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NUMERICAL ANALYSIS OF STRAIN INHOMOGENEITIES DURING DEFORMATION ON THE BASIS OF THE THREE DIMENSIONAL DIGITAL MATERIAL REPRESENTATION

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Abstract

The main objective of the DMR system presented in the work is to create the digital microstructure with its features (grains, sub grains, grain boundaries) represented explicitly. Particular attention in the paper is put on designing three dimensional DMR. These digital structures are used to generate finite element meshes that exactly replicate geometry of grains. Finally obtained meshes are used during simulation of the deformation process to analyze stress concentration along grain boundaries. Details of implemented algorithms are presented in the paper. The advantages and disadvantages of this approach are discussed, as well.

Key words: digital material representation, cellular automata, mesh generation

1. INTRODUCTION

The FE method is the main tool used in industry to simulate large scale forming processes and it gives good results. This method describes material behavior as a continuum and it is based on a general stress-strain relationship. Since large scale problems containing bilions of grains are usually considered, the major assumtion 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 to solve problems occurring during metal forming, as well as to develop the technologies for processes of rolling, forging, stamping, etc. However, the fast development of modern steel grades (TRIP, TWIP, DP, Bainitic, etc.) is one of the main challenges imposing significant changes to this commonly used approach. These materials are characterized by elevated material properties, which are the results of sophisticated microstructures with combination of e.g. large and small grains, inclusions, precipitates, nano-particles, different phases, etc. Interaction between features at the micro scale and the surrounding material under loading conditions results in specific properties at the macro scale.

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

2. DIGITAL MATERIAL REPRESENTATION

The concept of Digital Material Representation was recently proposed and is dynamically evolving (Bernacki et al., 2007; Cornwell et al., 2006; Loge et al., 2008; Madej, 2010). The main objective of the DMR is creation of the digital representation of microstructure with its features (i.e. grains, grain orientations, inclusions, cracks, different phases etc.)

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represented explicitly. Generation of material microstructure with specific geometrical features and 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 behaviour under exploitation conditions and the more accurate, in the case of geometry and properties, the digital representation is the more accurate results can be obtained. That is why a lot of research is put on development of methods responsible for creation of the 2D and 3D representations of analysed microstructures.

To obtain an accurate description of the 2D microstructure an Image Processing methods are usually applied. As an input data for this analysis a SEM/EBSD results can be used. That way not only information regarding microstructure geometry is obtained but also information about initial crystallographic orientation is provided. This approach was successfully used in (Raabe & Becker, 2000; Loge et al., 2010). Unfortunately the approach is time consuming and expensive, because each numerical simulation based on DMR require a SEM/EBSD analysis. That is why image processing is also applied to the optical microscopy images, that are much more affordable. However, in this case, only information regarding grain morphology is obtained see e.g. (Milenin & Kustra, 2008; Rauch & Madej, 2010). Presented approaches are even more demanding 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 microscopy can be used during the serial sectioning procedure to provide input data for image processing and reconstruction algorithms. The conventional approach to serial sectioning based on manual labour is extremely time consuming and requires a series of subsequent polishing and optical or scanning electron microscopy operations (Sidhu & Chawla, 2004). The solution may by application of specially designed equipment e.g. Robo-Met.3D^{TM} (Spowart, 2006; Spowart et al., 20010) that automatically provide a series of 2D images that are subjected to 3D reconstruction algorithms. The procedure consists of three major steps. The first involves a very precise polishing, where the sample is polished for a required time. Then, the robot arm moves the sample through rinsing and etching stages to finally position prepared surface above a metallographic microscope, where one or a series of 2D images are automatically obtained. This procedure is repeated desired number of times. As mentioned, after images are acquired, additional image processing and reconstruction procedures are applied to obtained 3D microstructure representation. At this stage of development the procedure is limited only to obtaining optical microscopy images, but they can be obtained from a large area of the sample. To obtain a series of 2D images from the scanning microscopy in an automated manner a SEM/FIB/EBSD technique can be used. The FIB – focused ion beam plays a crucial role in this procedure. The collision of the ion beam with the sample surface is confined to a small area removal of the material. This is followed by a 2D EBSD map acquisition. This procedure is performed in a subsequent manner and results in milling of the parallel serial sections of the material. Finally a reconstruction algorithms are applied to obtained a 3D representation. The major advantage of this method is possibility to obtained not only 3D morphology of particular grains but also information about their crystallographic orientation (Xu et al., 2007). Unfortunately, relatively small areas of material can be reconstructed by this approach. Presented methods are already in quite common use and despite their advantages they have one major disadvantage. All these techniques are classified as destructive methods. The solution to this problem may be application of high energy synchrotron radiation to provide a 3D visualization of polycrystalline materials (Poulsen, 2004). But this method is still highly expensive.

Methods presented in the literature review provide an exact 2D or 3D digital representation of analysed microstructures, however they require a series of costly and time consuming experimental research and metallographic analysis. That is why they are not appropriate for large number of numerical simulations. Due to that constrained, Authors decided to use artificial methods for fast creation of statistically equivalent digital microstructures.

When statistically representative digital microstructures are considered the most commonly used method is the Voronoi tessellation (Cao et al., 2010, Loge et al., 2008; Madej, 2010). But this method provides an artificial grain geometry as seen in figure 1. To obtain more reliable microstructures the Cellular Automata (CA) method can be used. Authors previously performed a lot of research on 2D creation and application of digital material representation idea (Madej, 2010; Madej, 2010b; Rauch et al., 2010). The present work is mainly focused on extending the capabilities of developed DMR model into the 3D space.

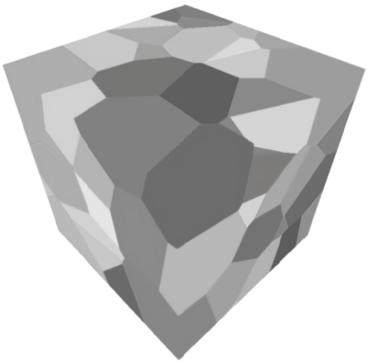


Fig. 1. The digital microstructure containing 100 grains obtained from the Delaunay triangulation.

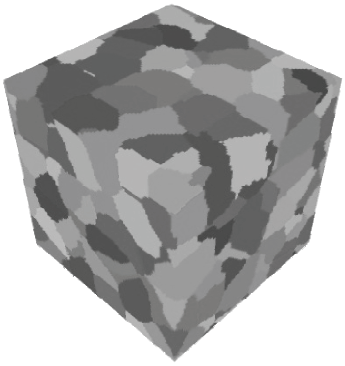


Fig. 2. The digital microstructure containing 170 grains obtained from the CA base algorithm with hexagonal random neighbourhood in 3D space.

The first step in the CA method is to establish the discrete space composed of cellular automata. With reference to 2D space, it will be a grid consisting of squares, whereas in 3D space it will be composed of cubes. In the next step of the CA grain growth algorithm, a set of CA cells is selected randomly, and then an internal variable describing cell state is set to "already grown." These cells represent grain nuclei. The second step of the algorithm is focused on grain growth. The transition rule for this stage is defined as follows: when a neighbour 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 impingement with other grains. After that they grow only in the area where no grains are observed. This process is performed until the entire space is fulfilled with grains. In the cellular automata method, several neighbourhoods can be selected. A detailed study on this subject can be found in (Madej, 2010b). From that study it was concluded that due to the stochastic character of the hexagonal random neighbourhood it provides an accurate representation of a real microstructure after annealing or static/metadynamic recrystallization. This neighbourhood was used in this work in the case of 3D microstructures as seen in figure 2.

3. FINITE ELEMENT MESH GENERATION

An approach to incorporate obtained 3D digital microstructures into commercial FE software through user defined subroutines has been developed by the Authors (Madej at al., 2009; Madej, 2010b). Based on the input data from the DMR regarding topology and properties, the generation of the uniform triangular mesh is performed in the commercial FE software. Each finite element within this mesh verifies with the underlying DMR to which grain it belongs. When particular groups of mesh nodes are located inside separated grains, this means that different grains are distinguished. These groups of elements take on properties (e.g., flow stress models) from the underlying digital microstructure. Additional user defined variables are introduced into the FE code to transfer and store information from the DMR into the FE solution. Example of generated mesh and obtained results after simple channel die test are presented in figure 3. Details of this approach can be found in another Authors work (Madej, 2010b).

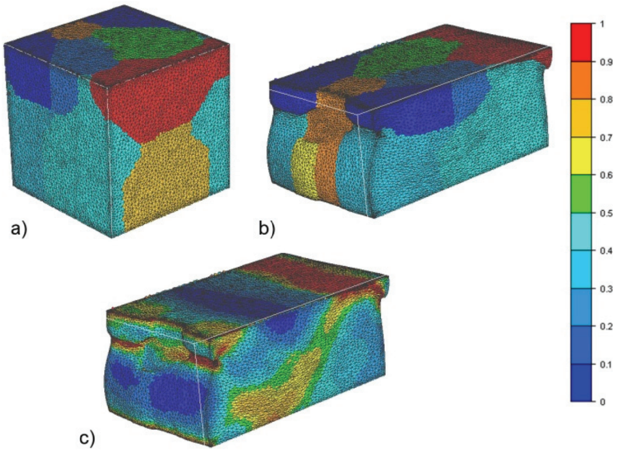


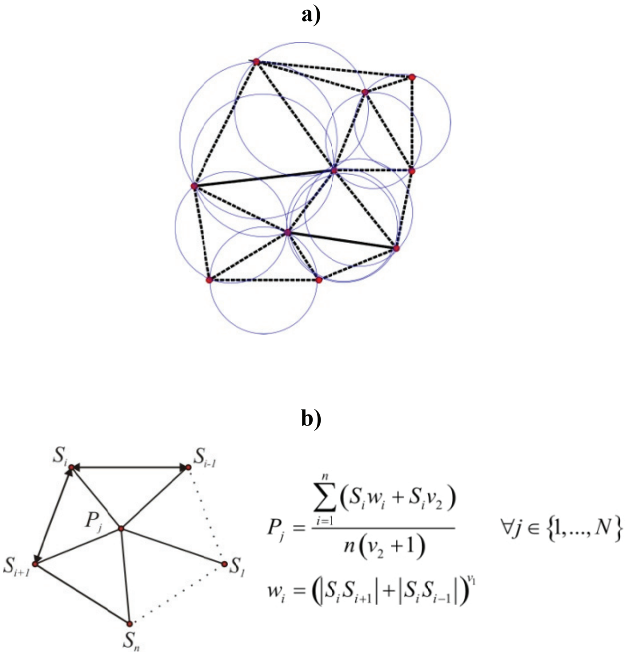
Fig. 3. Illustration of the a) initial 3D DMR with uniform mesh, b) deformed mesh, c) equivalent strain distribution after deformation.

Due to e.g. various crystallographic orientations of analysed grains a strain and stress gradients are expected to occur along grain boundaries as well as close to triple point junctions. To properly capture this behaviour a very fine finite element meshes have to be used, what in 3D case leads to excessive computational time. To reduce computational time and maintain high accuracy of the solution along mentioned grain boundaries a specific nouniform FE meshes that are refined along the grain boundaries have to be used. Since the functionality of refinement of the FE elements along grain boundaries is not available in the commercial FE codes, Authors decided to develop an in-house code for finite element nonuniform mesh generation called *DMRmesh*. The 2D approach to solve this problem is described in (Madej at al., 2009; Madej, 2010b). To create similar mesh in 3D case more advanced algorithms have to be used. Developed solution is briefly described below.

Information provided from the digital microstructure regarding position of the grain boundary, as well as grain nuclei, is used to create required refined meshes (figure 4). The digital microstructures with non periodical and periodical boundary conditions are inputs for the mesh generation stage. To control finite element refinement along the grain boundaries, a simple function is introduced that specifies number of new nodes located in the areas of interest. If too many elements are in a particular location, no new nodes are allowed.

Fig. 4. Initial position of the grain boundary points in 3D space.

Finally based on the available nodal points the Voronoi tessellation algorithm is applied to create the nonuniform meshes. The common 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 result, 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). Additionally, in order to obtain finite elements with regular shapes, the modified weighted Laplace smoothing algorithm is implemented (figure 5b) in the present work.



$$P_j = \frac{\sum_{i=1}^{n}\left(S_i w_i + S_i v_2\right)}{n\left(v_2+1\right)} \qquad \forall j \in \{1,\dots,N\}$$

$$w_i = \left(\left|S_iS_{i+1}\right| + \left|S_iS_{i-1}\right|\right)^{v_1}$$

Fig. 5. *a) illustration of the Delaunay triangulation, b) modified weighted Laplace smoothing algorithm, where: $\{S_1,\dots,S_n\}$, n – set and number of neighbours of the point P_j, respectively, w_i – weight assigned to point S_i, v_1, v_2 – coefficient, N – number of points.*

Each point S_i in the neighbourhood of the analysed P_j point has a specific weight w_i what can be seen in figure 5b. Additionally two coefficients v_1 and v_2 are introduced in order to strengthen influence of particular node on the final P_j position after Laplace smoothing. Finally, an optimisation procedure is applied, if after smoothing algorithm a mesh still contains low quality elements e.g. elongated in one direction. In this case a series of additional nodal points are added to the 3D space and mesh generation algorithm is performed again. Several iterations usually have to be applied to obtain satisfactory quality of the mesh. Eventually, a regular shapes of finite elements are obtained in the entire 3D space in the centre of the grains as well as close to the grain boundaries in the refined region. The last stage of the procedure is assigning the finite elements to particular grains. An iterative grain assignment algorithm is implemented into the *DMRmesh* code. A two dimensional representation of subsequent steps of this algorithm is presented in figure 6.

The algorithm is performed in an iterative manner as seen in figure 6a-d. Subsequent elements are assigned to particular grain until the grain boundary edges represented by circular nodes are not met as seen in figure 6d. As a results a final three dimensional mesh that exactly replicates grain geometry is created (figure 7).

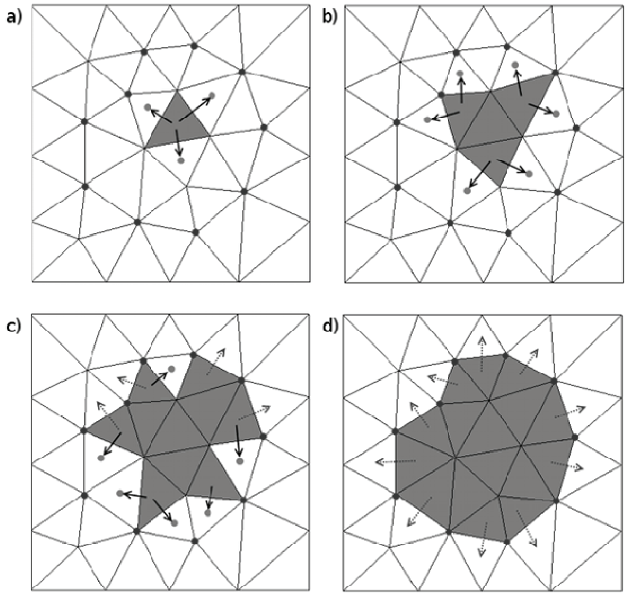


Fig. 6. Illustration of the grain assignemtn algorithm, solid black arrows representes possible growth direction, dotted gray arrows represent restricted growth diretions.

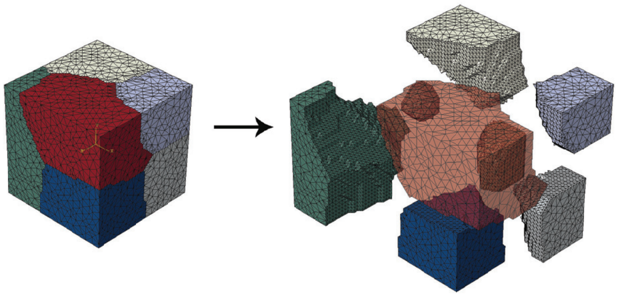


Fig. 7. Illustration of the finite element mesh generated on the basis of the digital material representation.

Presented meshes are then used as input for the finite element modelling of material behaviour subjected to simple compression.

4. THREE DIMENTIONAL DMR COMPRESSION

The CPFEM model described in (Madej, 2010b) is incorporated into the commercial finite element Abaqus software via user defined subroutines and is combined with the refined meshes described in the previous chapter. In the refined meshes, each finite element has a unique label that determines to which grain it belongs. Using these labels it is possible to cluster all the finite elements into separate groups. That way a specific crystallographic orientation is assigned to the subsequent grains, and then the mesh is used during finite element calculations. All other material properties are the same for the grains. Examples of results obtained for the deformation of the aluminium polycrystalline sample containing 10 grains in three crystallographic orientations: cube, shear and hard are shown in figure 8.

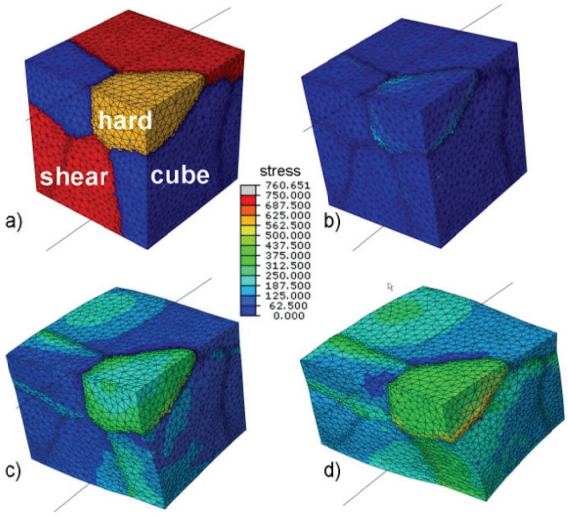


Fig. 8. a) initial digital material representation with refined FE mesh, b-d) equivalent stress evolution during loading.

Results presented in figure 8b-d clearly show advantages provided by the developed refined mesh generator. The stress concentration develops along grain boundaries and is accurately predicted by the refined meshes. The centre of the grain where material flow is more homogenous is described by coarse mesh what lead to reduction of computational time.

5. CONCLUSION

As presented, the developed digital material representation, in the sense of geometry and properties, was incorporated into the commercial finite element software. Examples of numerical simulations obtained using uniform meshes were presented. Uniform FE mesh provided very interesting results of inhomogeneous deformation at the micro scale level. However, the uniform FE approach has some disadvantages, that is why a nonuniform FE mesh generator was developed within this work. An increase in the accuracy of numerical simulations by application of the implemented refined finite elements was presented as well. Obtained meshes exactly replicate the shape of the grain boundaries.

At this stage of the research the 3D digital material representation can be applied to simulate local material behaviour at the micro scale level. The next part of the research will be focused on extending capabilities of the model to perform multi scale simulations both at micro and macro scale level. Results obtained in 2D space are very encouraging see e.g. (Madej, 2010b).

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ANALIZA NIEJEDNORODNOŚCI ODKSZTAŁCENIA Z WYKORZYSTANIEM TRÓJWYMIAROWEJ CYFROWEJ REPREZENTACJI MATERIAŁU

Streszczenie

Podstawowym celem pracy jest stworzenie modelu wykorzystującego cyfrową reprezentację materiału do analizy wpływu elementów mikrostruktury na zachowanie się materiału w trakcie odkształcenia. Cyfrowa reprezentacja materiału zapewnia możliwość uwzględnienia elementów mikrostruktury np. ziarna, granice ziaren, różne fazy itp. w sposób jawny w trakcie symulacji. W ramach pracy stworzone zostały algorytmy tworzenia trójwymiarowej cyfrowej reprezentacji wraz z dedykowaną siatką elementów skończonych, która wiernie odzwierciedla geometrię ziaren. Opracowana cyfrowa reprezentacja materiału polikrystalicznego jest następnie wykorzystana w trakcie analizy koncentracji naprężeń wzdłuż granic ziaren w trakcie testu spęczania próbki sześciennej. Wady i zalety opracowanego podejścia zostały również przedstawione w niniejszej pracy.

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