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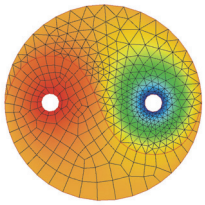

DIGITAL MATERIAL REPRESENTATION OF POLYCRYSTALS IN APPLICATION TO NUMERICAL SIMULATIONS OF INHOMOGENOUS DEFORMATION

LUKASZ MADEJ

Department of Applied Computer Science and Modeling
AGH - Akademia Gorniczo Hutnicza, Krakow, Poland
lmadej@agh.edu.pl

Abstract

Results of research on application of modern numerical methods for analysis of influence of microstructure heterogeneities on material processing are presented in this work. Various approaches that represent state of the art in this area are discussed. The main focus, however, is put on the micro-scale behavior, where advantages of digital material representation can be taken into account. Digital representation allows to model microstructure with its features like crystallographic orientation, grain boundaries or phase boundaries taken in an explicit manner. Two fast and computationally efficient methods for creation of statistically representative microstructures are presented in the paper: the cellular automata technique and Voronoi tessellation. Examples of capabilities of these two methods are presented and discussed. This section is supported by selected examples of numerical simulations of channel die compression test based on the digital microstructures.

Key words: digital material representation, finite element modeling, inhomogenous deformation

1. INTRODUCTION

The Finite Element (FE) method is commonly applied to create a complex description of a particular deformation, thermomechanical or heat treatment process. Applications of the FE method are wide, from modeling of simple plastometric tests (e.g., compression, tension, torsion) to modeling the complicated behavior of entire structures (e.g., cars, buildings, implants). FE models are able to replicate the real processes and phenomena that take place in materials, as well as in the surroundings. Plastometric tests at various deformation conditions (temperatures, strain rates) combined with an inverse analysis to eliminate various heterogeneities are usually performed to obtain accurate flow stress data necessary for the FE analysis. Since large scale problems containing billions of grains are usually considered, the major assumption of this approach is that behavior and interaction of particular grains is homogenized in the form of a single flow stress model. This procedure is well established and widely used in simulations of existing and new manufacturing technologies e.g. rolling, forging, stamping, etc. However, this commonly used approach faces now several challenges. One of them is fast development of modern steel grades (TRIP, TWIP, DP, Bainitic, etc.) and aluminum, magnesium or copper alloys that are characterized by elevated material properties. These special properties are the result of sophisticated microstructures with combination of e.g. large grains, small grains, inclusions, precipitates etc. (Beladi et al., 2009; Robertson et al., 2008; Sabirov et al., 2008; Timokhina et al., 2007). Gener-

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ally speaking microstructure features influences every aspect of mechanical as well as thermo-mechanical material response to processing and exploitation conditions. An omnipresent miniaturization that requires development of new micro forming technologies is another recent challenge. Since the sample is no longer a large aggregate of billions of grains but it may contain only hundreds of grains, an interaction between each particular grain becomes important (Egerer & Engel, 2004; Jeswiet et al., 2008; Vollertsen et al., 2004; Wang et al., 2009). However, the need to incorporate material structure into the simulation is not only limited to metallic materials, similar problems are observed in other engineering materials (Coster et al., 2005; Ballani et al., 2006; Haug et al., 2007).

New numerical methodologies are needed to meet such new challenges. The Digital Material Representation (DMR), which is the subject of the present work, is one of the possible solutions.

First a state of the art in this matter is presented within the paper. Various methods of generation of the digital microstructures as well as examples of their applications are presented. This is followed by detailed description of the two methods used by the author to obtain digital microstructures of policrystals. The first well known in literature is Voronoi tessellation, the second is an author solution based on the cellular automata method. The advantages and disadvantages of these approaches are discussed. Finally obtained digital microstructures are incorporated into the commercial finite element software and examples of inhomogeneous material response to loading are highlighted.

2. MODELS BASED ON DIGITAL MATERIAL REPRESENTATION

To the Author's knowledge, finite element simulation by Deve and Asaro (1989) is one of the first studies that considered a very simplified polycrystalline structure. This work is mainly focused on experimental investigation of plastic failure modes in polycrystalline materials, although a numerical approach based on the crystal plasticity theory is also described. For the last few years various researchers intuitively were trying to incorporate microstructure during simulations (e.g. Beynon et al., 2000; Beynon et al., 2002; Das et al., 2002; Gandin & Rappaz, 1994; Gawąd & Pietrzyk, 2007; Lan et al., 2004; Madej et al., 2004; Raabe & Becker, 2000, 2007). This research and fast progress in the multi-scale modeling capabilities reported earlier in Madej et al.'s work (2008) gave a lot input into development of the idea of the Digital Material Representation (DMR).

The concept of the DMR has been proposed recently and it is dynamically evolving. The main objective of the DMR is creation of the digital representation of microstructure with its features represented explicitly. The DMR basic concept creates possibility to describe material at various scales. Such approach offers gathering and processing of metallurgical data, which is related to each other at the different levels of description. Thus, the complex DMR system consists of several software modules. Some of these modules are dedicated to selected single scales, e.g. characterization of material microstructure (micro-scale). On the other hand, the rest of the modules span some of the scales together to perform multi-scale calculations, e.g. micro shear and shear bands or dynamic recrystallization.

The more precise DMR is applied, the more realistic results of calculations regarding material behavior are obtained. Due to that conclusion, the detailed virtual analysis of simulation results can be performed, while errors of calculations are minimized. This allows the replacement of the conventional methods, dedicated to determination of material properties, by the computer automatic analysis, which connects DMR with modeling of manufacturing processes and with digital analysis of results (figure 1).

As presented, conventional numerical approach provide general information regarding e.g. strain distribution across the sample. The underlying microstructure is not taken into account in this case. On the other hand results obtained from the experimental approach clearly show how complex is underlying microstructure. Lack of detailed information regarding material behavior from conventional numerical approach at micro scale level is evident. That is why application of the DMR approach is so important, it provides a possibility to take this complex microstructure into account. That way a detailed numerical analysis of inhomogeneities in microstructure can be analyzed without the need to perform costly laboratory analysis composed of e.g. optical or SEM/TEM microscopy investigation.

For the purpose of numerical simulations the digital microstructures can be created as exact replicas of real microstructures. In this case an image of real microstructure is required, what always employs a series of experimental analysis. This procedure is becoming even more complex when 3D digital

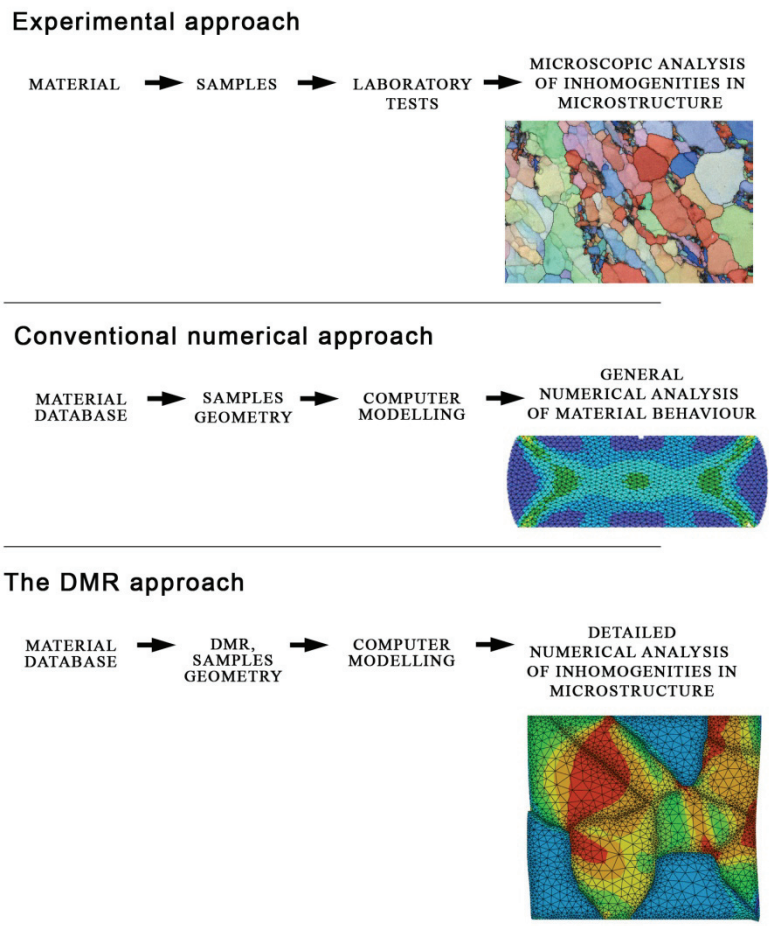

Fig. 1. *The DMR basic concept in comparison to conventional approach and experimental investigation.*

microstructures are required. To reduce the need for experimental analysis a statistically equivalent microstructures can be created using only numerical methods. That way a 2D and 3D digital microstructures can be obtained in a fast and efficient way.

A software dedicated to such virtual microstructures, developed in the CEMEF group of Mines-Paristech (Bernacki et al., 2007, 2009; Loge et al., 2008), gives the possibility to create digital material samples and to test their properties before and after processing. Two approaches are used to create such digital microstructures. The first is the Voronoi tessellation that provides statistically representative artificial microstructures. In the case when obtained digital structure is not in a good agreement with the experimental data, optimization algorithms are applied. The second approach is based on voxelized description of microstructure and allows to work with real 3D microstructures obtained, for example, by tomography. This approach, however, is much more complex, expensive and time consuming. The digital microstructure is then the basis for the finite element mesh generation and subsequent FE simulations of the processing conditions. The main application of this software is to create and characterize digital microstructures e.g. virtual electron back scattered diffraction. This software also provides data for the finite element simulation of large deformation or microstructure evolution during dynamic recrystallization. An example of the numerical simulation with this approach is presented in figure 2 (Bernacki et al., 2007). Similar approach is being developed at Cornell University by Dawson and Miller (2003). Research regarding 2D and 3D digital microstructures and their behavior during material deformation has also been conducted by Li and Zabaras (2009) and Sundararaghavan and Zabaras (2004) at Cornel University. This model is used to simulate microstructure development during large plastic deformations, as well as during heat treatment (i.e. static recrystallization).

A lot of research in the area of DMR was done by the joint group at Carnegie Mellon University, Alcoa Technical Center and National Institute of Standard and Technology (Brahme et al., 2006; Saylor et al., 2004; Rollett et al., 2004). Authors decided to use a 2D EBSD maps obtained in two directions, normal and perpendicular to the rolling direction, respectively, to create a 3D microstructure. Based on the geometrical information about the grain sizes in those directions a set of ellipsoids was generated. After a minimization procedure a set of optimally packed ellipsoids is obtained. Two approaches are proposed to fill the remaining areas between the ellipsoids. In the first the centers of ellipsoids are used as nucleation points and a simple grain growth algorithm is applied to fill the entire space by the grains. The second uses the Voronoi tessellation to create grain that are closely related to previously obtained ellipsoids. Both approaches can provide a periodical microstructures which later on are fulfilled with the information obtained from orientation distribution function. After this a microstructure is created in the geometrical and crystallographic sense. Authors proposed also a simple algorithm to create highly elongated microstructures that repre-

sent a microstructure after rolling. In this case some of the Voronoi cells vertices are scaled by a selected scaling factor. Authors used a commercially pure aluminum to create a 3D digital microstructure for simulation of the recrystallization.

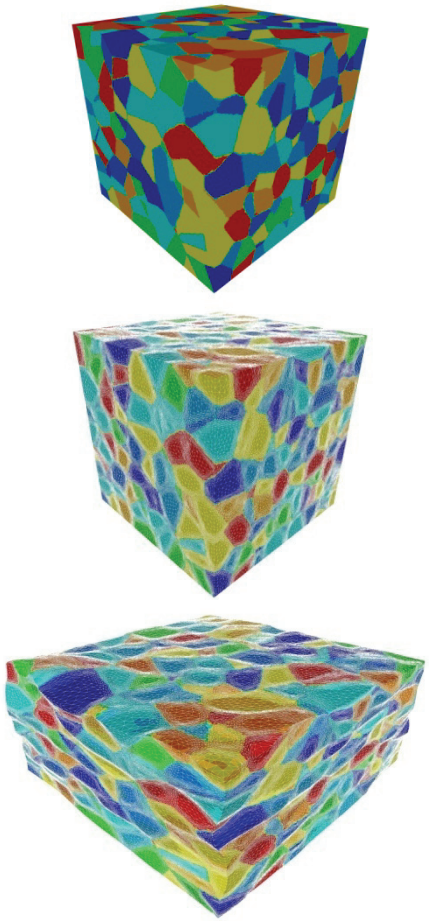

Fig. 2. *Digital representation of a microstructure before and after deformation (Bernacki et al., 2007)*

A problem of the generation of the 3D digital microstructures based on the experimental data was also considered by Lewis and Geltmacher (2006). The 3D microstructures were created on the basis of optical microscopy, serial sectioning and electron back scattered diffraction EBSD. To obtain reliable representation of the real microstructure a sectioning depth was selected as 3.3 μm. The average grain size of the investigated austenite grains was 30-80 μm what provided average number of 10-20 sections per grain. After each section an EBSD map was done what provided an information regarding crystallographic orientations across the microstructure. After a reconstruction procedure obtained 3D digital microstructure was meshed using the quadratic elements. Particular finite elements are assigned to underlying grains with the specific crystallographic orientation. The FE calculations are performed with the crystal plasticity approach. The main focus of this work was to investigate microstructure behavior under uniaxial stretch, plane strain tension and uniaxial tension condition. The sample was subjected to low deformation (about 0.2%) in order to evaluate which regions of the microstructure, under various stress condition, will start to deform plastically. The major drawback of this study is the limitation to a small degree of deformation.

Similar approach is presented by Cornwell et al. (2006). A software develop at Carnegie Mellon University is used for creation of the 3D digital microstructures. The developed approach is based on the information provided by the scanning electron microscope. Data provided by the experimental research are used to create distribution functions for size, shape and orientation of grains. The algorithm uses the Monte Carlo method to minimize the differences between the experimentally and numerically obtained distribution functions. Sorting is made through sets of configuration until the distribution functions converge. After this process digital microstructure is considered statistically equivalent. Based on the obtained geometry of the microstructure a 3D finite element mesh is created using the advancing front grid generating algorithm. Authors focused on deformation of the aluminum microstructures containing 134 grains. They have also used the crystal plasticity approach in order to evaluate influence of microstructure features on the strain localization.

Another approach, commonly used to create 3D microstructures, deals with serial sectioning. A software developed in Groeber et al.'s work (2008) takes as input a series of Electron Back Scattered Patterns from a serial sectioning experiment and reconstructs these 2D slices into the 3D microstructure. The authors of this work also pointed out the complexity of the approaches that are based on the EBSD data and proposed an artificial method for creation of digital microstructures. The approach developed to create statistically similar microstructures is generally a voxel-based algorithm interconnected with the Voronoi tessellations approach. This method also requires a series of experimental analyses, what is just a small simplification in comparison to the serial sectioning approach.

Advantages provided by the digital material representation were also highlighted in Zhao et al.'s paper (2007) by comparison of three different approaches to the problem. The first one is the simplest and it uses a homogenized constitutive model at the integration point level. Each integration point repre-

sents the averaged behavior of a large number of grain orientations. The second approach considers each element of the FE mesh as single crystal so the FE mesh is treated as polycrystalline conglomerate. The third one takes into account idealized geometry of the grains and represents them by a set of fine finite elements. Grains were represented by polyhedrons. The key element in the third method is again creation of the geometrical representation of microstructure e.g. using the Voronoi diagrams, to represent grains and to create the finite element mesh describing these grains. Zhao et al. (2007) pointed out that their approach lacks tools to automatically produce FE meshes conforming to create grains. That is why several simplifications are adopted, e.g. structured FE meshes are created independently using another software. The advantages provided by the third method based on DMR were clearly highlighted in comparison to the first two methods. Much better crystallographic material description was obtained. Problem of incorporating crystal plasticity into the digital material framework is also extensively studied in Loge et al.'s (2008) and Roters et al.'s (2010) works.

A digital microstructure based modeling is not only limited to taking into account the grain geometry. In Hu et al.'s paper (2008) both grains of the aluminum as well as hard particles are taken explicitly into account. Significant influence of the hard particles on the strain distribution and failure at the microscale level is investigated in this paper. The approach is based on the conventional rheological models assigned to different microstructure features, although advantages provided by the crystal plasticity are also considered as plans for future work. Similar work is described by Mishin and Farkas (1999), who investigated the effect of particle arrangement on the damage evolution in aluminum based composites. In this work a simplified geometry of the inclusions was obtained using the Voronoi method while more complicated shapes were obtained using the voxel approach. Another interesting work on particle reinforced metal matrix composites and porous sintered steels is mainly focused on the elastic deformations (Ayyar & Chawla, 2006). Image based modeling with the serial sectioning approach during obtaining digital microstructure is considered in this work.

Another approach, that is also worth mentioning, is focused on investigation of the material behavior not under monotonic but cyclic conditions on the basis of the digital microstructure (Barbe & Quey, 2007). Authors created a digital microstructure with the commonly used Voronoi approach and then the structure was meshed to capture the grains geometry during the FE simulations.

Finally, it should also be pointed out that the digital microstructures becomes very popular in many other areas of material science, e.g. to simulate sintered ceramics (Coster et al., 2005), concrete (Ballani et al., 2006) nano crystaline materials (Dobosz et al., 2009) or behavior of ferroelectric materials (Haug et al., 2007).

As it is seen in the presented review of research, the generation of the material microstructure with specific properties is one of the most important algorithmic parts of systems based on the DMR. Such DMR is further used in numerical simulations of processing or simulation of behavior under exploitation conditions. The more accurate the digital representation is the more accurate results can be obtained. Most commonly used method is Voronoi tessellation, voxel method and serial sectioning, but also other methods like cellular automata are capable to generate microstructure and they are discussed within the framework of this work.

3. CREATION OF DIGITAL MATERIAL REPRESENTATION

As mentioned earlier, the Voronoi tessellation is commonly used method dedicated to generation of initial microstructures, as well as to interpretation of some metallographic phenomena. The idea of this method is based on the mapping of the bounded area onto the group of specific polygons $P=\{p_1,\ldots,p_n\}$, generated around a set of n distinct 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 $x = 1\ldots n$.
– Each point inside the polygon is closer to s_x than to any other point from S.

For the purposes of the present work points from the S set represent grains nuclei, while the polygon areas around these points, called Voronoi cellulars, represents final grains in the microstructure.

Several algorithms used to determine Voronoi diagram can be distinguished. One of them, based on the Brutal Forces approach, points out bisectrixes between each pair of points and then eliminates bisectrixes, which do not satisfy Voronoi assumptions (De Berg et al., 2000). Nevertheless, this algorithm is very time consuming. Thus, the Fortune algorithm (De Berg et al., 2000), which is much more efficient, has been chosen for the purposes of the DMR system.

The main idea of the Fortune algorithm is based on the sliding line, which moves constantly through the input set of points *S* (grain nuclei). The step-by-step procedure of this method is presented in figure 3.

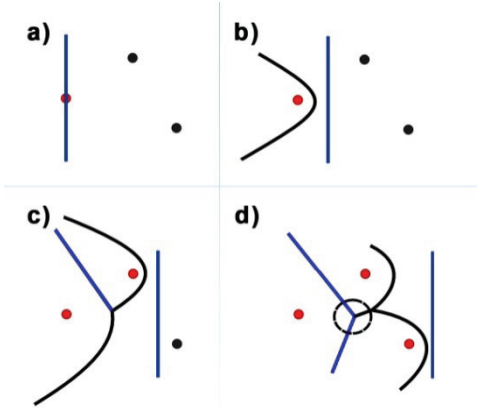

Fig. 3. *Schematic idea of the Voronoi diagram generation by the Fortuna algorithm (De Berg et al., 2000).*

In the first step the vertical line reaches the first point, which is marked with red color (figure 3a). When the sliding line passes through the point, the new parabolic line is created (figure 3b). This parabola slides in the same direction as the leading vertical line and the peak of the parabola is located exactly in the middle between the leading line and the original starting point. During the motion the parabola extends its range iteratively. The procedure of parabola creation is repeated each time the vertical line passes a non-marked point. The new parabola and the old ones cross each other in the two points, creating systematically the bisectrixes. If more than three points are marked, the "circle events" take place and Voronoi junction points are determined. The connections between Voronoi junction points creates the final Voronoi diagram. Implementation of the Fortune algorithm was applied to investigate the phenomenon of grain growth at the 2D space. Examples of obtained results for different number of grains are presented in figure 4.

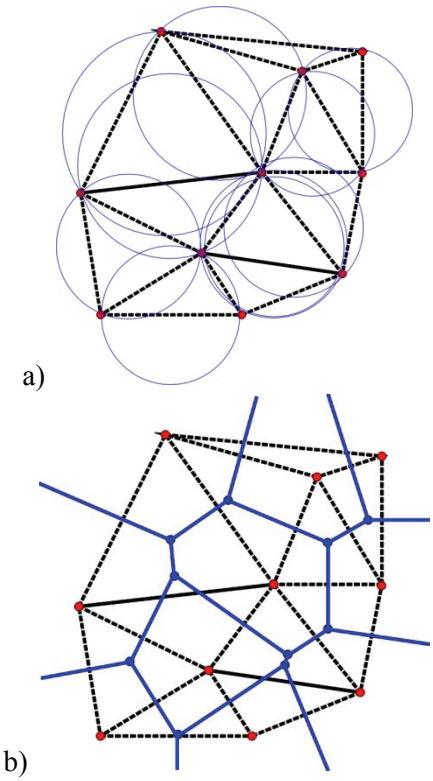

Fig. 5. *a) schematic idea of the Delaunay triangulation, b) Voronoi diagram.*

In the 3D space the third algorithm based on the Delaunay triangulation is used to create a Voronoi diagram. The general algorithm for triangulation starts by forming the super triangle enclosing all the points from set *V* that has to be triangulated. Then incrementally, a process of inserting the points *p* into the set *V* is performed. After every insertion step a search is made, to find the triangles whose circumcircles enclose *p*. Identified triangles are then deleted from the set. As a results an insertion polygon containing *p* is created. Edges between the vertices of the insertion polygon and *p* are inserted and form the new triangulation. After all the points are inserted the Delaunay triangulation is created (figure 5a). When all the centers of the circumcircles are connected, the Voronoi diagram is obtained (figure 5b).

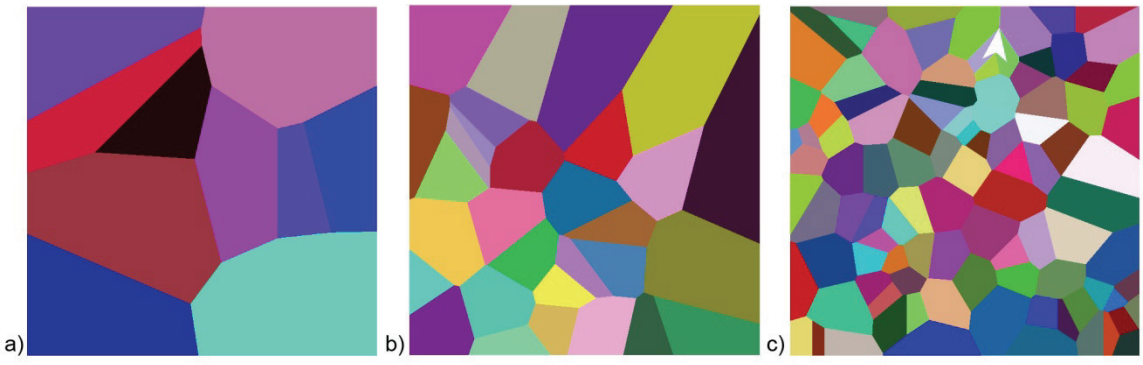

Fig. 4. *Results of simulation for different number of grains a) 10, b) 30, c) 50.*

Example of the 3D digital microstructure obtained from the presented algorithm is shown in figure 6.

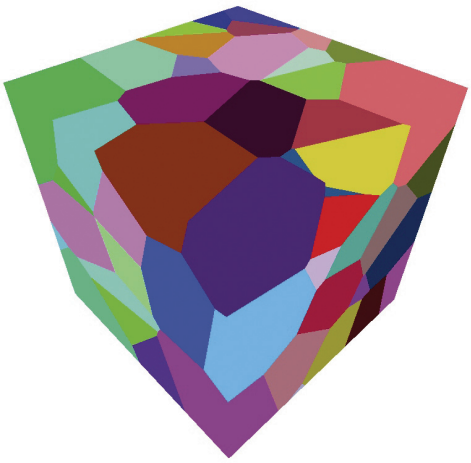

Fig. 6. *The digital microstructure containing 100 grains obtained from the Delaunay triangulation.*

The principle of cellular automata is based on the three basic concepts:

– The cellular automaton space (it is grid of finite number of cells described by several internal variables).
– The cell neighborhood (qualifies its closest neighbors).
– The transition rules that control the changes in the cells states.

In every time step, the internal variable describing state of each cell in the lattice is determined by the previous states of its neighbors and the cell itself, by a set of precisely defined transition rules f:

$$\gamma_i^{t+1} = f\left(\gamma_j^t\right) \tag{1}$$

where $j \in N(i)$, $N(i)$ – surrounding of the i^{th} cell, γ_i – state of the i^{th} cell.

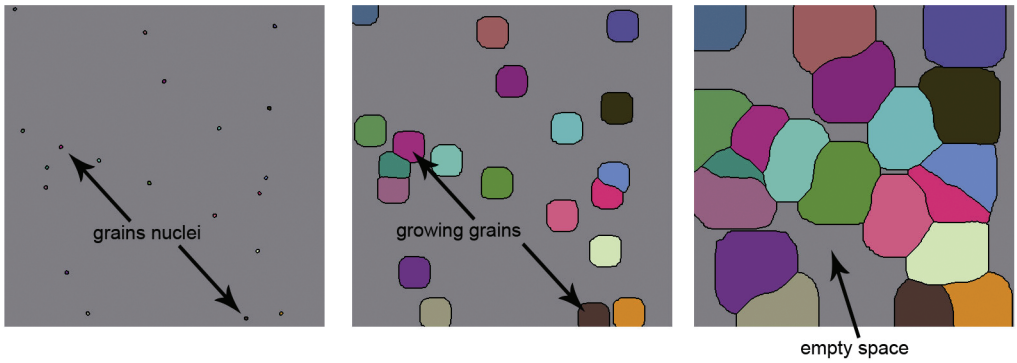

Fig. 7. *Stages of CA grain growth algorithm.*

Obtained shapes of grains are still far from shapes of real grains observed under the optical microscopes, and this is the main disadvantage of this approach.

To overcome the problem with the artificial grain geometry, the cellular automata method can be applied. This technique was originally developed in the early 1960s by Janos Von Neumann (1966) to simulate the behavior of discrete, complex systems. In the early stages the low capability of the computers was the main obstacle limiting development of this method. With the increasing computational power of present computers this technique becomes more popular. During the last few years the CA method has also been applied to model material behavior during plastic deformation (Madej et al., 2009a). In this work the CA based algorithm is applied to generation of initial microstructure, which is further on used in some specific thermo-mechanical simulations.

Modeling of the grain growth in the microstructure can be easily performed on the basis of the CA method. The implemented algorithm for the purposes of this research is a simplified version of the CA grain growth algorithm. More advanced algorithms based on the energy conditions can be found in Liu et al.'s work (1996).

The first step in the CA method is to establish the discrete space composed of cellular automatons. With reference to the 2D space it will be a grid built of squares, whereas in 3D spaces this grid will be composed of cubes. In the next step of the algorithm a set of CA cells is selected randomly and then internal variable describing cells state is set to "*already grown*". These cells represent grains nuclei. The second step of the algorithm is focused on a grain growth. The transition rule for this stage is defined as follows: when a neighbor of a particular cell in the previous time step is in the state "*already grown*", then this particular cell can also change its state. Particular grains grow with no restrictions

until the impingement with other grains. After that they grow only in the empty space area where no grains are observed as seen in figure 7. This process is performed until entire space will be filled with grains.

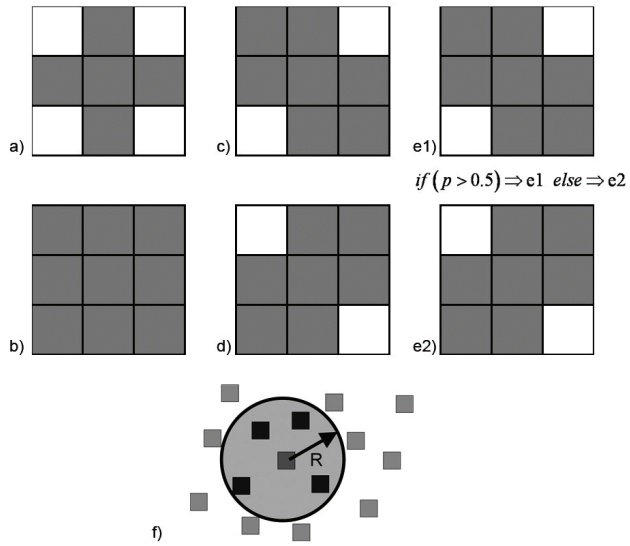

Fig. 8. *Examples of the CA neighborhoods: a) von Neumann, b) Moore, c) hexagonal left, d) hexagonal right e) hexagonal random ($p \in \langle 0,1 \rangle$ – probability), f) random.*

rounded only by five cells and in hexagonal by six cells. Neighboring cells change randomly in every time step as seen in figure 8c,d. Finally, a random neighborhood is implemented where number of neighboring cells depends on the defined radius *R* (figure 8e). The larger the radius *R* the more CA cells fall into the neighborhood area. Similar approach is used at the 3D space.

Examples of the obtained 2D and 3D microstructures using various CA neighborhoods are presented in figure 9 and 10. The CA space size used in 2D simulation was set to 500x500px which is equal to 500x500 μm. In the 3D the space size was set to 300x300x300 μm. Based on the space and required grain size the number of initial grain nuclei can be easily calculated.

As it is shown in figure 9 or 10, application of Moore or Von Neumann neighborhood is not satisfactory due to unnatural shapes of final grains. Much better effect is obtained by, hexagonal random, due to their stochastic character. These microstructures can statistically represent geometry of real microstructure after annealing or static/metadynamic recrystallization. As seen in figure 9 application of the

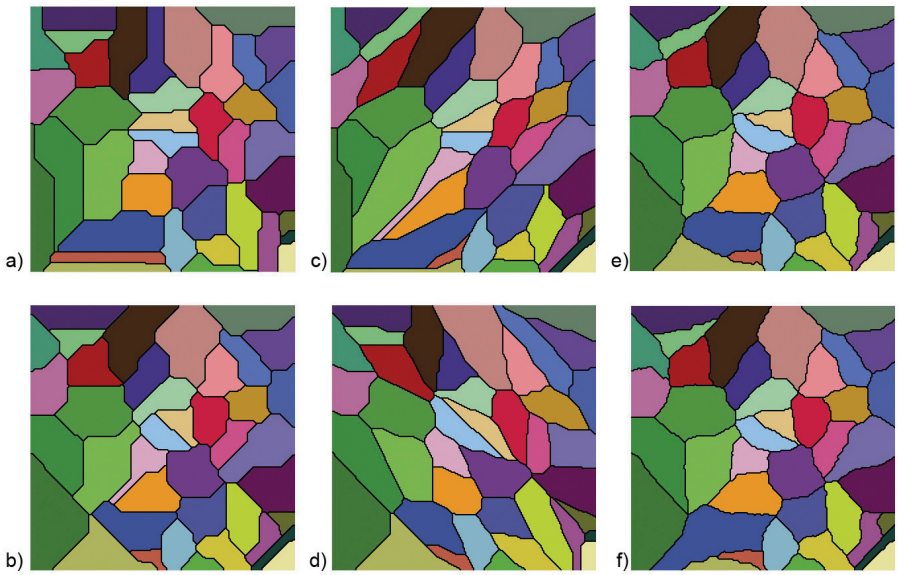

Fig. 9. *Microstructures obtained by a) von Neumann, b) Moore, c) hexagonal left, d) hexagonal right e) hexagonal random, f) random for 40 grains.*

Due to the fact that transition rules depend on the type of the neighborhood, several different neighborhoods are implemented to investigate differences between them. Two of them are commonly used: Von Neuman and Moore neighborhoods (figure 8a,b). The particular cell is surrounded by four neighbors and eight neighbors, respectively. Another example are pentagonal and hexagonal neighborhoods. In pentagonal neighborhood the cell is surhexagonal left or right neighborhood can be useful when a microstructure after rolling process have to be created. These two neighborhoods provide microstructures with elongated grains in particular direction. The grain size distribution of the obtained microstructure can be easily compared with the experimental results. If the generation of the microstructure do not provide required grain size distribution the processes can be performed one more time.

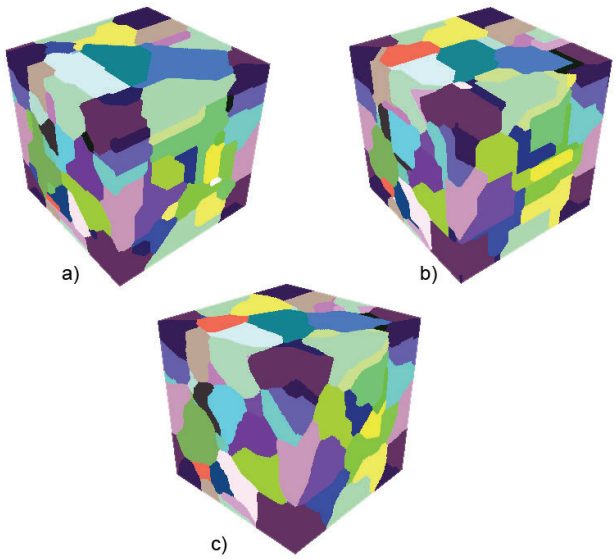

Fig. 10. *Results of microstructure obtained by a) Von Neuman, b) Moore, c) hexagonal random in 3D space.*

To obtain CA space continuity the periodic boundary conditions can be introduced. For simplicity, only the 2D representation of the boundary conditions is presented in figure 11. As seen the CA cells that are located at the edges of the CA space consider as neighbors CA cells located at other edges. That way no free edges in the CA space are observed.

9	3	6	9	3
7	1	4	7	1
8	2	5	8	2
9	3	6	9	3
7	1	4	7	1

Fig. 11. *Periodic boundary condition in the 2D case.*

Microstructures generated with and without periodic boundary conditions are shown in figure 12.

Using this methodology more sophisticated microstructures can be crated containing various phases or other microstructure features, e.g. inclusions (figure 13).

Adding inclusions into the microstructure is also based on the CA grain growth algorithm. Selected locations along the grain boundaries become a nuclei of a inclusion. In the subsequent steps, inclusion grows until the desired size is obtained. The more complicated case is obtaining the reliable digital representation of the dual phase microstructures. The phase transformation algorithm that is based on physical aspects of the process have to be considered. The process parameters e.g. cooling rate play a significant role in this case. Information on the developed phase transformation algorithm that provides a digital representation of two phase microstructures can be found in other author works (Madej et al., 2010; Pietrzyk et al., 2010).

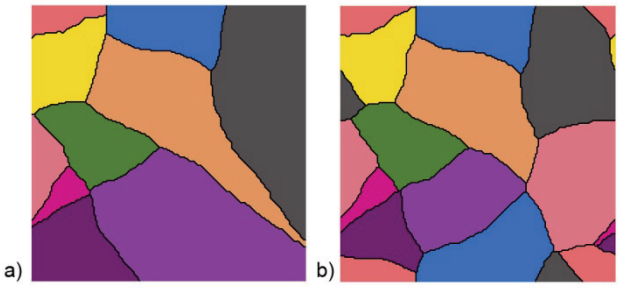

Fig. 12. *Microstructure with 10 grains generated a) without and b) with periodic boundary conditions.*

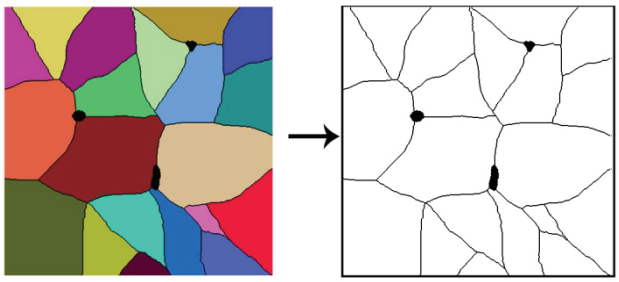

Fig. 13. *Initial microstructure with added inclusions.*

It can be concluded that the CA approach with the appropriate neighborhood can replicate real microstructure, with features like grain boundary or inclusions.

When the initial microstructure is created in the sense of the topology, then it can be analyzed and fulfilled with properties, e.g. crystallographic orientation. The main key in the DMR platform is possibility to assign material properties to particular grains. At this stage of the author research these properties can be represented by a scalar or by a vector containing three elements. When scalar value is considered the assigned information can represent one parameter in the simple flow stress model. When a vector is assigned it can represents three parameters in the flow stress model. For example, when a crystal plasticity model is used, this vector can represent a three Euler angles that precisely determine grain crystallographic orientation. However, more complicated data structures (e.g. tensors) that represent material properties can also be assigned to particular grain.

When the topology of the initial microstructure is created and material properties to each grain are assigned then the digital material can be further

transferred into numerical model that will simulate material behavior under deformation conditions. As mentioned earlier, various method can be used, e.g. cellular automata or finite element methods. Examples of application of the designed initial digital microstructure during finite element micro-scale simulations are presented in the following chapter.

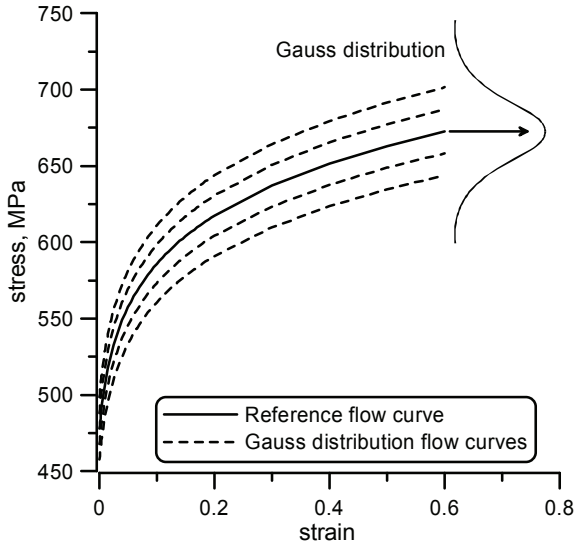

Fig. 14. *The diversification in the flow curves for each grain introduced using the random Gauss distribution.*

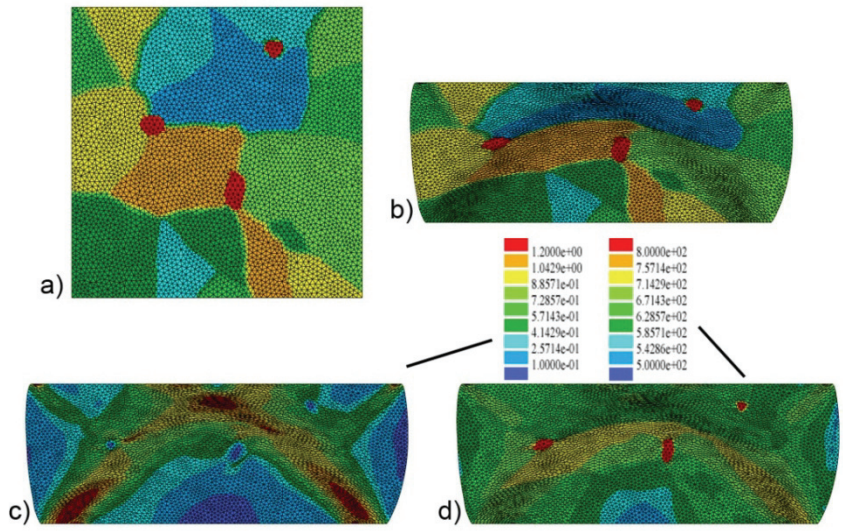

Fig. 15. *a) initial microstructure, b) final microstructure, c) strain distribution, d) stress distribution after 50% deformation.*

4. NUMERICAL SIMULATION BASED ON DMR

Simulations of the channel die compression test of the microstructure from figure 13 were performed. The digital microstructure was incorporated into the commercial FE Forge2 software using the user defined subroutines. The Norton-Hoff type constitutive equation is used. This procedure is designed to be performed automatically and do not require any other actions than running conventional FE simulation. Thus, it can be used by engineers with no experience in the field of numerical methods. The algorithm is as follows:

- Based on the input data from the image processing, the generation of the triangular mesh is performed. Particular groups of mesh nodes are located inside separated grains and inclusions.
- The flow curve that represent ferritic steel is taken from the literature (Delannay et al., 2007) and is assigned to the particular grains. The elevated yield point is assigned for the hardly deformable inclusions.
- Possibility of capturing differences in grains flow due to various crystallographic orientations is the advantage of the DMR. The easiest way to capture this is diversification in the flow curves for each grain is introduction of the random Gauss distribution (figure 14). To get detail information about texture evolution a crystal plasticity models should be used (Roters et al., 2010; Resk et al., 2009).
- Starting the FE simulation is the final step.

The non periodic boundary conditions were applied with free edges what leads to unconstrained material flow. Selected conditions represent behavior of micro sample containing 20 ferrite grains with hardly deformable inclusions during micro compression test at room temperature. The load is applied on the top surface of the sample. The Coulomb law with friction coefficient set to 0.2 was used. The strain and stress distribution obtained from the simulations are shown in figure 15.

Zones with high strain localization are clearly visible in the form of major bands in figure 15. This is due to the influence of microstructures and inclusions. Also higher strain values are in the area surrounding inclusions. The strain localization in this case may be a precursor material failure that initiates at e.g. the hard inclusions. When hot deformation is considered areas around the inclusions due to high strain localization may be zones where dynamic recrystallization will initiate, what is observed experimentally.

In the present approach FE simulation was performed with the homogenous FE mesh and it provided very interesting results of inhomogenous deformation at the micro-scale level. However the homogenous FE approach has some disadvantages, that is why a heterogeneous FE meshes can also be used. This problem was the subject of investigation in (Resk et al., 2009) as well as in other author works (Madej et. al., 2009b).

5. CONCLUSIONS

The results of research on development of digital representation of microstructure and the advantages provided by this technique were presented in the paper. Based on the research performed by the Author it can be concluded that:

- application of the Voronoi and cellular automata methods can provide statistically representative microstructures with varying grain sizes very fast. This is important when large number of calculations is required. However the grain geometry obtained from Voronoi tessellation is very regular. The cellular automata algorithm, in general, provides much better microstructures in terms of their geometrical features.
- selection of an appropriate neighborhood in the cellular automata method in order to obtain realistic geometry of the grains in the digital microstructure is crucial. It seems that random hexagonal and random neighborhoods provide microstructures that represents material structure after annealing process. Application of other neighborhoods e.g. hexagonal left can provide microstructure similar to the microstructure after e.g. rolling process.
- cellular automata method is also more efficient than Voronoi tessellation when generation of the two phase materials is considered. Microstructures with e.g. various phases, inclusions or voids can be easily created and used in numerical simulations as shown in figure 13.
- if required an image processing methods should be applied to create digital microstructures that exactly replicate real metallic materials. This procedure is becoming more complex when 3D microstructures are considered. However, capabilities of modern experimental techniques (SEMFEG/EBSD with FIB) combined with an image analysis and reconstruction algorithms gives the possibility to obtain accurate 3D digital representations of microstructure. Author's research in this field are described in Cybulka et al.'s (2007), Rauch and Madej works (2010).

In future studies the inverse analysis method will be applied to obtain desired initial microstructure that during the deformation will provide specific material properties. Also more accurate crystal plasticity based approaches will be added to properly describe rotation of the grains during deformation.

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WYKORZYSTANIE CYFROWEJ REPREZENTACJI MATERIAŁU DO SYMULACJI NIEJEDNORODNOŚCI ODKSZTAŁCENIA

Streszczenie

W pracy przedstawiono modele numeryczne stosowane przede wszystkim w skali mikroskopowej, ponieważ szczególny nacisk położono na wykorzystanie zalet cyfrowej reprezentacji materiału. Cyfrowa reprezentacja materiału stwarza możliwość wiernego odwzorowania rzeczywistej mikrostruktury materiałów polikrystalicznych z jej cechami charakterystycznymi w formie jawnej (np. orientacja krystalograficzna, granice ziaren, granice faz, wtrącenia itp.). Przedstawiono przegląd dotychczasowych zastosowań koncepcji cyfrowej reprezentacji materiału oraz omówiono propozycję własnych rozwiązań do tworzenia w/w mikrostruktur. Omówiono dwie metody generacji cyfrowych mikrostruktur: metodę wieloboków Voronoi oraz metodę automatów komórkowych. Przedstawiono również przykłady wyników uzyskanych z symulacji procesu spęczania w próbie kanalikowej prowadzonych metodą elementów skończonych w oparciu o wygenerowane cyfrowe mikrostruktury.

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