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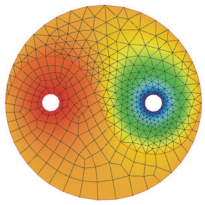

REALISTIC DESCRIPTION OF DUAL PHASE STEEL MORPHOLOGY ON THE BASIS OF THE MONTE CARLO METHOD

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Abstract

Development of appropriate algorithms for fast and reliable creation of digital representations of dual phase (DP) microstructures is described in the paper. Modified Voronoi tessellation and cellular automata grain growth algorithms are described first to highlight difficulties in a realistic description of the DP morphology by artificial numerical approaches. To solve the presented limitations a modified Monte Carlo algorithm dedicated to creation of 2D and 3D virtual representations of DP steel is proposed. Details of the developed approach as well as examples of obtained results are presented within the work. Finally, obtained 3D digital representations of dual phase steel are subjected to numerical simulations of cold cube compression tests to investigate differences occurring in the two phases during plastic deformation.

Key words: Digital material representation, dual phase steel, Monte Carlo method

1. INTRODUCTION

A realistic description of microstructure has been an interest of scientists for several decades. From the 1990's development of new generation multiscale modelling methods has been observed, and it created the possibility of higher quality simulations. Analysis of these methods shows that from one side, they can provide an exact 2D or 3D digital representation of analysed dual phase microstructures, but on the other hand they require a series of costly and time consuming experimental research and metallographic analysis. That is why they are not appropriate for a large number of numerical simulations. Due to the mentioned disadvantages the Author's interest is in applying artificial methods for fast creation of statistically equivalent digital microstructures. Development of these methods for the dual phase steels is the objective of the paper.

2. STATE OF THE ART IN MODELLING MATERIAL BEHAVIOUR IN METAL FORMING PROCESSES

A series of deterministic models, based either on closed form equations describing the flow stress dependence on external variables or on differential equations describing the evolution of internal variables, has been published in scientific literature (Szeliga & Pietrzyk, 2010). These approaches are used to describe material behaviour as a continuum, and they are based on general relationships between strains and stresses. Due to the fact that large scale problems containing billions of grains are considered, the major assumption of the mentioned approaches is that behaviour and interaction of particular grains/phases are averaged in the form of one single flow stress model. These models are commonly used in simulations for the majority of metal

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forming processes and give reasonably accurate results.

They fail, however, to accurately describe innovative steels (TRIP, TWIP, DP, Bainitic, nano-Bainitic etc.) as well as other modern metallic materials (e.g., aluminum, magnesium, titanium or copper alloys) that are being developed in various research laboratories around the world (Beladi et al., 2009; Robertson et al., 2008; Sabirov et al., 2008; Timokhina et al., 2007). Elevated properties of these materials are the results of highly sophisticated microstructures composed of large grains, small grains, inclusions, precipitates, etc.

One of those new steel grades widely used in the automotive industry is dual phase steel. DP steel thin strips have been successfully applied in the production of automobile structural parts because they are characterized by a combination of good malleability, high bake hardenability and crash worthiness. As previously mentioned, these elevated properties are the result of properly designed microstructure morphologies. The DP microstructure consists mainly of a ferritic matrix (about 70-90%) with hard martensitic islands (about 10-30%). The required combination of steel properties is usually obtained by proper balance between chemical composition of DP steels and processing parameters in order to obtain proper size, shape or position of the hard martensitic phase in the soft ferrite matrix. As seen, in these materials behaviour and interactions between particular grains are extremely important. The assumption of averaging the grain behaviour in only one flow curve becomes questionable in that case.

These issues are driving forces for the development of modern numerical models that are based on the digital material representation (DMR) approach. The main objective of the DMR is to create the digital microstructure with its features (grains, sub grains, grain boundaries, different phases, etc.) represented explicitly and not in an averaged form. The generation of the microstructure morphology with its subsequent features is one of the most important algorithmic parts of the DMR model because the more realistic the digital representation is, the more accurate the results that will be obtained. The problem of generation of digital material representations of single phase microstructures is widely discussed in Madej et al. (2011).

However, when digital representation of a dual phase microstructure is required the approaches become much more complicated in comparison to single phase materials.

One of the most commonly used solutions to obtain digital material representation of a dual phase microstructure is to use an optical or electron microscope picture and apply image processing methods (Brahme et al., 2006; Rauch & Madej, 2010). This approach provides the possibility to obtain an exact representation of complex shapes of ferritic and martnesitic phases, as seen in figure 1.

The possibility to replicate even highly complex shapes of martensite phase is the main advantage of this approach. Details of the applied image processing method are presented in Rauch and Madej (2010). The image based approaches have already been successfully used in modelling strain inhomogeneities, as well as other phenomena such as failure initiation and propagation at the micro scale level (Sun et al., 2009; Ramazani et al., 2012; Kadkhodapour et al., 2011). However, when investigation of the two phase microstructures obtained, e.g., after various cooling rates is considered, this approach is problematic because it requires an image of real microstructure. Aźseries of experimental research has to be performed first to provide these data. The entire procedure becomes even more de-

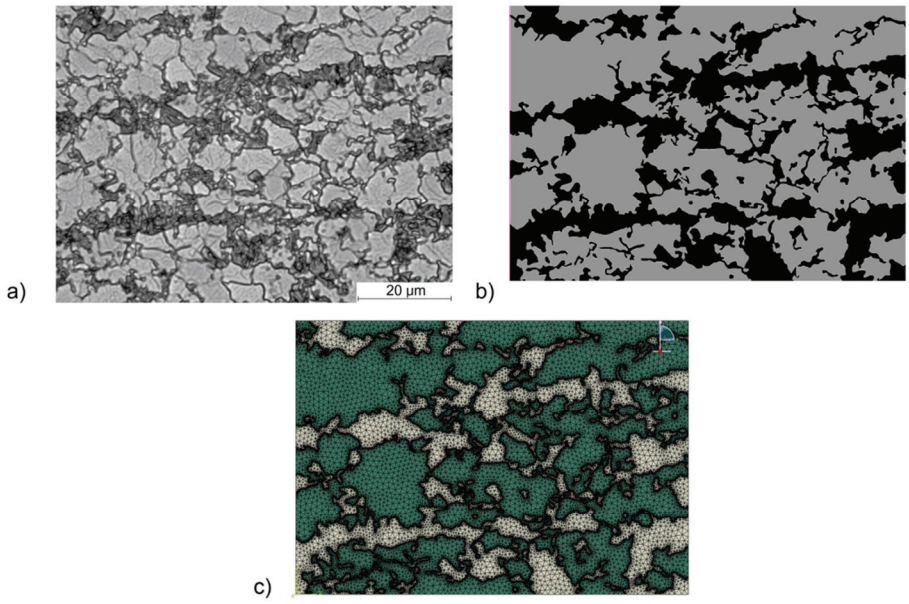

Fig. 1. *a) optical microscope image, b) binary representation and c) digital material representation with finite element discretization of dual phase steel.*

manding and time consuming when 3D digital representations are required. In 3D cases the DMR is usually created based on the reconstructed 2D slices obtained using a destructive method. Again an optical or scanning electron microscope can be used during the serial sectioning procedure to provide input data for image processing and reconstruction algorithms. An example of a non-destructive method is high energy synchrotron radiation used to provide a 3D visualization of dual phase materials (Poulsen, 2004). However, this method is very expensive.

As was mentioned in the introduction, the majority of multiscale modelling methods that provide digital representation of microstructure requires a series of costly and time consuming experimental research and metallographic analysis. That is why they are not appropriate for a large number of numerical simulations. Development and application of alternative methods for fast creation of statistically equivalent digital microstructures is described below.

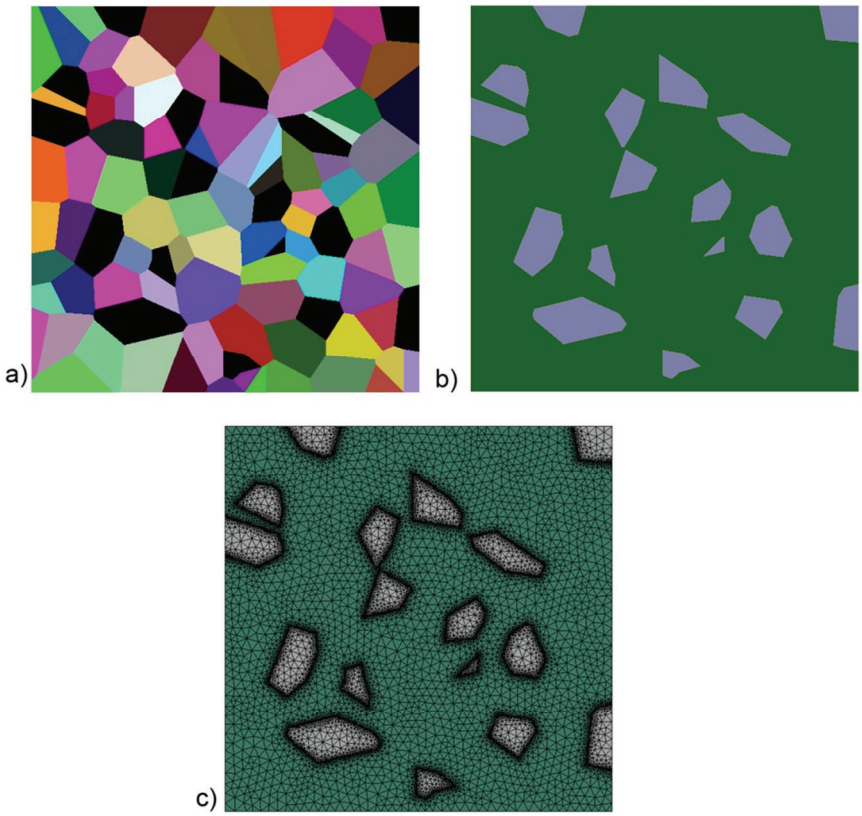

Fig. 2. *Examples of 2D digital microstructure representing dual phase material obtained by Voronoi tessellation, a) separated grains, b) binary form of microstructure, c) generated specific finite element mesh.*

3. DIGITAL MATERIAL REPRESENTATION OF DUAL PHASE STEELS

Voronoi tessellation is one of the most commonly used methods that can be classified into this group of alternative methods. A detailed discussion on generation of digital representation of single phase microstructures can be found in Madej (2010), while a brief summary and modifications to obtain a dual phase microstructure are presented in this section. The idea of this method is based on the mapping of the bounded area onto a group of specific polygons $P=\{p_1,\ldots,p_n\}$ generated around a set of initial points $S=\{s_1,\ldots,s_n\}$. Each polygon p_x is characterized by the two following features: it is connected exactly to one point s_x, where $x=1\ldots n$, and each point inside the polygon is closer to s_x than to any other point from S. For the purposes of this work points from the set S represent grain nuclei, while the polygon areas around these points, called Voronoi cells, represent final grains in the microstructure. Several algorithms can be used to determine the Voronoi diagram (De Berg at al., 2000). After the Voronoi diagram is created, the next step to obtain a dual phase microstructure is to randomly select subsequent grains and assign them to martensite phase, as seen in figure 2a. Finally, a simple binarization algorithm with the defined threshold level is applied, resulting in a two phase representation (figure 2b). The amount of martensite phase can be precisely controlled using this simple approach. Eventually, the generated morphology is subjected to a discrimination algorithm, creating a finite element mesh as seen in figure 2c. The non uniform mesh is created using a DMRmesh software developed in Madej et al. (2011). The FE mesh is highly refined along the phase boundaries to properly capture significant solution gradients that are expected in that region due to large differences in hardening behaviour of ferrite and martensite.

The Voronoi Tessellation approach is often used in scientific literature, despite the limitation that this method provides only a rough description of real morphology of dual phase microstructure (Kok & Korver 2009; Ma & Hartmaier, 2012). The geometry of the martensitic island as well as the shape of phase boundaries are far from

the real shape of these features observed under optical microscopes.

To partially overcome these disadvantages, a modified cellular automata algorithm was implemented by the Author. Details of the CA grain growth algorithm in application to digital material representation of single phase materials was studied in detail in earlier works (e.g., Madej, 2010). However, some major steps as well as necessary modifications to obtain a dual phase microstructure are recapitulated below.

The first step in the CA algorithm is to establish a discrete space composed of $n \times m$ cellular automata. With reference to 2D space it will be a grid consisting of squares. In the next step of the algorithm a set of cells is selected randomly, and then an internal variable describing the cell state is set to "grain-id", where id is used to distinguish cells belonging to different grains (id = 1,2…n, where n – number of grains). Selected CA cells represent grain nuclei that will grow in the second step of the algorithm. The transition rule for this stage is defined as follows: when a neighbour of a particular cell in the previous time step was in the state "grain," then this particular cell can also change its state:

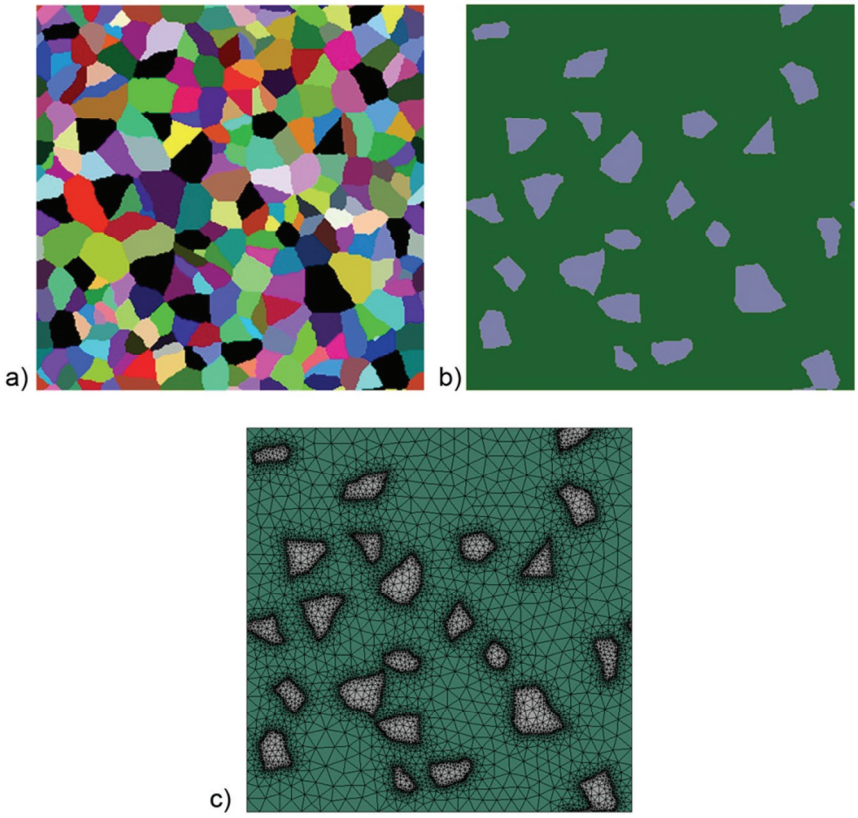

Fig. 3. *Examples of 2D digital microstructure representing dual phase material obtained by modified cellular automata algorithm a) separated grains, b) binary form of microstructure, c) generated specific finite element mesh.*

$$\mathrm{Y}_m(t_{i+1}) = \begin{cases} grain-id \Leftrightarrow \mathrm{Y}_l^m(t_i) = grain-id \\ \mathrm{Y}_{m(MSB)}(t_i) \end{cases} \quad (1)$$

where: $\mathrm{Y}_m(t_{i+1})$ – state of the m^{th} cell at the t_{i+1} time step, Y_l^m - state of the l^{th} neighbour of the m^{th} cell.

Particular grains grow with no restrictions until impingement with other grains. After that, they grow only in the area where no other grains are observed. This process is performed until the entire space is filled with grains. Using this method, microstructures with significantly different grain sizes can be created. Similar to the previous method, in order to obtain representation of dual phase microstructures, selected grains are randomly assigned to martensite phase (figure 3).

As presented, using a modified cellular automata algorithm, the shapes of phase boundaries are not as regular as in the case of Voronoi tessellation. Nevertheless, obtained DP morphologies on the basis of these two approaches are far from the shapes of real phases observed under optical microscopes (see figure 1). The specific shape of the martensitic phase is related to morphology of initial microstructure before phase transformation as well as to the cooling velocity applied during the real process. Neither Voronoi nor cellular automata algorithms can replicate these final complex morphologies in a qualitative manner. Only quantitative information regarding amount of martensite fraction is replicated. As mentioned, despite these limitations, both methods are quite commonly applied in literature during investigation of dual phase behaviour under deformation conditions.

However, to improve predictive capabilities of digital representation of dual phase microstructures and solve the mentioned limitations, the Author decided to develop a grain growth algorithm on the basis of the Monte Carlo method.

4. MONTE CARLO BASED ALGORITHM

Monte Carlo (MC) is a general name for a group of algorithms based on a completely random sampling of a solutions space Ω for application in mathematical and physical simulations (Blikstein & Tschiptschin 1999; Metropolis et al., 1953). The algorithm is composed of several major steps:

– generation of input data that describe an initial state of material in the form of a two or three-dimensional matrix of cells. A random state Q_i that belongs to $\Omega = \{Q_0, \ldots, Q_{n-1}\}$ is assigned to each cell in the investigated space as seen in figure 4.

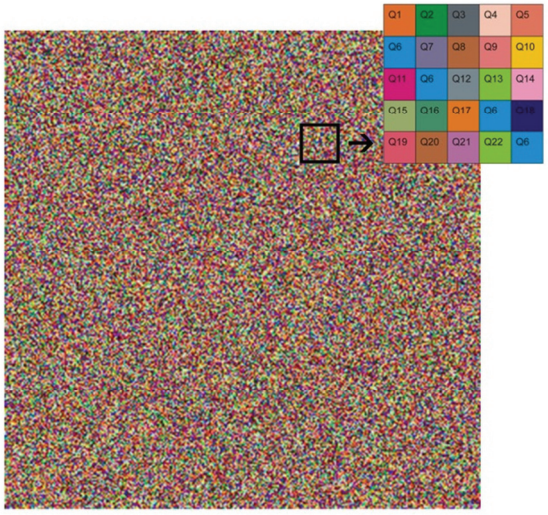

Fig. 4. *Example of a random distribution of 50 states in 2D space.*

– random sampling of the entire space is then performed in order to calculate the energy change of the subsequent cells (figure 6a):

$$E_i = J_{gb} \sum_{<i,j>} \left(1 - \delta_{S_i S_j}\right) \tag{2}$$

where: J_{gb} - coefficient used to determine the grain boundary energy, δ_{SiSj} - the Kronecker delta.

Sampling is performed according to the Metropolis algorithm until all cells are selected (Metropolis et al., 1953). In the present model aźMoore neighbourhood containing 8 neighbours was selected as seen in figure 5.

– random changes in cell states from the Q-1 available states is another step of the algorithm. After the change of the state, the energy of the system is again calculated using eq. (2). The energy difference is calculated as:

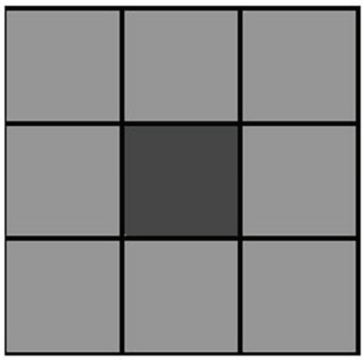

Fig. 5. *Examples of Monte Carlo Moore neighbourhoods.*

$$\Delta E = E_{i+1} - E_i \tag{3}$$

Finally the probability of change in the cell state is calculated:

$$p(\Delta E) = \begin{cases} 1 & \Delta E \le 0 \\ \exp\left(-\dfrac{\Delta E}{kT}\right) & \Delta E > 0 \end{cases} \tag{4}$$

where ΔE – energy difference of the selected cell prior and after random change of the state, k – Boltzmann constant, and T – temperature of the simulation.

If the calculated difference of energy takes a negative value, a new value of cell state is accepted (figure 6b), otherwise the state is accepted with a probability p (figure 6c). With successive MC steps, the energy value of the entire system is reduced, and digital microstructure with clearly visible phases can be observed.

Due to the stochastic nature of the MC method, the major limitation is long computational time. In order to accelerate the algorithm, several modifications to the standard approach were implemented. The first concerns the sampling of the new state of the cell. Contrary to the mentioned approach, where sampling of a new state was from the entire Q-1 available states, in the modified version sampling is realized only from states among those directly adjacent to the analyzed cell. Another modification of the algorithm is based on a division of the cells into two groups lying inside the grain and those that are at the grain boundary. As a result only cells lying along the grain boundary have the possibility to change the state and minimize energy of the system. A change of the cell lying inside the grain always leads to an increase in energy value. Finally it is assumed that during a particular MC step, each cell can be selected only once.

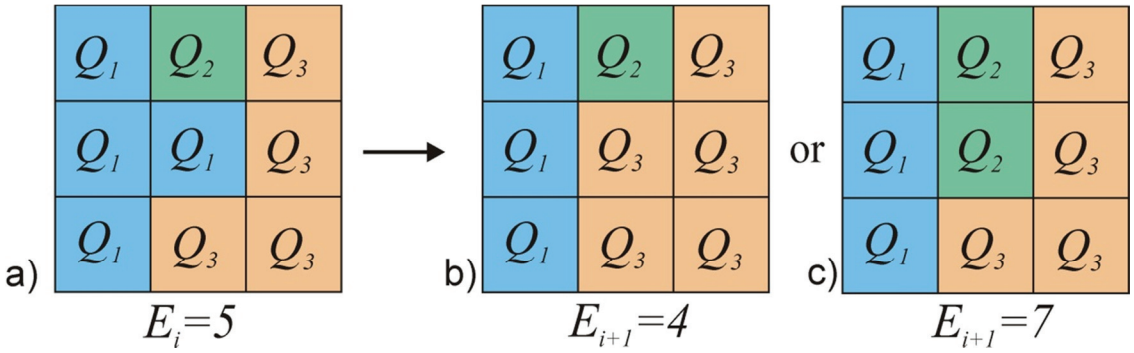

Fig. 6. *Illustration of the energy calculation process for a) initial state, b,c) two possibilities of the final state.*

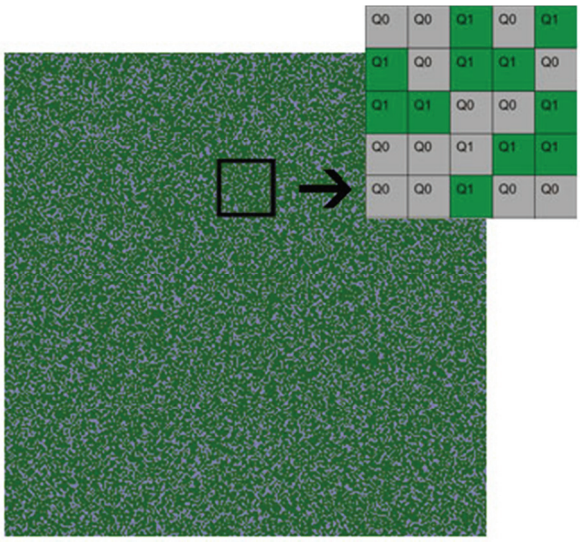

Fig. 7. *Examples of a random distribution of 2 states in 2D solution space.*

that observed experimentally for dual phase steel can be obtained (figure 8). The remaining steps of the algorithm MC remain unchanged in this case.

The amount of martensite phase in the final microstructure can be precisely controlled by proper selection of the amount of MC steps. As presented using the MC approach, not only a quantitative but also a qualitative description of DP morphology can be obtained.

Finally, it must be mentioned that the possibility to obtain a realistic digital representation of a 3D dual phase microstructure is a major advantage of the proposed approach. In the case of dual phase steels, the possibility to model complete 3D morphology is import since special distribution of hard martensite phase significantly affects inhomogeneous deformation of the ferrite matrix. As mentioned in the first part of the paper, creation of 3D represen-

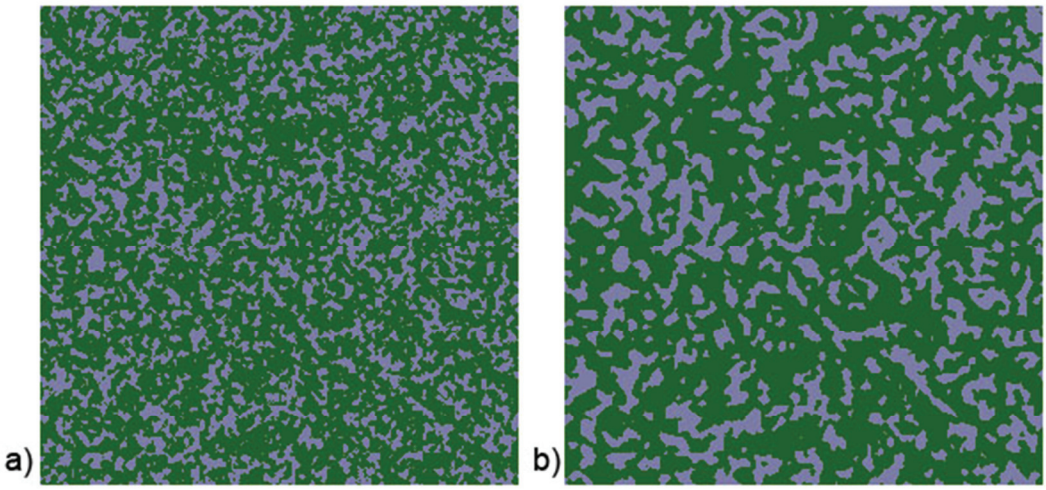

Fig. 8. *Subsequent steps of the MC algorithm with the assumption of only two MC states $\Omega = \{Q_0, Q_1\}$.*

Using the MC approach, it is possible to obtain a digital representation of polycrystalline microstructures similar to those using the cellular automata method. However, when the amount of cell states Q is limited in the solution space Ω only to two ($\Omega = \{Q_0, Q_1\}$) as seen in figure 7, morphology close to

tations on the basis of experimental analysis is extremely time consuming and expensive. The developed MC approach is free of these disadvantages.

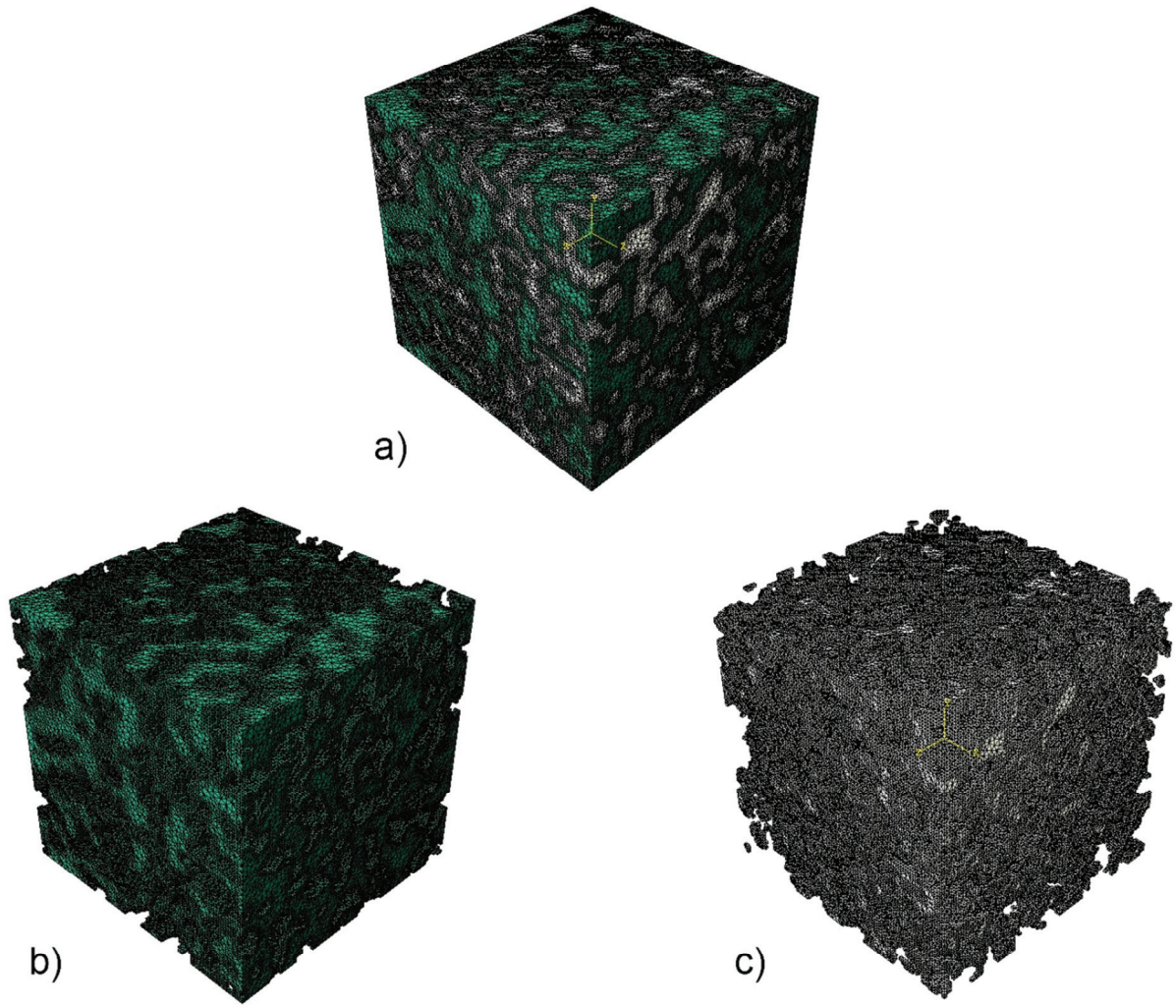

Fig. 9. *a) Digital representation of a dual phase steel in 3D space, b) separated ferrite phase and c) separated martensite phase.*

An example of the 3D representation of a DP steel with generated finite element mesh is shown in figure 9. The finite element mesh was generated with the approach described in the Author's earlier works (Madej et al., 2011). To describe solution gradients along particular phases a specific refined mesh was created. When the topology of the initial microstructure is created, and material properties are assigned to each grain, then the digital material can be further transferred into a numerical model that will simulate material behaviour under deformation conditions. The main key in the DMR model is the possibility to assign material properties to particular grains. At this stage of the research these properties can be represented as either scalar or vector values. However, there is no problem in assigning other data structures such as tensors to particular grains. In the present paper the flow curves assigned to particular grains describe behaviour of particular phases, namely ferrite and martensite. The flow stress data were reported in Delannay et al. (2007) and are shown in figure 10.

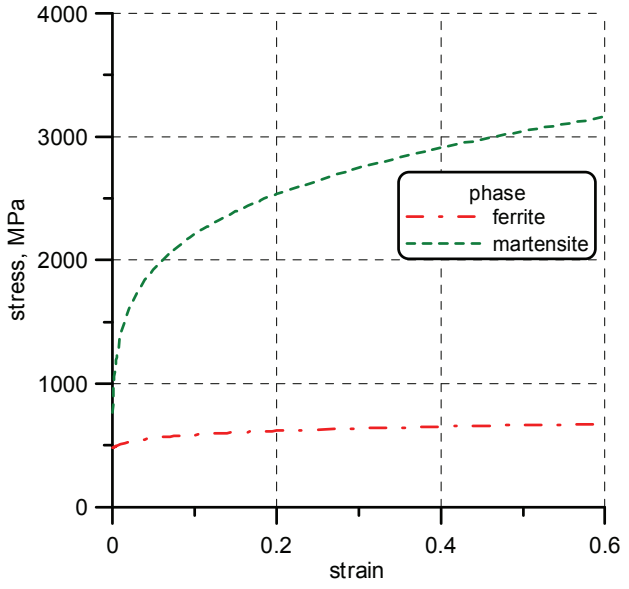

Fig. 10. *Flow stress models for different phases in steel (Delannay et al., 2007).*

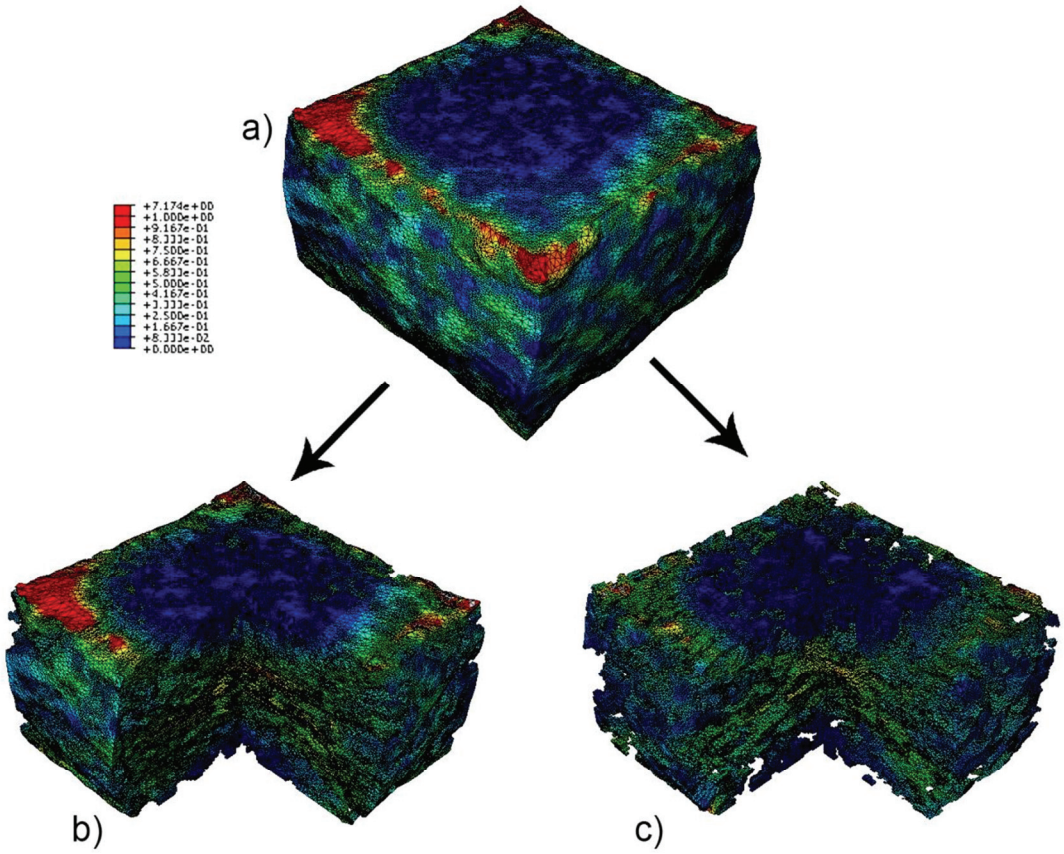

Fig. 11. *Equivalent plastic strain distribution in a) complete digital representation of a dual phase steel, b) separated ferrite phase and c) separated martensite phase (sample size 300×300×300 μm).*

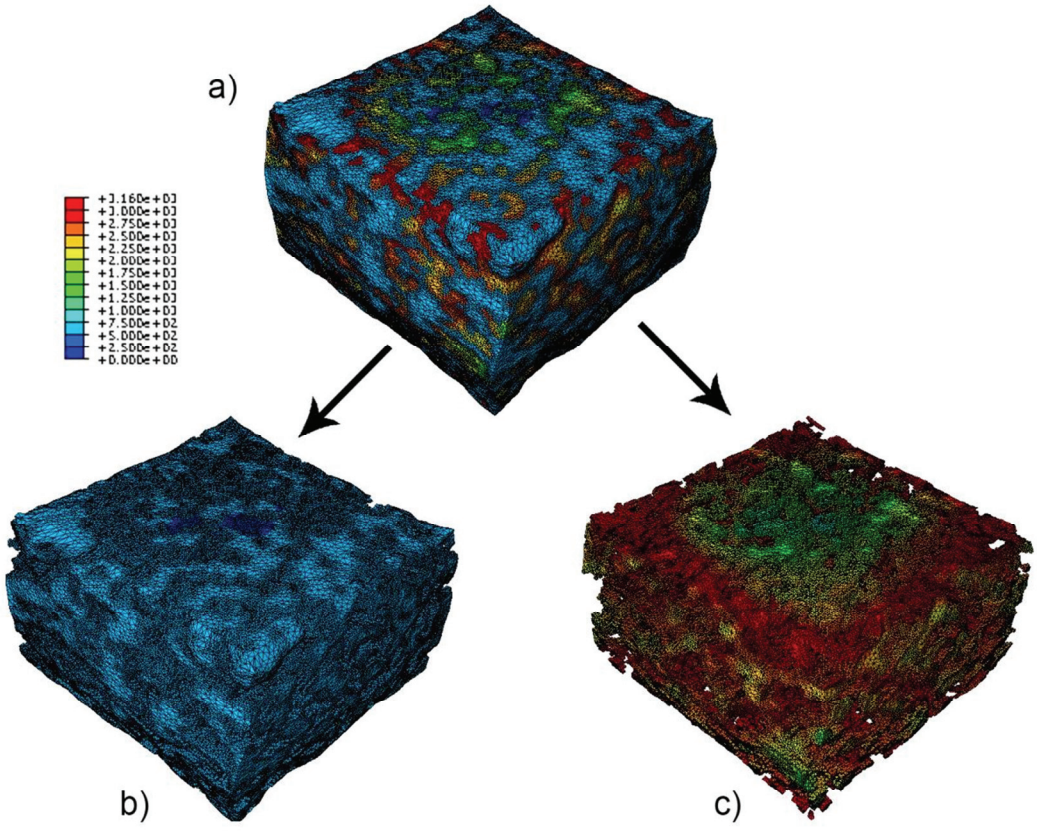

Fig. 12. *Equivalent plastic stress distribution (MPa) in a) complete digital representation of a dual phase steel, b) separated ferrite phase and c) separated martensite phase (sample size 300×300×300 μm).*

An example of the application to a 3D standard cube compression test is shown in figures 11 and 12. Deformation degree was set to 30% of initial sample height, while the coulomb friction coefficient was 0.1.

The strain localization is clearly visible in figure 11 in ferrite phase; however, martensite phase also reveals signs of regions carrying high strain values. Regions with large strain localization forming characteristic bands aligned 40-45^{o} to the deformation direction are observed in both cases. Even higher differences in material behaviour are observed when stress distribution in these phases is investigated, as seen in figure 12.

Because martensite is rich in carbon, high stress values observed in this region will be precursors of brittle failure that eventually will propagate to ductile ferrite phase. The problem of dual phase steel failure taking into account the influence of microstructure morphology will be investigated in future work.

5. CONCLUSIONS

The results of research on the development of a digital representation of dual phase microstructure, and the advantages provided by this technique were presented in this paper. Examples of various approaches to create digital material representation of two phase steel were discussed. Particular attention was put on development of the method used for fast creation of digital microstructures: Voronoi tessellation, cellular automata and Monte Carlo algorithms. Based on the presented research it can be concluded that:

- the first two algorithms provide the possibility to obtain only quantitative digital representation of microstructure for further FE simulation. The complex morphology of dual phase steel is neglected in this case.
- the Monte Carlo method with the assumption of only two cell states can provide qualitative and quantitative representation of dual phase steels. Both complex morphology of martensite phase as well as the amount of martensite fraction can be taken into account using this approach. The same advantages are reported for 2D as well for 3D cases. It is expected that a similar approach can be used to recreate representation of more complex microstructures, e.g., in TRIP steel.
- 3D realistic description of morphology of dual phase microstructure provides the possibility of a detailed virtual investigation of strain and stress inhomogeneities occurring at the micro scale level and can be a valuable support for experimental research. These inhomogeneities play a crucial role during other phenomena occurring during material deformation, e.g., brittle and ductile fracture initiation/propagation, which will be further investigated.

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NUMERYCZNA ANALIZA PROCESU ZACISKANIA TULEI

Streszczenie

W opracowaniu przedstawiono wyniki analizy numerycznej procesu zaciskania tulei między innymi na linach stalowych przy pomocy obrotowych segmentów bruzdowych. Omówiono obszary zastosowań wyrobów typu liny i cięgna oraz przedstawiono sposoby wykonywania na nich zakończeń. Analizę numeryczną procesu przeprowadzono w oparciu o metodę elementów skończonych (MES), wykorzystując komercyjny pakiet oprogramowania DEFORM - 3D. Omówiono modele geometryczne zastosowane w obliczeniach oraz wpływ kształtu wykroju na jakość wyrobu. Uzyskane wyniki analizy numerycznej wykorzystano w projekcie przyrządu do praktycznej realizacji tego procesu.

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