a discrete case the linear-path function is:

$$\zeta_{LP}^{l}(m,k) = \frac{1}{(p_M - p_m)(q_K - q_k)} \sum_{p=p_m}^{p_M-1} \sum_{q=q_k}^{q_K-1} \chi^{l}(\tilde{y}) \tag{17}$$

where:

$$\begin{aligned} p_m &= \max[0,-m], \quad & p_M &= \min[N_x, N_x - m] \\ q_k &= \max[0,-k], \quad & q_K &= \min[N_y, N_y - k] \end{aligned} \tag{18}$$

For periodic unit cells the linear-path function is:

$$\zeta_{LP}(m,k) = \frac{1}{N_x N_y} \sum_{p=1}^{N_x} \sum_{q=1}^{N_y} \chi(\mathbf{b}) \tag{19}$$

Calculation of the linear-path function from equation (17)-(19) is expensive. The efficiency of the solution can be improved without noticeable lost of the accuracy. The following simplifications can be introduced:

- The size of the template is reduced according to the maximum inclusion size.
- Number of analysed line segments is reduced and only certain set of line orientations is considered.
- Not all positions of the original image are considered. Line segments are placed at random positions and this process is repeated N_r times.

After these simplifications are introduced the linear-path function is:

$$\zeta_{LP}(m,k) = \frac{1}{N_r} \sum_{j=1}^{N_r} \chi(\mathbf{b}_j) \tag{20}$$

The vector $\mathbf{b}_j = \{p_j + m, q_j + k\}$. The random positions of the coordinates have to fulfil:

$$\begin{aligned} \max[0,-m] \le p_j \le \min[N_x, N_x - m] - 1 \\ \max[0,-k] \le q_j \le \min[N_y, N_y - k] - 1 \end{aligned} \tag{21}$$

for random microstructures and

$$\begin{aligned} 0 \le p_j \le N_x - 1 \\ 0 \le q_j \le N_y - 1 \end{aligned} \tag{22}$$

for periodic unit cells.

4. SENSITIVITY ANALYSIS OF SHAPE COEFFICIENTS

Selection of the parameters, which are the most representative for the DP steel microstructure, was one of the objectives of the work. This selection was made on the basis of the sensitivity analysis, which included evaluation of the importance of the parameters. The ranges of possible values of the parameters are given in table 1.

Table 1. *The ranges of possible values of the parameters.*

Parameter	symbol	units	Range
volume fraction	ζ_1	-	[0,1]
area/volume	ζ_2	1/m	[3/R, ∞]
area/volume	ζ_3	-	[0,∞]
Roundness	ζ_4	m^3	[0,∞]
ellipsoid fit	ζ_5	-	[-1,1]
contour to centre	ζ_6	-	[0,1]
border index	ζ_7	-	[1,∞]
mean curvature	ζ_8	$1/m^2$	[0,∞]
total curvature	ζ_9	1/m	[0,∞]
Malinowska	ζ_{10}	-	[0, ∞]
Blair-Bliss	ζ_{11}	-	[0,1]
Danielsson	ζ_{12}	-	[0, ∞]
Haralick	ζ_{13}	-	[0,1]

Sensitivity analysis was performed on the basis of coefficients values obtained for general set of dual phase steels characterized by different fraction of martensite phase. The pieces of these microstructures and presented in figure 4. Steel A is typical DP steel composed of 125 small separated grains without included background phase. The fraction of martensite phase in steel B exceeds 30%, thus it cannot be treated as typical DP steel, however, the shape coefficients can be still reliably calculated. In steel C the martensite phase took part in more than 50% of material sample. This caused very sophisticated shapes of analysed object with many foreign inclusions, which highly influence reliability of coefficients based on perimeter-area ratio or on an object's centre of gravity. Steel B contains 65 grains, while steel C only 38.

The analysis of calculated coefficients was performed twofold i.e. for one selected microstructure, and in comparison to other microstructures. In the first case, distributions of the calculated coefficients were estimated on the basis of obtained histograms. The analysis of distributions showed that some of the coefficients, e.g. Malinowska or border index (figure 5), are localized around one peak value. These peaks can be treated as expected values and they can be applied in optimization function as optimal values of particular coefficients.

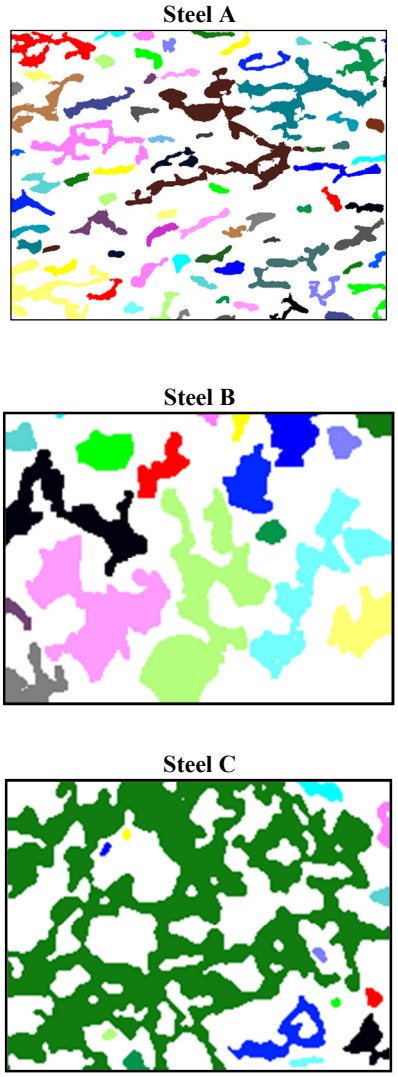

Fig. 4. *Samples of microstructures obtained from DP steels with different phase fraction (steel A: 26.31% of martensite, steel B: 39.77%, steel C: 53.03%).*

The one-peak distributions are complemented by other types of plots e.g. distributions with more peaks, uniform distributions or monotonic distributions. The plot with more peaks would suggest that the coefficients are localized nearby two or more values, therefore SSRVE should be composed of two or more inclusions, characterized by particular expected values. The Haralick (ζ_{13}) is an example in the case of steels A and B (figure 6). It can be applied in optimization procedures for each inclusion of SSRVE separately.

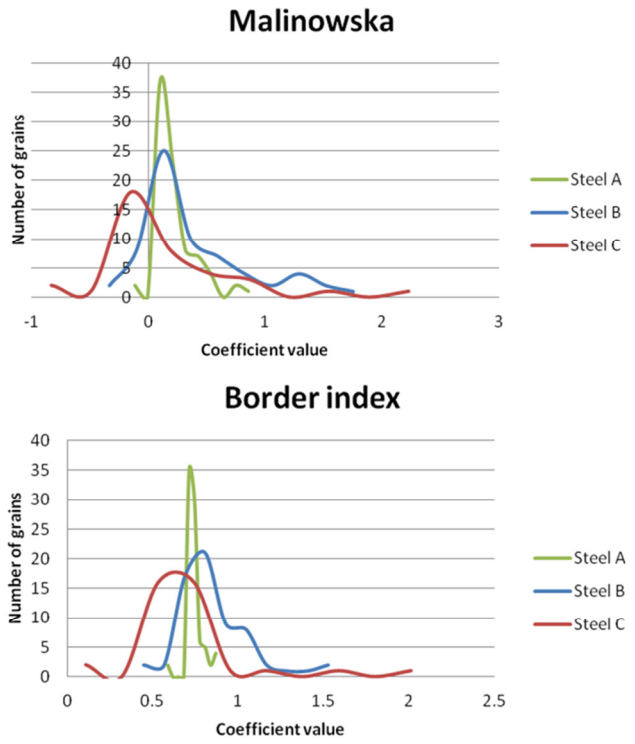

Fig. 5. *Distribution of Malinowska (ζ_{10}) and border index (ζ_7) coefficients for selected microstructures characterized by singular value of the coefficient.*

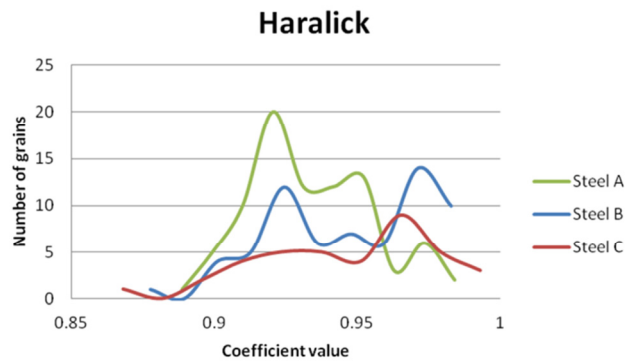

Fig. 6. *Distribution of Haralick and maximum curvature coefficients for selected microstructures characterized by double or triple value of the coefficient.*

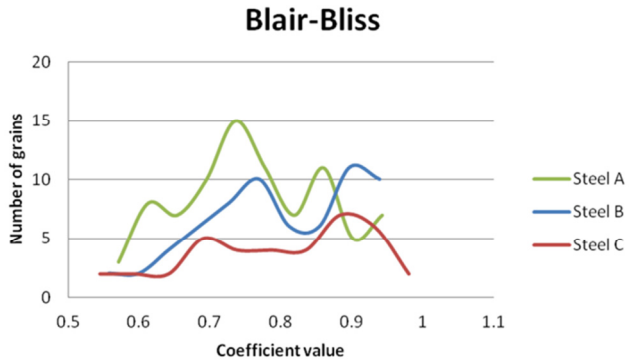

Fig. 7. *Distribution of Blair-Bliss coefficients for selected microstructures characterized by a specific range of values, where the coefficient has noticeable predominance.*

Besides strongly localized values, the coefficients, which are characterized by almost uniform distribution exist, e.g. Blair-Bliss coefficient for steel C, presented in figure 7. Information about uniform distribution can be passed to the cost function as a constraint for possible solutions.

The least useful coefficients are characterized by monotonic (ascending or descending) distributions, e.g. contour to centre or ellipsoid fit for steel A or C, presented in figure 8. Independently of the number of inclusions inside SSRVE, these coefficients cannot be reliably incorporated into a cost function.

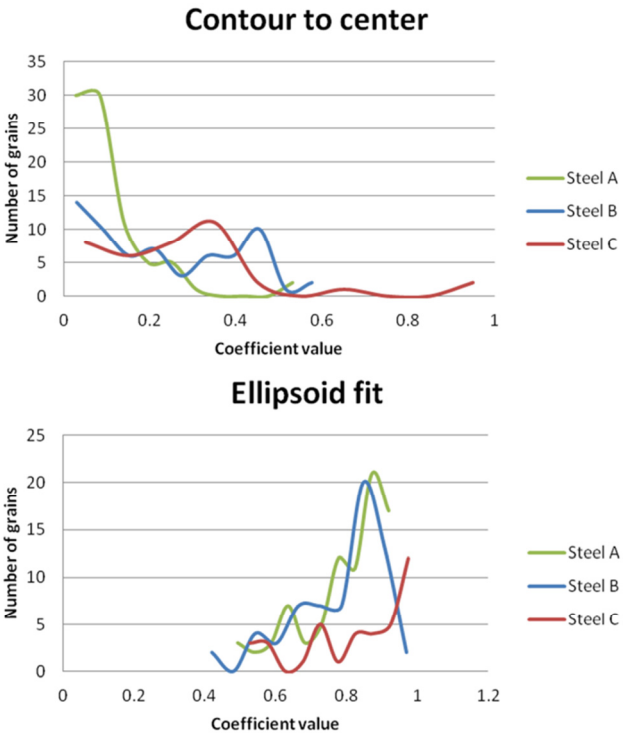

Fig. 8. *Distribution of contour to centre and ellipsoid fit coefficients for selected microstructures characterized by an uniquely described trend.*

Although histograms give detailed information about distribution of particular coefficients, they have to be validated according to the table 1, which presents the possible range of values for each coefficient. The validation has to take into account the numerical errors, caused by the approximated calculation of geometrical features of analysed objects e.g. underestimated perimeter and overestimated area in Malinowska coefficient results in final value less than zero (figure 5). Those values are ignored during the optimization procedure used to create SSRVE. According to the results of validation and sensitivity analysis, the coefficients are chosen and applied into the cost function described in chapter 5.2.

5. CONSTRUCTION OF THE SSRVE FOR DP STEELS

Basic principles of the construction of the SSRVE and examples of calculations for selected microstructures are presented in this chapter. The process of SSRVE creation consists of the image analysis, calculation of shape coefficients, construction of a cost function for optimization procedures, implementation of a proper optimization procedure and selection of the most suitable results.

5.1. Image analysis

The process of segmentation is very sophisticated and the results obtained can be highly diversified even for the same input data and algorithm. This phenomenon depends mainly on the parameters established for the selected algorithm. Moreover, the automated assessment of the results is very difficult, thus, it is hard to design a universal segmentation method able to work on various types of images. The methodology for analysis of DP microstructure images is proposed in this chapter.

Filtering and reconstruction

The image pre-processing stage consists of the two supplementary approaches, i.e. filtering and reconstruction. For the purposes of filtering the Dynamic Particles (DP) algorithm was designed and implemented (Rauch & Kusiak, 2007). The main advantage of the solution is its universality, which allows the application of the DP method not only for images but also for signals and sophisticated multidimensional data. The basis of this method is in the definition of the particle, which can be treated as an *N*-dimensional object, which in the case of images is a set of 3D vectors [X-axis, Y-axis, greyscale value] related to particular pixel inside the analysed images. The main idea of the DP algorithm consists in the appropriate movement of each particle according to the following set of differential equations:

$$\begin{cases} m_i \dfrac{d\vec{v}_i}{dt} = -\nabla V_{ij} - f_c \vec{v}_i \\ d\vec{r} = \vec{v}_i dt \end{cases} \tag{23}$$

where m_i is mass and v_i is the velocity of the i-th particle, V_{ij} is the potential between particles i and j, depending on the distance between them, f_c is a friction coefficient responsible mainly for the convergence of calculations.. The magnitude of the force that causes the movement of the considered particle is reduced by the friction coefficient $f_c < 1$. It was found that, according to the Newtonian laws of motion, if all of the pre-conditions would be fixed properly, the entire system would remain stable and convergent to the expected results. Additionally, the friction coefficient f_c can be modified during the calculations of the algorithm, which influences the final smoothness of the results, as well as the stop criterion of the DP algorithm. Images filtered by the described method is passed further to the process of image segmentation, which will allow to distinguish each particular material grain as a separated object from the input image.

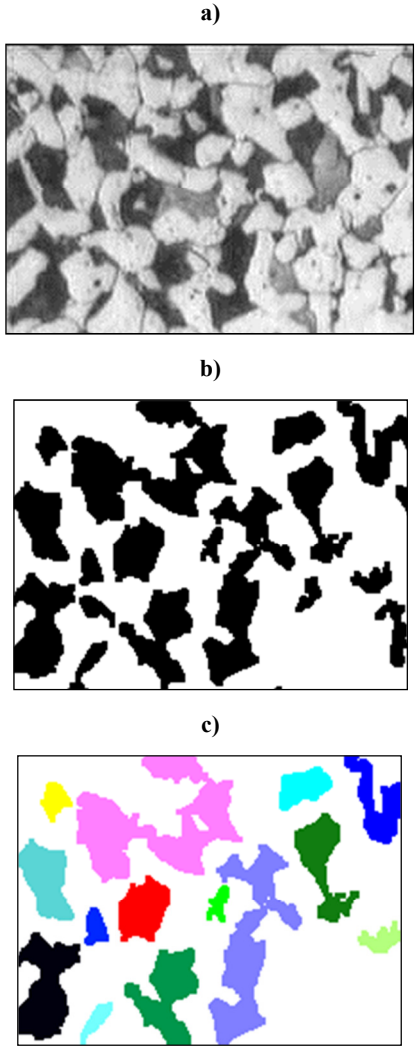

Fig. 9. *Results of image segmentation, (a) original DP image, (b) divided phases, (c) separated grains.*

Segmentation

The process of segmentation consists of two steps, i.e. separation of phases and detailed analysis of grains inside each phase. Several images of DP steel were analysed and it was observed that there is the possibility to automatically find the greyscale threshold, which separates the light and dark phases on the image. The value of such a threshold usually

covers the first minimum or the first inflexion point located on the histogram on the left side of the peak (Rauch & Madej, 2010). Then, separated areas of different grains can be processed by detailed grain boundary detection algorithms to separate particular grains within each phase. At the moment, this process can be omitted, especially in the case of background phase, during the analysis for the purposes of SSRVE creation. All of the coefficients described in chapter 2 do not take into account information about the background phase. Instead, the whole analysis is focused in the inclusion phase.

Calculation of shape coefficients is performed on the results of segmentation (figure 9c).

where: w_i – weights, n – number of coefficients, $\sum_{i=1}^{n} w_i = 1$, ζ_i – average i-th shape coefficient of original microstructure, ζ_{iSSRVE} – i-th shape coefficient of SSRVE. The calculations are performed with assumption that inside SSRVE there is only one inclusion. The current implementation of optimization procedure is based on genetic algorithm (GA), where chromosome is composed of m elements representing coordinates of crucial points determining SSRVE shape. These points are connected with spline functions forming smooth shape of SSRVE inclusion. Calculation of cost function is performed iteratively for each proposition of new SSRVE shape.

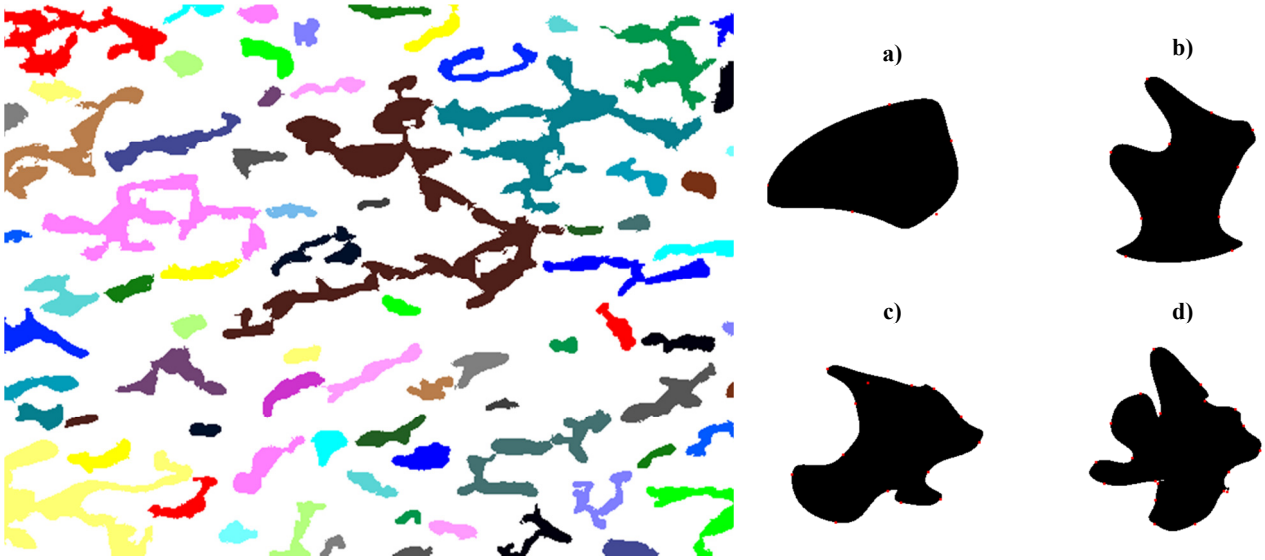

Fig. 10. *Results of one-particle SSRVE creation by using a) 5, b) 10, c) 15 and d) 20 reference points.*

5.2. Optimization procedure

A method for the construction of simple periodic structures for the special case of randomly distributed circular inclusions with constant equal diameters was proposed by Povirk (1995). The positions of circular inclusions with given diameter were found by minimizing the objective function, which was defined as a square root error between spectral density of the periodic RVE and non-periodic real microstructure. This idea inspired (Schroeder et al., 2011) to formulation of the objective function accounting for several parameters, which characterize the microstructure. In the present work this function was adapted to the following form:

$$\Phi = \sqrt{\sum_{i=1}^{n} \left[w_i \left(\frac{\zeta_i - \zeta_{iSSRVE}}{\zeta_i} \right)^2 \right]} \qquad (24)$$

5.3. Examples of calculations

The examples of calculations presented in this chapter were performed for steel A. The following parameters were assumed for optimization procedure:

- Expected values obtained from 10-class histograms – phase fraction = 26.31%, Malinowska coefficient = 0.617, border index = 0.855, maximum curvature = 2.627,
- Images parameters – original microstructure: width = 640px, height = 427px; SSRVE: width = height = 300px,
- Optimization parameters – maximum number of iterations = 20, minimum fitness = 0.001, the cost functions composed of the following coefficients: phase fraction ($w_1 = 0.4$), Malinowska coefficient ($w_2 = 0.2$), border index ($w_3 = 0.2$), max curvature ($w_4 = 0.2$).

The obtained results for different number of reference points are presented in figure 10. The final value of the cost function for 5 reference points is 0.006085, for 10 points is 0.00098, for 15 points is 0.000961 and for 20 points is 0.000466. In the cases of SSRVE built of 15 and 20 reference points, the optimization procedure stopped after 10 and 7 iterations respectively.

The SSRVE is described by splines connected in reference points, thus, it can be freely scaled without losing any information. Therefore, RVE constructed from periodically joined SSRVEs can be built in many ways, dependently on SSRVE size. The issue of SSRVE size adaptation remains unsolved and it is one of the directions for the future work. The example of RVE composed of SSRVE is presented in figure 11.

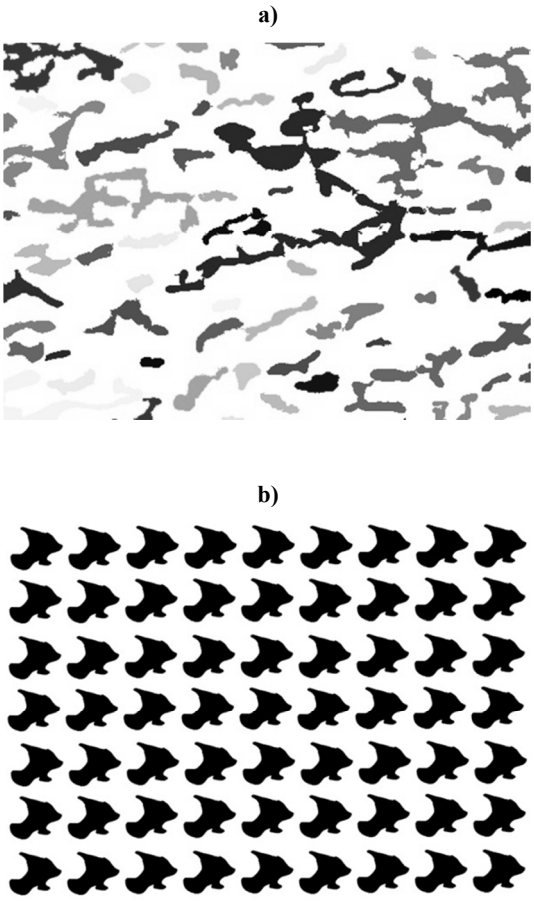

Fig. 11. *The example of original image (a) with related RVE (b) composed of periodically connected SSRVEs.*

6. CONCLUSIONS

The paper presents analysis of shape coefficients applied to creation of SSRVE for DP steels. Thirteen coefficients were selected. Nine of them describe geometrical shape of analysed object in 2D and 3D domain, while remaining four are dedicated to processing of digital images. All of these coefficients were implemented in the form of numerical procedures, which allowed to obtain coefficients distributions. The results showed that a set of coefficients, which can be applied to subsequent optimization method, has to be composed individually for each microstructure. Three different microstructures were analysed in this work, but only Malinowska coefficient has similar values and distributions in all the cases. Additional conclusions can be enumerated as follows:

1) The analysed coefficients return reliable results for microstructures with clearly separated grains of inclusion phase. The modification of existing coefficients has to be incorporated for large grains with sophisticated shapes and enclosed background phase.
2) Number of elements inside SSRVE:
   a) can be determined by the analysis of histograms with more than one noticeable peak, like in Haralick coefficient in this work,
   b) influences the final value of the cost function, however, it may depend on applied optimization method, its parameters and randomness.
3) Numerical errors:
   a) The procedures calculating perimeter and area of an analyzed object does not take into account real shape of an object but its digitalized approximation, e.g. in the case of Malinowska coefficient, its value is sometimes lower than zero going out of range, what is caused by underestimated value of object's perimeter in the numerator of the coefficient's fraction,
   b) Low reliability of calculation procedures estimating curvature of the object's contour may cause problems in interpretation of results by using only singular value. Therefore, mean and total curvature parameters should be replaced with information about distribution of these parameters around the contour for more accurate description of all grains in original microstructure,
   c) Dimensionality of coefficients' units requires normalization of an image before calculation process starts.
4) Maximum curvature and histogram of this value is correlated with fraction of inclusion phase in the whole sample. The larger phase fraction is in a sample, the less place remains to be filled with an inclusion phase. Thus, the curvature parame-

ter has to be analyzed more deeply to detect existing correlations.

Future work should focus mainly on the development of the cost function with characterization of material behaviour based on strains and stresses analysis.

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ANALIZA MOŻLIWOŚCI WYKORZYSTANIA WSPÓŁCZYNNIKÓW KSZTAŁTU DO TWORZENIA STATYSTYCZNIE REPREZENTATYWNEGO ELEMENTU OBJĘTOŚCI DLA STALI DP

Streszczenie

Symulacje wieloskalowe FE^2 wymagają złożonych obliczeniowo procedur zarówno w skali makro jak i mikro. Wysiłki, zmierzające do poprawy efektywności programów realizujących takie obliczenia, skupiają się głównie na zrównolegleniu implementacji algorytmów numerycznych lub uproszczeniu budowy elementu reprezentatywnego. Jednym z podejść realizujących takie uproszczenie jest metoda statystycznie podobnego reprezentatywnego elementu objętości (SSRVE). Głównym celem metody jest poprawa efektywności obliczeń poprzez redukcję liczby elementów skończonych wykorzystywanych w skali mikro do dyskretyzacji przestrzeni obliczeniowej. Cel osiągany jest poprzez transformację obrazu rzeczywistej złożonej mikrostruktury materiału na uproszczoną sztucznie wygenerowaną mikrostrukturę, charakteryzującą się zbliżonymi własnościami jak jej oryginalny odpowiednik. Niniejszy artykuł dedykowany jest analizie procesu tworzenia SSRVE dla stali DP pod kątem wykorzystania współczynników kształtu do opisu własności wysp martenzytu, a następnie ich odwzorowania w SSRVE. Wykonana w tym celu analiza wrażliwości została opisana wraz z własnościami charakteryzującymi wykorzystane współczynniki. Wyniki samej analizy wrażliwości wraz z przykładowym SSRVE zostały przedstawione w niniejszej pracy.

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