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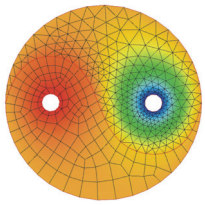

GENERATION OF DEDICATED FINITE ELEMENT MESHES FOR MULTISCALE APPLICATIONS WITH DELAUNAY TRIANGULATION AND ADAPTIVE FINITE ELEMENT - CELLULAR AUTOMATA ALGORITHMS

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Abstract

The main aim of the work is development and comparison of algorithms for mesh creation that can be further used to investigate material behavior under loading conditions, on the basis of digital material representation. Particular attention is put on development of conforming meshes for two-phase materials. Two approaches are investigated within the present work. The first is based on mesh refinement along particular microstructure features. The second incorporates the cellular automata phase transformation model into the finite element adaptation technique. Description of the two approaches and an example of application of the obtained meshes to analyze multiscale material behavior under plastic deformation condition are presented.

Key words: finite element mesh generation, digital material representation, inhomogeneous deformation, mesh refinement

1. INTRODUCTION

The recently observed significant need of the automotive and aerospace industries for new metallic materials that can meet strict requirements regarding weight/property ratio is a driving force for fast development of modern steel grades. A wide range of innovative steels (TRIP, TWIP, DP, Bainitic, nano-Bainitic etc.) as well as other metallic materials like aluminum, magnesium, titanium or copper alloys is 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; Kuziak et al., 2011). Complex thermomechanical operations are applied to obtain highly sophisticated microstructures with combination of large grains, small grains, inclusions, precipitates, multi-phase structures etc. These microstructure features and interactions between them at the micro scale level during manufacturing or exploitation stages eventually result in highly elevated material properties at the macro-scale level. Parallel to the experimental research on development of these materials, there is a need for a robust numerical model supporting the mentioned investigations. However, due to the complex nature of these microstructures, their behavior should not be homogenized in the form of a single flow stress model, like in the conventional approach to numerical simulations (Pietrzyk et al., 2004; Malinowski et al., 2004). On the contrary, to capture the mentioned micro scale interactions during numerical analysis, behavior of particular microstructure features need to be explicitly taken into account.

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One of the possible solutions, to deal with the explicit representation of microstructure features during numerical analysis, is an approach based on the Digital Material Representation (DMR) (Bernacki et al., 2007; Madej, 2010a). This technique and similar ones based on the same assumptions (image based analysis, digital microstructures analysis, virtual microstructures analysis) are intensively studied and developed by researchers.

Basic features and problems of the DMR are reasonably well addressed in scientific literature (Bernacki et al., 2007; Madej, 2010a). The problem of meshing the representative volume element (RVE) representing part of the material is one of the most important problems scientists face. Thus, the objective of the present work is to briefly present the Authors' recent achievements in the field of development of the DMR approach and to apply advanced techniques of the mesh generation to improve the reliability and quality of simulations based on the DMR.

2. BASIC FEATURES OF THE DMR

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 a homogenized manner. The created digital representation can be used, for example, to investigate inhomogeneous strain evolution around particular microstructure features during various materials processing operations. A lot of research in the area of DMR was done by the groups at Carnegie Mellon University by Dawson (2000), Alcoa Technical Center (Brahme et. al., 2006, Rolett et al., 2004), National Institute of Standard and Technology (Saylor et al., 2004), CEMEF Mines-Paristech (Bernacki et al., 2007; Bernacki et al., 2009; Logé et al. 2008), Imperial College (Zhang et al., 2011), The Catholic University of Leuven (Delannay et. al., 2006), Warsaw University of Technology (Kurzydlowski, 2010), AGH University of Science and Technology (Madej, 2010a; Rauch & Madej, 2010; Gawad et. al., 2008). The literature review on this subject is presented in another work by Madej (2010a).

There are two major issues that have to be solved during creation of the numerical model on the basis of the DMR approach. The first is generation of the material microstructure with specific grain morphologies and properties. This 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 the obtained results will be. The most commonly used methods are Voronoi tessellation, voxel method and serial sectioning, but also other methods such as cellular automata, sphere growth, inverse analysis or Monte Carlo are capable to generate polycrystalline microstructure. The problem of generating accurate digital material representations with various algorithms was extensively studied by one of the Authors in (Madej 2010b, Madej et. al., 2011c) and is not addressed in the present work.

The second issue that influences accuracy of the results obtained from simulations with DMR is the mesh density and its topology. Limited amount of research is devoted to this subject (see for example Bernacki et. al., 2008). This issue is investigated in detail within the framework of the present paper.

As a case study, a digital material representation of a two phase microstructure was selected. Description of the approach to obtain digital representation of two phase microstructure was in detail described by Madej (2010c) and only briefly summarized in the present paper. Based on the obtained results during and after phase transformation, three various approaches to create FE meshes are discussed, and examples of applying multi-scale modeling are presented.

3. DIGITAL MATERIAL REPRESENTATION OF A TWO PHASE MICROSTRUCTURE

The problem of the digital material representation for two phase microstructures is discussed using steels as an example. Out of the few methods that can be used to create two phase microstructure, the Cellular Automata (CA) technique was selected in the present work. In this approach, the CA cell in the cellular automata space is described by several state and internal variables in order to properly describe the state of the material. Each cell can be in three different states: ferrite (α), austenite (γ) or in ferrite-austenite (α/γ) as a cell lying in-between two phases. The internal variables describe, for example, how many ferrite phases are in a particular cell $x_{cellferrites,}$ or what are the carbon concentrations in each cell $c_{concentration}$. These internal variables are used in the developed transition rules that replicate mechanisms of phase transformation. The two major transition rules are defined to describe nucleation and growth of the ferrite phase. At the beginning of each time

step the number of nuclei is calculated. The grain nuclei are then generated randomly along the austenite grain boundaries. When a cell is selected as a nucleus its state changes from austenite (γ) to ferrite (α). At the same time all the neighboring cells of the ferrite (α) cell change their state to ferrite-austenite (α/γ). In the next time step these newly formed ferrite nuclei grow into the austenite phase. This process is controlled by a set of physically based equations describing for instance the velocity of the γ/α interface. When a ferrite phase grows according to the mentioned equations, the cells change their states from the austenite (γ) to ferrite (α) phase. When a change in the cell state occurs, the corresponding carbon concentration changes according to the FeC diagram. As mentioned previously, details of this approach can be found in (Madej 2010c). Examples of results obtained from the developed model during subsequent stages of the cooling of low carbon steel are shown in figure 1.

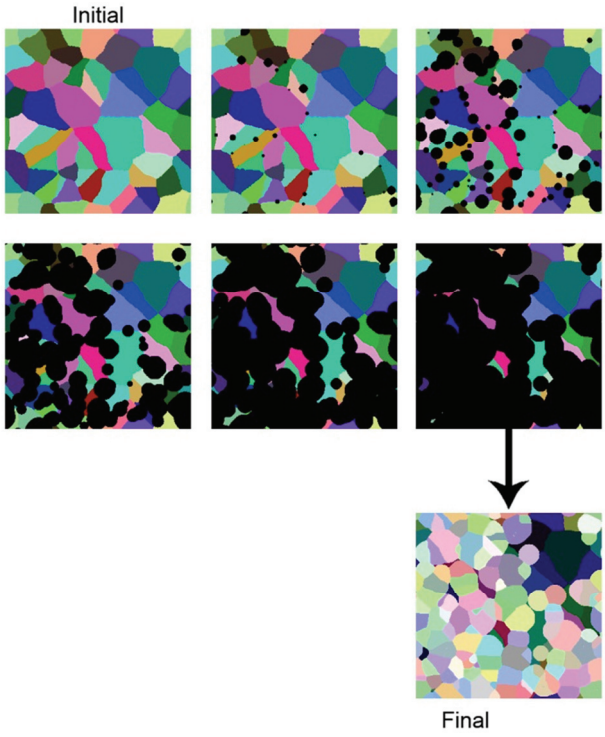

Fig. 1. *a) microstructures obtained after subsequent cooling stages (black color represents progress phase transformation front) b) final microstructures with separated ferrite and austenite grains.*

The developed phase transformation model was used to create a two phase representation of digital microstructure for subsequent mesh generation and numerical analysis. The prospective objective of this analysis can be simulation of dual phase or multi phase steels (AHSS - advanced high strength steels), which are now frequently used by the automotive industry. In these steels, combination of high strength and good workability is obtained by combination of the soft ferrite matrix with the tough islands of martensite and/or bainite (Thomser et al., 2009; Pietrzyk et al., 2010). In the present work, a simplifying assumption is made that at a certain stage of the transformation, accelerated cooling is applied, and remaining austenite is transformed into hard constituents. Thus the resulting microstructure is composed of soft ferrite (black areas in figure 1) and hard bainite or martensite. Due to the nature of the obtained microstructure, a significant gradients of solution (strain, stress etc.) are expected during numerical modeling. To enable accurate simulation of deformation of this microstructure the problem of appropriate mesh generation is discussed in the following chapters.

4. UNIFORM MESH GENERATION FOR THE DMR

An approach to incorporate obtained digital microstructures in the commercial FE software through user defined subroutines has been developed by Madej and co-workers (Madej et al., 2009; Madej, 2010b,c). Based on the input data from the DMR, regarding topology and properties, the generation of the uniform triangular mesh can be performed in the commercial FE software Forge2D. 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 properties from the underlying two phase digital microstructure. Additional user defined variables are introduced into the FE code to transfer and store information from the DMR into the FE solution. Details of this approach can be found in another work by Madej (2010b). Examples of FE meshes with various densities created using commercial software on the basis of the two-phase digital microstructure are shown in figure 2.

As mentioned, due to significant differences in properties of subsequent phases or various crystallographic orientations of analyzed grains, strain and stress gradients are expected to occur along the phase or grain boundaries. To properly capture this behavior related to grain morphology, very fine finite element meshes have to be used, which leads to excessive computational time. As seen in figure 2, the finer the FE mesh is, the better the description of the phase boundary shape is. With coarser meshes

some microstructure features can even be neglected. However, to reduce computational time and maintain high accuracy of the solution along mentioned phase/grain boundaries, a decision was made to use specific non-uniform FE meshes that are refined along the phase/grain boundaries. Since the functionality of refinement of finite elements along phase/grain boundaries is not available in the commercial FE codes, the Authors decided to develop an in-house code for finite element non-uniform mesh generation. Two approaches were implemented and tested. The first is based on the final morphology of the two-phase microstructure where the mesh density is prescribed prior to mesh generation. The second is based on the FE adaptation applied during the phase transformation process. Details of both investigated solutions are described below.

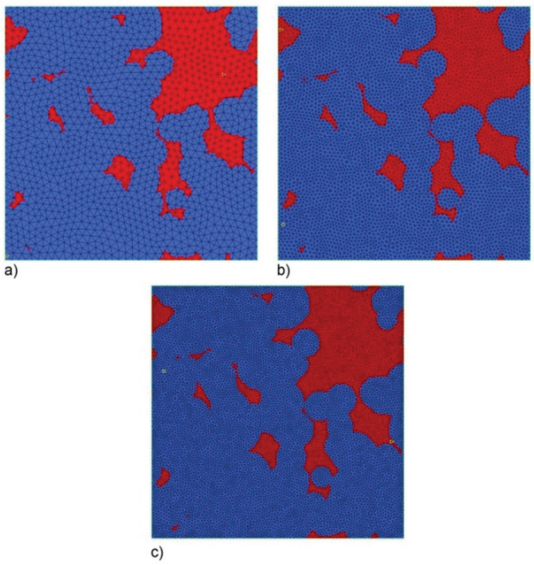

Fig. 2. *FE meshes with various densities created using commercial software on the basis of the two-phase digital microstructure.*

5. NONUNIFORM MESH GENERATION

Information provided from the digital microstructure regarding position of the grain boundary or other microstructure features is an input for the mesh generation algorithm that has the capability to create FE meshes refined along particular microstructure elements. As mentioned earlier in the present research, a digital microstructure of a two-phase material is used as input data. The image of the microstructure is transferred into the 2D or 3D space of cells representing the morphology of each microstructure feature by different colors. The digital microstructures with non periodic and periodic boundary conditions can be used during the mesh generation stage.

The developed algorithm is composed from several subsequent steps that are briefly described below.

– The first step is focused on establishing border nodes, which map the boundary between the grains, phases or other microstructure features. This stage is of importance as accurate reconstruction of the borders lead to a good quality of conforming meshes that exactly describe investigated microstructure geometries. Density of nodes is controlled by the α parameter. There are two approaches that can be used during boundary reconstruction. In the first method, nodes are added at the corners of each cell's wall, which is adjacent to the cell of another color. In th way nodes are added along phase boundaries. This solution accurately reproduces the division of areas stored in the digital material representation. However, this high level of accuracy during border reconstruction is associated with the occurrence of the stepped boundary between analyzed features (different phases, grains etc.) as shown in figure 3.

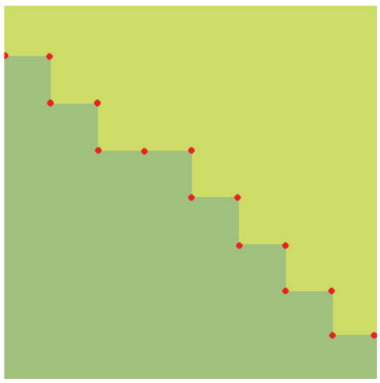

Fig. 3. *Nodes are located at the corners of each cell's wall between two microstructure features.*

To avoid this behavior, a second method of border reconstruction can be used. In this approach nodes are created in the middle of the walls dividing cells assigned to various features. This method allows the creation of a border based also on lines at an angle of 45 degrees. However, matching elements based on the DMR image requires additional corrections due to some misalignment as shown in figure 4. As a consequence, during elimination of the presented sharp elements, a smoothing of the boundary is visible.

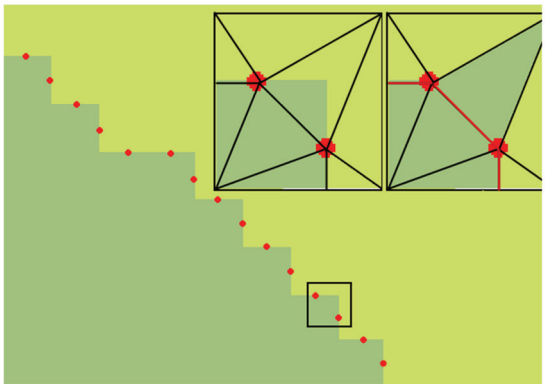

Fig. 4. *Nodes are located in the middle of the walls dividing cells between two microstructure features.*

– The second step involves generation of nodes in the interior of investigated features. By assigning the appropriate position to each nodal point a precise control of the density of elements is obtained. To control the size of finite elements in the area of the feature boundaries and in the interior of those features, a simple algorithm is introduced that controls the density of nodes located in the areas of interest. Each nodal point is additionally described by a defined radius r. If another node is found within the radius r, the location is rejected, otherwise a new node is created. Different values of r are defined for nodes close to the feature boundary or close to the center of the feature. In this way, a specific node distribution along the feature boundary is obtained.
– Finally, based on the available nodal points the Delaunay triangulation algorithm is applied to create non-uniform meshes. The Delaunay triangulation algorithm was chosen because it allows discretization only on the basis of available input nodes. Additionally, in the algorithm the process of adding subsequent nodes to the mesh is based on the reconstruction of the local area of meshes associated with the added vertex. These properties make this method an efficient tool for introducing changes in density of the elements at every stage of the discretization process.
The common algorithm for triangulation starts by forming the super triangle enclosing all the points from set V that have 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.
– After the Delaunay triangulation, algorithms responsible for improvement of the mesh quality are applied. The criterion for improvement of the elements is determined by the value of the smallest angle in the element β. The basic algorithm is based on the modified weighted Laplace smoothing approach (figure 5). The position of subsequent nodes is calculated as:

$$P_j = \frac{\sum_{i=1}^{n}\left(S_i w_i + S_i v_2\right)}{n\left(v_2+1\right)} \qquad \forall j \in \{1,\ldots,N\} \tag{1}$$
$$w_i = \left(\left|S_i S_{i+1}\right| + \left|S_i S_{i-1}\right|\right)^{v_1}$$

where: $\{S_1,\ldots,S_n\}$, n – set and number of neighbors of the point P_j, respectively, w_i – weight assigned to point S_i, v_1, v_2 – coefficient, N – number of points.

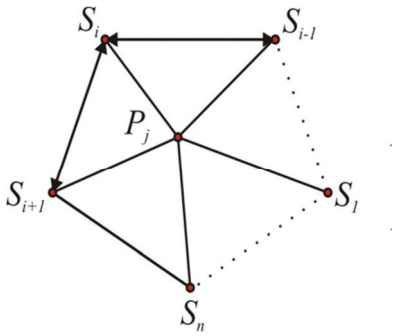

Fig. 5. *Modified weighted Laplace smoothing algorithm.*

After the smoothing algorithm, the mesh still may contain degenerated elements elongated in one direction. In this case a series of additional nodal points is added to the investigated space, and the mesh generation algorithm is performed again. Another technique is to use the finite element edge swapping algorithm. Several iterations have to be applied to obtain satisfactory quality of the mesh.
– The last stage of the mesh generation algorithm is to assign obtained finite elements to particular grains. An iterative grain assignment algorithm is implemented into the *DMRmesh* code. Details of this algorithm can be found in another work by Madej and co-workers (2011a,b).

As a result, a final conforming mesh dedicated to numerical simulation that exactly replicates grain geometry is generated (figure 6). In this case, a mesh

is created for a two-phase microstructure that is obtained after the end of phase transformation. Thus the algorithm is based on a final digital material representation revealing the position of the phase boundary in 2D space. As mentioned previously, the level of accuracy in the description of the phase boundary depends on proper selection of mesh parameters, namely: density of points along the phase boundary α and minimal finite element internal angle β. These parameters are set up prior to mesh generation and remains the same along the entire interface. The FE mesh presented in figure 6 was created with $\alpha = 0.5$, $\beta = 30^{o}$ and precisely describes the shape of the phase boundary without any simplifications, but it is also characterized by a large amount of finite elements. Examples of meshes created with various sets of parameters (α,β) are presented in figure 7 and 8. As shown, the correctness of the description of the microstructure features increases with an increasing amount of finite elements. Influence of the mesh density on the obtained solution will be addressed in the following chapter. In this approach, evolution of phase transformation does not influence the morphology of the FE mesh.

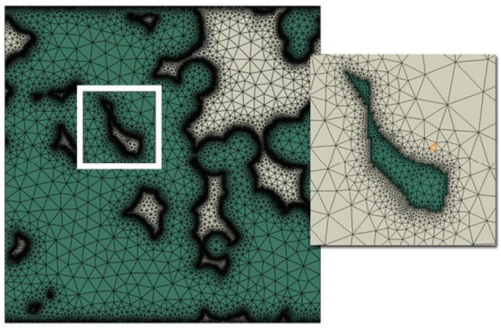

Fig. 6. *Final morphology of the FE mesh after the end of phase transformation.*

The obtained meshes are then used as input for the multi scale finite element modeling of material behavior subjected to multi scale tension simulation.

The presented approach is extremely efficient with the only limitation being that the mesh density remains the same along every microstructure feature. To create an FE mesh that can additionally adjust a level of refinement in particular locations, another technique was used in the present work.

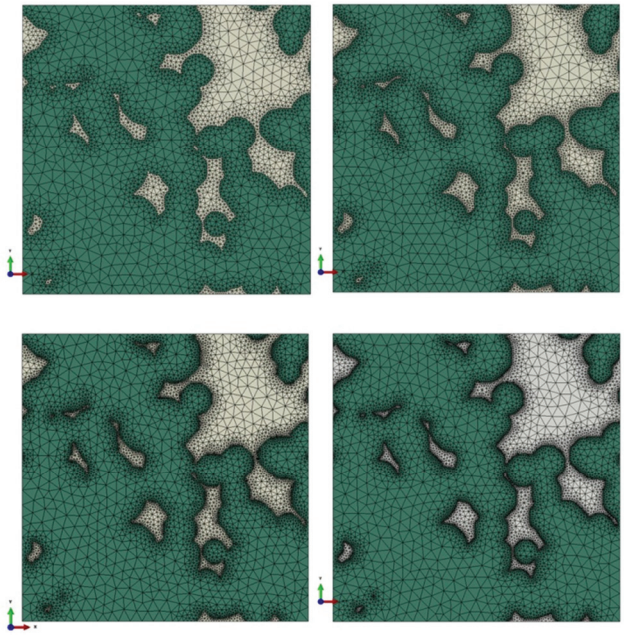

Fig. 7. *Morphology of the FE mesh after the end of phase transformation for increasing α = 1,2,3,4 and constant $\beta = 30^{o}$.*

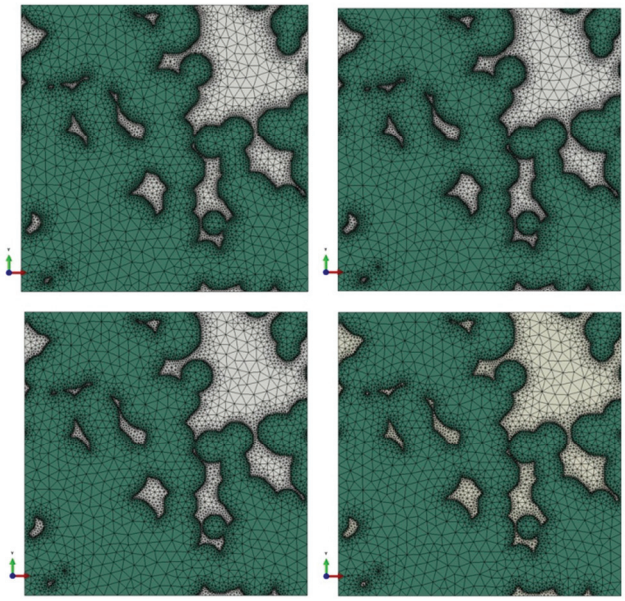

Fig. 8. *Morphology of the FE mesh after the end of phase transformation for constant α = 1 and decreasing $\beta = 30^{o}$, 25^{o}, 20^{o}, 15^{o}.*

6. LOCAL MESH REFINEMENT AND ADAPTATION

As mentioned above, the main aim of this part of the research is to enable creation of FE meshes with different mesh density at phase boundaries. The approach presented above takes into account only geometrical properties of modeled materials. Another possibility is to consider the properties of numerical solutions as well. Mesh adaptivity can be used for this purpose, where elements of an original, initial mesh are subsequently divided based on some

refinement indicators. Mesh adaptivity has an advantage in that indicators for mesh refinement can be based on some error estimates, as well as on geometrical features.

In the present work the sample is subject to loading in the elastic regime while phase transformation proceeds. At the same time, mesh adaptation is performed leading to final morphology of the FE mesh. Details of this approach are described below.

The conventional adaptive finite element method is considered in the analyzed case. The combination of the FE and CA methods in the form of the concurrent CAFE (cellular automata finite element) model is applied. The information about progress in phase transformation is transferred from the CA to the FE at every calculation step. In this way, detailed information on the influence of the evolving phase boundary on inhomogeneous deformation is obtained. Based on the error estimation, performed according to the classical Zienkiewicz-Zhu superconvergent patch recovery method (Zienkiewicz & Zhu, 1992), mesh adaptation is realized. The minimum level of refinement of each FE element is described by the γ parameter. In the present implementation the division of the global mesh to the patches of elements is applied and, for each patch, the recovered stress tensor σ^* is obtained for its central node through L2 projection. Then calculation of the Zienkiewicz-Zhu error estimator is based on the standard equation:

$$e_\sigma^* = \sigma^* - \sigma_h \tag{2}$$

where: σ_h - standard stress tensor computed using derivatives of shape functions. The error indicator for each finite element is calculated as the energy norm:

$$\|e\| = \sqrt{\int_\Omega e_\sigma^{*T} D^{-1} e_\sigma^* d\Omega} \tag{3}$$

where: D – the elasticity matrix with material constants. In the case of multi-phase microstructures, different material properties are assigned to subsequent phases.

The whole procedure is applied to numerical calculations of phase transformation during loading in the elastic regime according to the scheme presented in figure 9. The investigated evolution of the ferrite phase during deformation is presented in Figure 1.

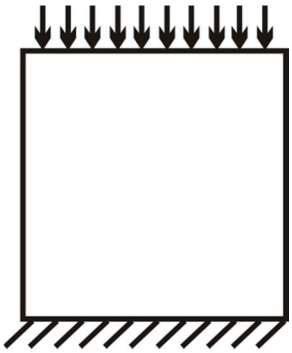

Fig. 9. *Schematic illustration of the boundary conditions during FE calculations.*

The FE adaptation procedure is performed after every CA time step, when information about the progress of the growing ferrite phase into the surrounding material is obtained, as schematically presented in figure 10 (the meshes in figure 10 are just examples and do not correspond to the actual meshes used in the numerical experiments).

The mesh is subsequently refined and de-refined along the moving phase boundary, and the material coefficients are changed due to the information obtained from the CA. Change in material properties due to phase transformation influences the numerical solution. The elements in the mesh are divided if the error in the element is greater than the average error multiplied by an adaptation parameter ***r***. As mentioned, at the same time elements can be clustered if

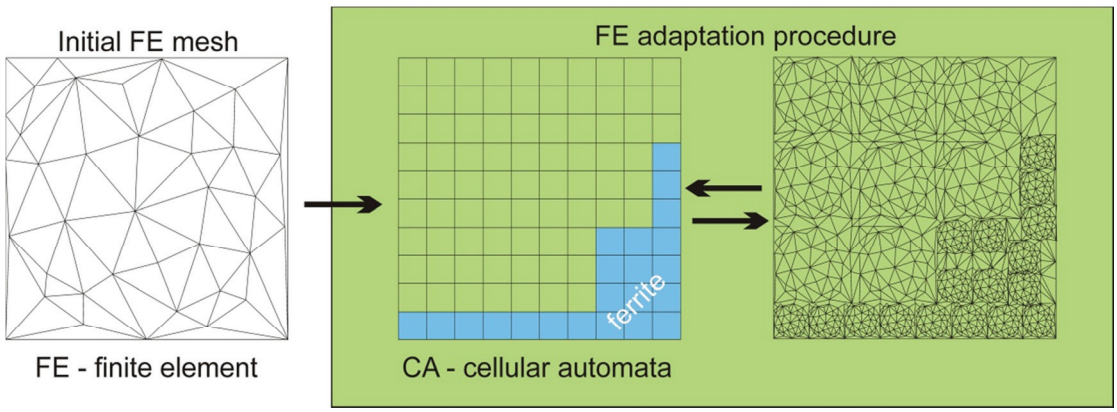

Fig. 10. *Schematic illustration of the concurrent cellular automata – finite element model.*

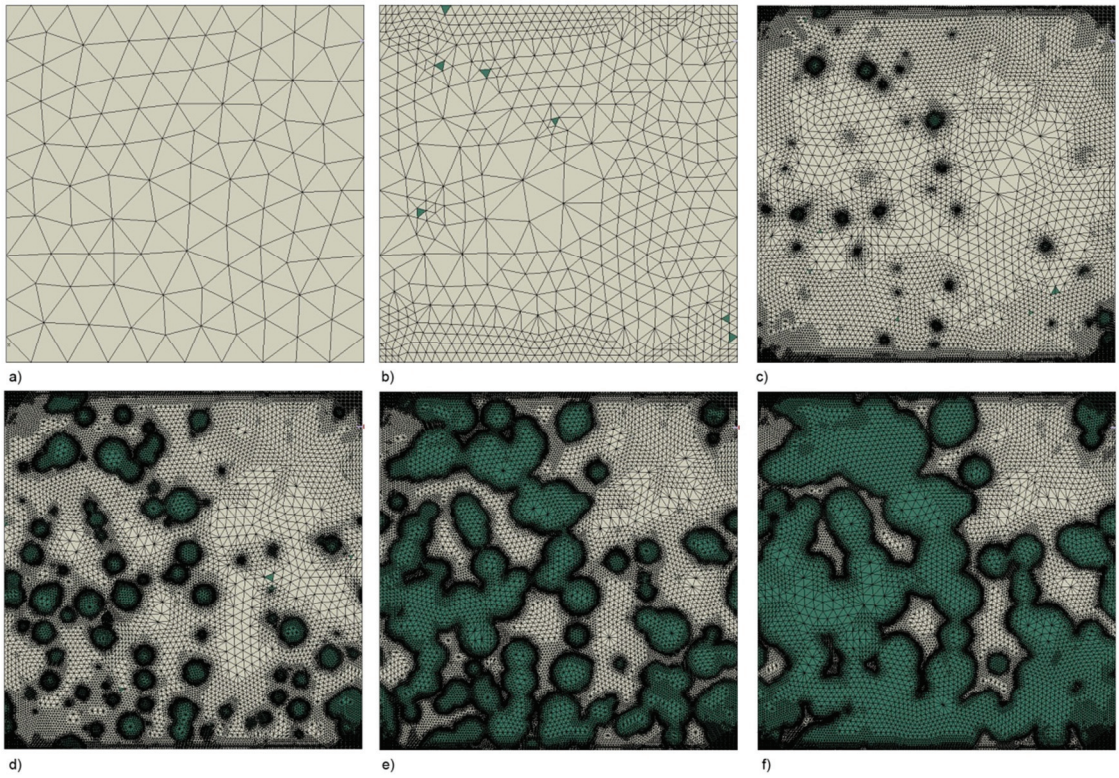

Fig. 11. *Subsequent stages of FE adaptation during phase transformation.*

the total error in all descendant elements is smaller than the average error multiplied by an adaptation parameter ***d***. There is also a limit on the size of an element through which the division is carried. So the element refinement is performed only to the defined level of accuracy. With this approach, it is possible to precisely control the adaptation coefficients in order to obtain the optimum proportion between the accuracy and the calculation time. In the present work only information on obtained stress distribution is taken into account during mesh adaptation. As a result detailed information on morphology of the FE mesh in subsequent phase transformation steps can be obtained as seen in figure 11. Figure 11 clearly shows the correlation between refinement/de-refinement of the FE mesh and evolving ferrite phase during transformation. As a result, a specific FE mesh refined along the phase boundaries is obtained as seen in figure 12. Due to the fact that adaptation is sensitive to the calculated stress gradient during loading, the level of refinement along various microstructure features is different (see figure 12). Density of the grid at grain boundaries and on the limits of the area where the force was applied, is evidence of the existence of the higher stresses and hence the higher value of an error. This is a major advantage of the method since a good quality mesh for further numerical simulation of plastic deformation is obtained. Another advantage of adaptation is the possibility of almost unlimited division of the mesh in elements, in which the solution gradient is greater, with simultaneous clustering of elements in which an error is significantly smaller. Additionally, information on the position of the phase boundaries can be supplied to the mesh refinement procedure. In this way even better accuracy of the interface reconstruction can be obtained.

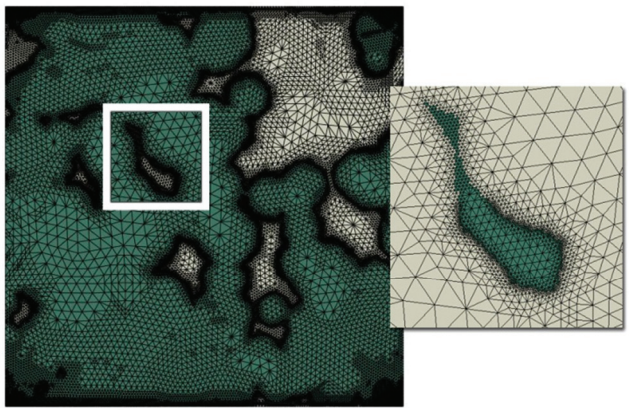

Fig. 12. *Final morphology of the FE mesh after the end of phase transformation.*

Again, a lot of attention has to be put on proper selection of the γ parameter, as the increasing size of the minimum level of refinement can result in an inaccurate description of the phase boundary as seen in figure 13.

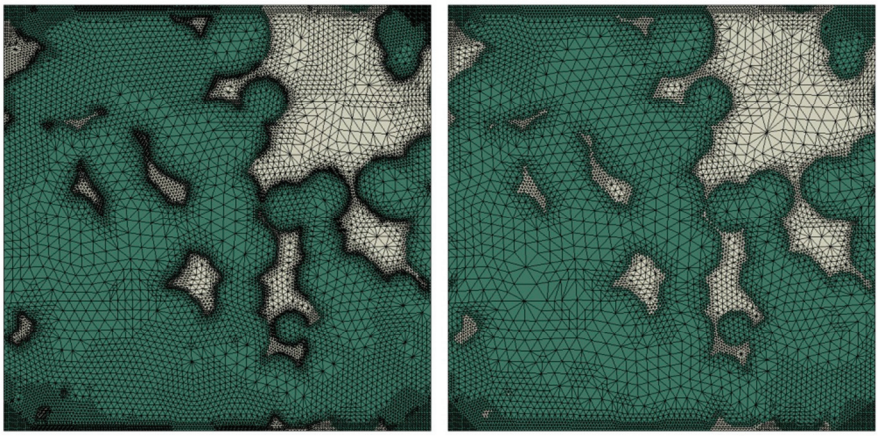

Fig. 13. Final morphology of the FE mesh after the end of phase transformation for increasing γ = 0.02 and 0.015.

large plastic deformation. Calculations were performed using the commercial Abaqus FE software. The solution is based on the isotropic hardening model combined with the Levy-Mises flow rule. An isotropic model can be explained as an expansion of the yield surface without any change in the position of its centre in the defined stress space.

A typical laboratory tensile test for investigating material behavior under loading conditions was selected for the investigation. The displacement boundary conditions were applied to obtain 10% of deformation as seen in figure 14a. To properly capture both macro and micro scale deformation conditions, a concurrent multiscale model was created. The main idea of this model is based on the assumption that macro scale material behavior is modeled as a global model, with a relatively coarse finite element mesh, which assures acceptable computational time. At the same time, a region in this global mesh is selected, and a finite element mesh created on the basis of the digital material representation is at-

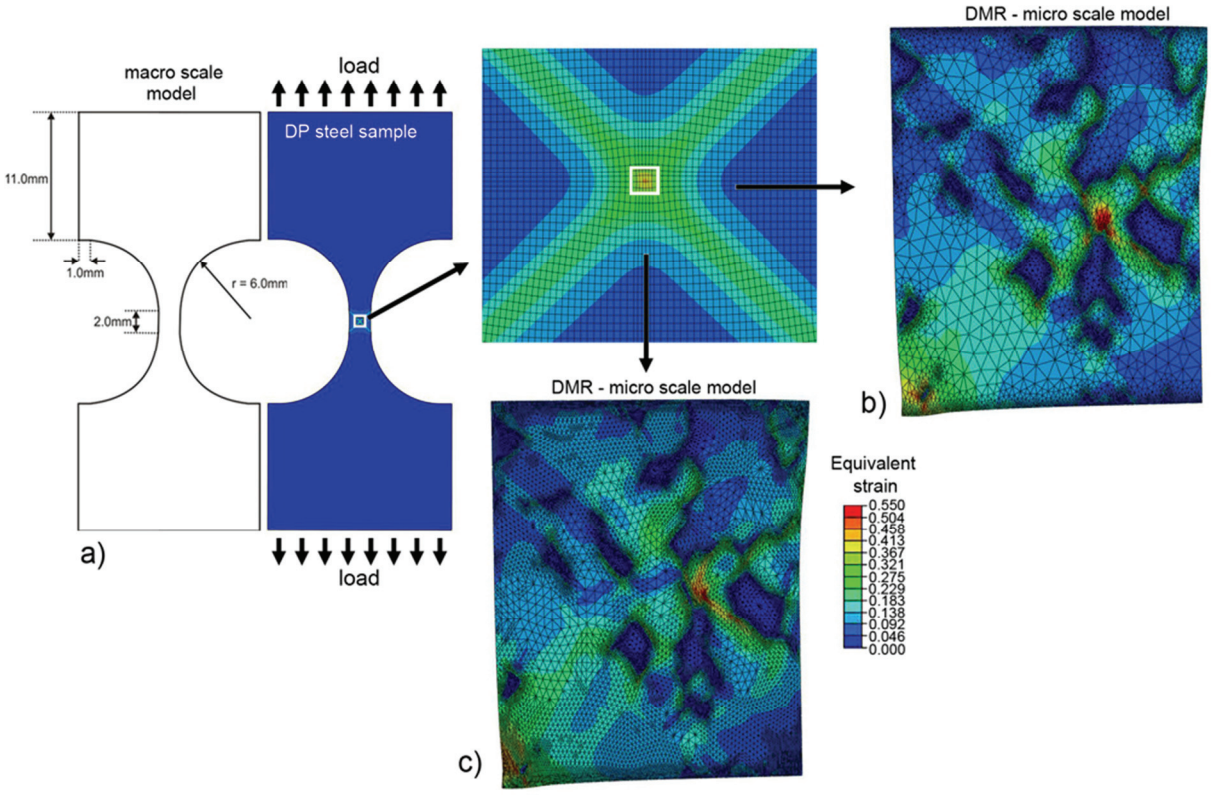

Fig. 14. Equivalent strain distribution obtained during a tensile test at the a) macro scale and b) micro scale with mesh created by non-uniform generation, c) micro scale with mesh obtained through adaptation.

The FE meshes, obtained with the two latter techniques, are input data for further multiscale analysis of material behavior during plastic deformation.

7. MULTISCALE MODELING ON THE BASIS OF THE DMR

The obtained FE meshes presented in figures 6-8, 12, and 13 are used during the multiscale investigation of two-phase microstructure behavior under

tached to represent material behavior at the micro scale. The displacement field calculated at the macro scale level is used at every time step as a boundary condition for the micro scale solution. As a result, the FE model provides general information concerning strain, stress, etc. at the macro scale level as well as detailed information about microstructure behavior at the micro scale level. Details on this approach regarding a flow stress model for macro as well as micro scale are presented elsewhere by Madej (2010a,b).

As an example, the equivalent strain distribution obtained both at the macro and micro scales for the two most accurate FE meshes (figure 6 and 12) is presented in figure 14.

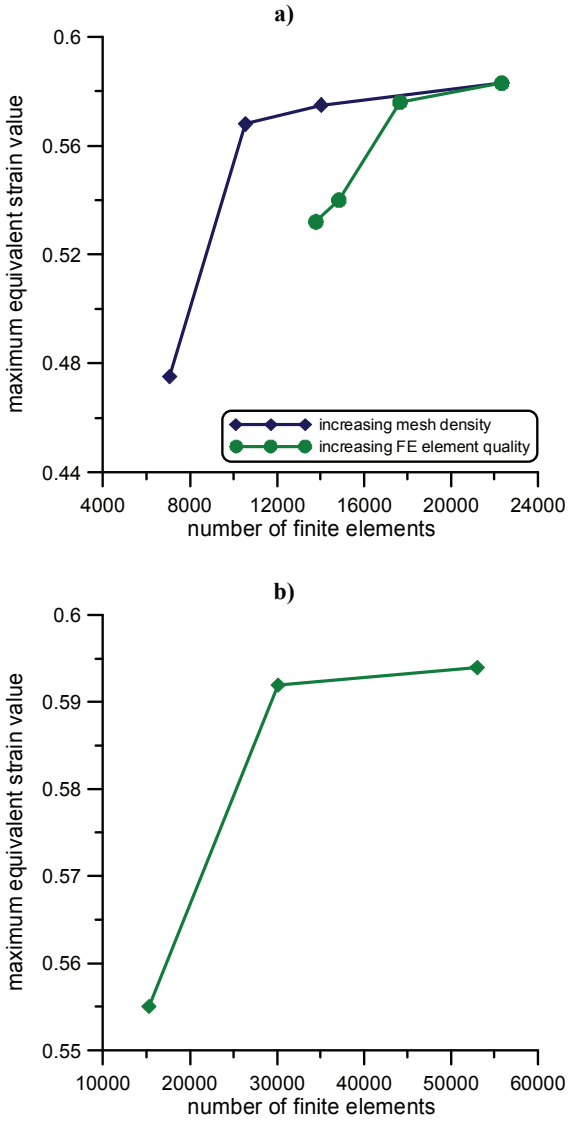

Fig. 15. *Influence of number of finite elements on accuracy of the numerical solution. Meshes were obtained by a) increase of the α and β parameters, b) decrease of the γ parameter.*

Similar calculations were performed for all investigated meshes to highlight that increasing accuracy of the phase boundary description to some extent influences also the accuracy of the FE solution during multi scale simulation. Various combinations of mesh generator parameters (α,β or γ) significantly influence the number of FE elements. However, a clear threshold value in the number of elements can be identified, where influence of the mesh becomes less pronounced (see figure 16). The problem of minimization of mesh generation time will be addressed in future research.

8. CONCLUSIONS

Both presented approaches for generating FE meshes for multiscale modeling have their advantages and disadvantages. The first method based on non-uniform mesh generation works well when there is only one mesh required for the simulation procedure. In such a case, the mesh dedicated to a given geometry of the problem is created with optimal computational cost. The drawback of the method is the relatively long time required to adapt the particular morphology. Expensive procedures of remeshing combined with mesh improvement algorithms have to be applied. Additionally the same level of refinement is maintained along various microstructure features and has to be specified prior to mesh generation.

The second method, based on refinements and de-refinements, offers flexibility and speed in changing the mesh. It can be used for creating a single mesh for a simulation; however, in such a case not all of its potential is exploited. Nevertheless, even such a simple problem as the one presented in the paper reveals some of its advantages. One of the most important advantages is the possibility to refine and de-refine finite elements based on solution error estimates, which provides a desired FE mesh on the basis of physically motivated mechanisms. In this way a dedicated mesh refined in specific areas can be obtained for further multi scale calculations. Additionally, FE meshes after subsequent phase transformation stages are also available, which expands the possibility to perform numerical analysis of material behavior under deformation. However, it should be stated, that further research in this area is required to support fast development of the digital material representation approaches.

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REFERENCES

Beladi, H., Adachi, Y., Timokhina, I., Hodgson, P.D., 2009, Crystallographic analysis of nanobainitic steels, *Scripta Materialia*, 60, 455-458.

Bernacki, M, Chastel, Y, Digonnet, H, Resk, H, Coupez, T., Logé, RE, 2007, Development of numerical tools for the multiscale modelling of recrystallization in metals, based on a digital material framework, *Computer Methods in Materials Science*, 7, 141-149.

Bernacki, M., Chastel, Y., Coupez, T., Logé, R., 2008, Level set method for the numerical modelling of primary recrystallization in the polycrystalline materials, *Scripta Materialia*, 58, 12, 1129-1132.

Bernacki, M., Resk, H., Coupez, T., Logé, R.E., 2009, Finite element model of primary recrystallization in polycrystalline aggregates using a level set framework, *Modelling and Simulation in Materials Science and Engineering*, 17, 064006.

Brahme, A., Alvi, M.H., Saylor, D., Frify, J., Rollett, A.D., 2006, 3D reconstruction of microstructure in a commercial purity aluminum, *Scripta Materialia*, 55, 75-80.

Delannay, L., Jacques, P.J., Kalidini, S.R., 2006, Finte element modeling of crystal plasticity with grains shaped as trunced octahedrons, *International Journal of Plasticity*, 22, 1879-1898.

Gawad, J., Paszyński, M., Matuszyk, P., Madej, L., 2008, Cellular automata coupled with hp-adaptive Finite Element Method applied to simulation of austenite-ferrite phase transformation with a moving interface, *Steel Research International*, 79, 579–586.

Kurzydłowski, K.J., 2010, Modelling of the microstructure and properties in the length scales varying from nano- to macroscopic, Bulletin of the polish academy of sciences, Technical sciences, 58, 217-226.

Kuziak, R., Pidvysots'kyy, V., Węglarczyk, S., Pietrzyk, M., 2011, Bainitic steels as alternative for conventional carbon-manganese steels in manufacturing of fasteners - simulation of production chain, *Computer Methods in Materials Science*, 11, 443-462.

Logé, R.E., Bernacki, M., Resk, H., Delannay, L., Digonnet, H., Chastel, Y., Coupez, T., 2008, Linking plastic deformation to recrystallization in metals, using digital microstructures, *Philosophical Magazine*, 88, 3691-3712.

Madej L., Mrozek A., Kuś W., Burczyński T., Pietrzyk M., 2008, Concurrent and upscaling methods in multi scale modelling – case studies *Computer Methods in Materials Science*, 8, 1-15.

Madej, L., Cybułka, G., Perzynski, K., Rauch, L., Pietrzyk, M., 2009, Multi-scale modeling based on Digital Material Representation, eds. E. Onate, D. R. J. Owen, B. Suárez, *Proc. Conf., Complas 2009*, Barcelona, CD.

Madej, L., 2010a, Digital material representation – new perspectives in numerical simulations of inhomogenous deformation, *Computer Methods in Materials Science*, 10, 143-155.

Madej, L., 2010b, *Development of the modeling strategy for the strain localization simulation based on the Digital Material Representation*, AGH University Press, Krakow.

Madej, L., 2010c, Influence of microstructure features on strain distribution during micro forming on the basis of Digital Material Representation, *Steel Research International*, 81, 1438-1441.

Madej, L., Cybulka, P., Perzyński, K., Rauch, L., 2011a, Numerical analysis of strain inhomogeneities during deformation on the basis of the three dimensional Digital Material Representation, *Computer Methods in Materials Science*, 10, 375-380.

Madej, L., Rauch, L., Perzyński, K., Cybułka, P., 2011b, Digital Material Representation as an efficient tool for strain inhomogeneities analysis at the micro-scale level, *Archives of Civil and Mechanical Engineering*, 11, 661-679.

Madej, L., Szyndler, J., Pasternak, K., Przenzak, M., Rauch, L., 2011c, Tools for generation of digital material representations, *Proc. Conf. MS&T 2011*, Columbus, Ohio, CD.

Malinowski, Z., Głowacki, M., Pietrzyk, M., Madej, W., 2004, Finite element model for efficient simulation of ring rolling, *Proc. Conf. MS&T 2004*, New Orleans, Louisiana USA, 397-401.

Pietrzyk, M., Madej, L, Rauch, L., Spytkowski, P., Kusiak, J., 2010, Conventional and mul-tiscale modelling of austenite decomposition during laminar cooling of hot rolled DP steels, *Proc. XXIX Verformungskundliches Kolloquium*, Planeralm, 41-46.

Pietrzyk, M., Pidvysotskyy, V., Paćko, M., 2004, Flow stress model accounting for the strain localization during plastic deformation of metals, *Annals of the CIRP*, 53, 235-238.

Rauch Ł., Madej Ł., 2010, Application of the automatic image processing in modeling of the deformation mechanisms based on the digital representation of microstructure, *International Journal on Multi Scale Modeling*, 8, 343-356.

Robertson, L.T., Hilditch, T.B., Hodgson, P.D., 2008, The effect of prestrain and bake hardening on the low-cycle fatigue properties of TRIP steel, *International Journal of Fatigue*, 30, 587-594.

Rollett, A.D., Saylor, D., Frid, J., El-Dasher, B.S., Barhme, A., Lee, S-B., Cornwell, C., Noack R., 2004, Modelling polycrystalline microstructures in 3D, *Proc. Conf. Numiform*, eds Ghosh, S., Castro, J.C., Lee, J.K., Columbus, 71-77.

Sabirov, I., Estrin, Y., Barnett, M.R., Timokhina, I., Hodgson P.D., 2008, Tensile deformation of an ultrafine-grained aluminium alloy: Micro shear banding and grain boundary sliding, *Acta Materialia*, 56, 2223-2230.

Saylor, D.M, Fridy, J., Bassem, S., El-Dasher, B.S., Kee-Youing, J., Rollett, A.D., 2004, Statistically representative three-dimensional microstructures based on orthogonal observation sections, *Metallurgical and Materials Transaction A*, 35A, 1969-1979.

Thomser, C., Uthaisangsuk, V., Bleck, W., 2009, Influence of marten-site distribution on the me-chanical properties of dual phase steels: experiments and simulation, *steel research international*, 80, 582-587.

Timokhina, I.B., Hodgson, P.D., Ringer, S.P., Zheng, R.K., Pereloma, E.V., 2007, Precipitate characterisation of an advanced high-strength low-alloy (HSLA) steel using atom probe tomography, *Scripta Materialia*, 56, 601-604.

Zienkiewicz, O.C., Zhu, J.Z., 1992, The superconvergent patch recovery and a posteriori error estimates, *International Journal for Numerical Methods in Engineering*, 33, 1331-1382.

Zhang, P., Balint, D. S., Lin, J., 2011, An integrated scheme for crystal plasticity analysis: Virtual grain structure generation, *Computational Material Science*, in press.

OPRACOWANIE ALGORYTMÓW DO TWORZENIA SIATEK ELEMENTÓW SKOŃCZONYCH NA BAZIE TRIANGULACJI DELAUNAYA I ADAPTACYJNEJ METODY ELEMENTÓW SKOŃCZONYCH SKORELOWANEJ Z METODĄ AUTOMATÓW KOMÓRKOWYCH

Streszczenie

Głównym celem pracy jest opracowanie i porównanie algorytmów generowania siatek, elementów skończonych, które można wykorzystać do badania zachowania materiału w warunkach odkształcenia z wykorzystanie idei cyfrowej reprezentacji materiału. W pracy szczególna uwaga została położona na odwzorowanie stopniem zagęszczenia elementów morfologii materiałów dwufazowych. W tym celu wykorzystano dwa różne algorytmy. Pierwszy oparty jest na utworzeniu siatki poprzez triangulacje Delaunay przy jednoczesnym jej zagęszczeniu wzdłuż poszczególnych elementów mikrostruktury. Drugi obejmuje wykorzystanie modelu przemiany fazowej opracowanego na bazie metody automatów komórkowych i sprzęgnięcie go z algorytmami adaptacji siatki podczas rozwiązania MES zagadnienia liniowej sprężystości. Opis w/w algorytmów oraz przykład zastosowania uzyskanych siatek do wieloskalowej analizy zachowania się mikrostruktury w warunkach odkształcenia plastycznego jest zamieszczony w ramach niniejszej pracy.

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