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STRAIN DISTRIBUTION ANALYSIS BASED ON THE DIGITAL MATERIAL REPRESENTATION

ANALIZA STANU ODKSZTAŁCENIA W OPARCIU O CYFROWĄ REPREZENTACJĘ MATERIAŁÓW

Results of research on application of modern numerical approaches for analysis of influence of microstructure heterogeneities on strain distribution during material processing are presented in this work. This work is part of the research towards development of the tool for detailed microstructure modeling. The main focus here 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. By combination of these digital structures with numerical simulation methods a possibility to improve quality of results was created. Developed method can be used to design specifically dedicated microstructures, which meet very strict requirements. In the first part of the work the review of various ideas of digital representation of materials is presented. It is followed by a short description of the application of the developed approach to creation of the digital microstructures. The main focus is put on the application of cellular automata technique. Afterwards, obtained digital microstructures of ferrite steel and two phase steels are used as an input data for the finite element analysis of the compression test. Selected results are also presented and discussed in the paper.

Keywords: digital material representation, cellular automata, image processing

W pracy przedstawiono postęp w badaniach nad zastosowaniem nowoczesnych metod numerycznych do analizy wpływu niejednorodności mikrostruktury na stan odkształcenia w materiałach poddanych obciążeniom. Przeprowadzone badania dotyczą przede wszystkim skali mikro, ponieważ szczególny nacisk w modelowaniu położono na wykorzystanie zalet cyfrowej reprezentacji materiału. Cyfrowa reprezentacja pozwala wiernie odwzorować rzeczywistą mikrostrukturę materiałów polikrystalicznych z jej cechami charakterystycznymi (np. orientacja krystalograficzna, granice ziaren, granice faz) w formie jawnej. Wykorzystanie takiej reprezentacji w połączeniu z metodami symulacji numerycznych stwarza możliwość uzyskania nowej jakości wyników, które mogą zostać użyte do projektowania dedykowanych mikrostruktur materiałowych zapewniających zadane własności. W artykule przedstawiono zarówno przegląd dotychczasowych zastosowań koncepcji cyfrowej reprezentacji materiału jak również propozycje własnych rozwiązań, takich jak np.: automaty komórkowe stosowane do modelowania zjawisk zachodzących w mikrostrukturze. Wygenerowane w ten sposób mikrostruktury dla stali ferrytycznej oraz stali dwufazowych poddano następnie symulacjom spęczania z wykorzystaniem komercyjnych pakietów metody elementów skończonych. Dyskusja otrzymanych wyniki również jest zawarta w niniejszej pracy.

1. Introduction

The FE method is the main tool used in industry to simulate large scale forming processes and it gives satisfactory results [1-4]. This method describes material behavior as a continuum based on general strain-stress relationship [5]. Plastometric tests at various deformation conditions (temperatures, strain rates, etc.) are usually performed to obtain accurate flow stress necessary for the FE analysis. An inverse method is applied to eliminate the effect of heterogeneities due to e.g. friction in the tests and to obtain strain-stress relationships that is insensitive to material geometry [6]. 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.

There are two main challenges imposing significant

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changes to this commonly used approach. The first is fast development of modern steel grades (TRIP, TWIP, DP, Bainitic, etc.) that are characterized by elevated material properties, which are the results of sophisticated microstructures with combination of e.g. large grains, small grains, inclusions, precipitates, nano-particles, different phases, Luders bands, Portevin-le-Chatelier bands, shear bands etc. Interaction between these features at the micro scale and the surrounding material under loading conditions results in mentioned properties at the macro scale [7-9].

Omnipresent miniaturization which requires development of new micro forming technologies is the second 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. The grains are characterised by different crystallographic orientation or different properties, what results in heterogeneous material flow during deformation [10].

New numerical methodologies are needed to meet these two challenges. Digital Material Representation (DMR), which is the subject of the present work, is one of the possible solutions. The main objective of the developed DMR system is to create the digital microstructure with its features (grains, sub grains, grain boundaries, etc.) presented explicitly. Created digital representation can be used in numerical simulations of forming processes for modern steels, as well as micro forming processes. Inverse analysis will create the possibility to design initial microstructure that would provide expected material properties after forming. That way a series of costly industrial trials can be minimized. Review of the selected simulations based on Digital Material Representation are shown below.

2. Digital Material Representation

The concept of Digital Material Representation was recently proposed and is dynamically evolving [11-16]. As mentioned the main objective of the DMR is creation of the digital representation of microstructure with its features represented explicitly. This approach allows to attach external numerical modules, which are able to simulate various microstructural phenomena like dynamic recrystallization, micro shear bands or fracture.

One of the most advanced software developed in [12] is called DigiMicro. This software gives the possibility to create digital material samples and to test their properties before and after processing. In the case when obtained digital structure is not in a good agreement with the experimental data, a series of optimization algorithms is applied. Final structure is then the basis for the finite element mesh generation and subsequent FE simulations of the processing conditions. Similar approach is proposed in [16]. Both models are used to simulate microstructure development in large plastic deformations, as well as during heat treatment (i.e. static recrystallization). Contrary to that, another interesting work [11] is mainly focused on the elastic deformations. In [11] image based modeling of particle reinforced metal matrix composites and porous sintered steels is considered. The main advantage of this work is that digital microstructures are obtained directly from the microscope images prior to deformation. In 3D cases the digital microstructure is created based on the reconstructed 2D slices obtained using a destructive method.

Generation of material microstructure with specific properties is one of the most important algorithmic parts of systems based on the DMR. As mentioned such DMR is further used in numerical simulations of processing or simulation of behaviour under exploitation conditions. The more accurate the digital representation is, the more accurate results can be obtained. Most commonly used method is Voronoi tessellation, however other method like Cellular Automata, Monte Carlo, Sphere Growth or Image Processing can also be found. Wide review of methods used for this purpose can be found in another Authors' work [17].

Development of the DMR software and its application to simulations of materials processing was the main goal of this work. Based on this software a complete cycle of analysis was perform, starting from creation of initial microstructure with grains represented explicitly through generation of the microstructure oriented FE meshes and finally finite element simulation of deformation processes.

3. Initial Microstructure Generation

The numerical representation of the microstructure has to replicate as realistically as possible several features of the polycrystal. It concerns shape of grains and properties prescribed to these grains. Therefore, beyond existing DMR methods, search for more accurate and realistic techniques is necessary. Authors decided to use a cellular automata techniques [18]. As described in [17], this method provides the best results in the case of grain geometry. The principle of cellular automata is based on 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, and by a set of precisely defined transition rules f :

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

where $j \in N$, N (i) – surrounding of the ith cell, γ_i – state of the ith cell.

The first step in the CA method is to establish the discrete space composed of cellular automatons. With reference to 2D space it will be a grid consisted of squares whereas in 3D spaces it 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 is the simple algorithm 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 was in the state "already grown", then this particular cell can also change its state. The grains grow with no restrictions until the impingement with the other grains. After that they grow only in the area where no grains are observed. This process is performed until entire space will be fulfilled with grains. Due to the fact that transition rules depend on the type of neighborhood, different neighborhoods have to be investigated to distinguish differences between them [17]. Example of obtained microstructures in 2D space using mentioned algorithm and containing different amount of grains are presented in Figure 1.

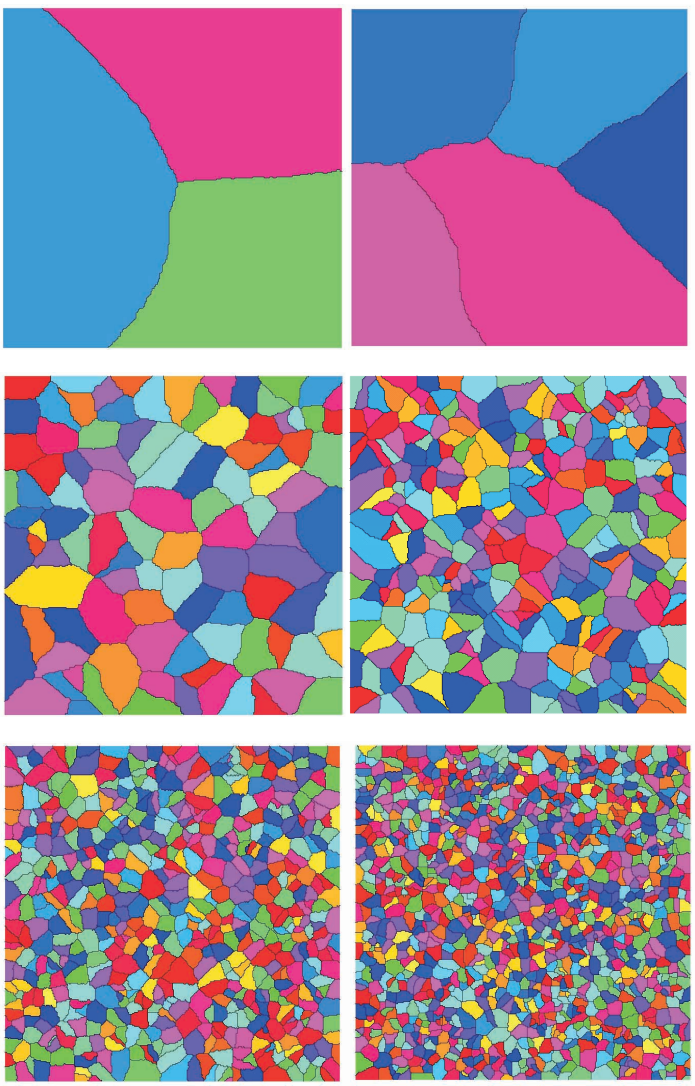

Fig. 1. Examples of 2D digital microstructures containing different amount of grains (3, 5, 100, 300, 600 and 1200 grains) generated by the cellular automata approach

These microstructures are an input data for homo- or heterogenic mesh generation algorithms and finally for FE modeling of material behavior under deformation conditions.

4. Finite element modelling based on DMR

The obtained digital microstructures can be incorporated into the commercial FE software by application of user defined subroutines. 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 DMR, the generation of the isotropic triangular mesh is performed. Particular groups of mesh nodes are located inside separated grains and different grains are distinguished (Figure 2).

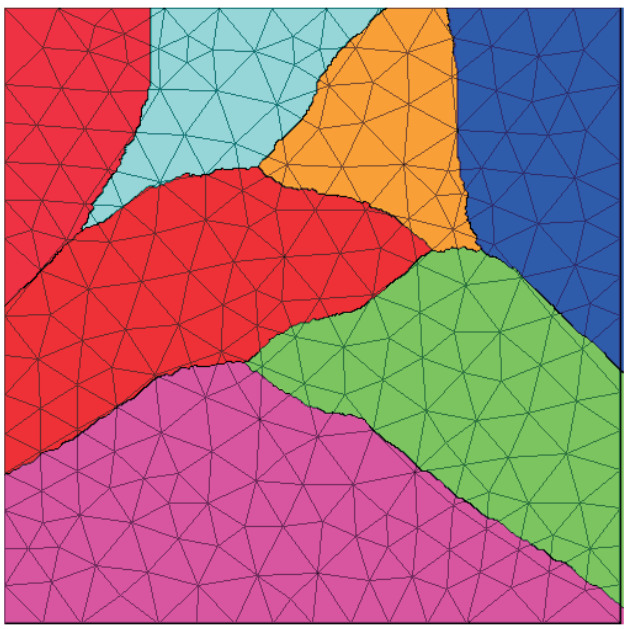

Fig. 2. Digital microstructure with homogenous mesh obtained using commercial Forge 2 FE code

- The selected flow curves describing particular material (ferrite, austenite) are assigned to the particular grains in the microstructure. These flow curves were reported in [19].
- Possibility of capturing differences in grains flow due to various crystallographic orientations is the advantage of this work. The diversification in the flow curves for each grain is introduced here using the random Gauss distribution (Figure 3).

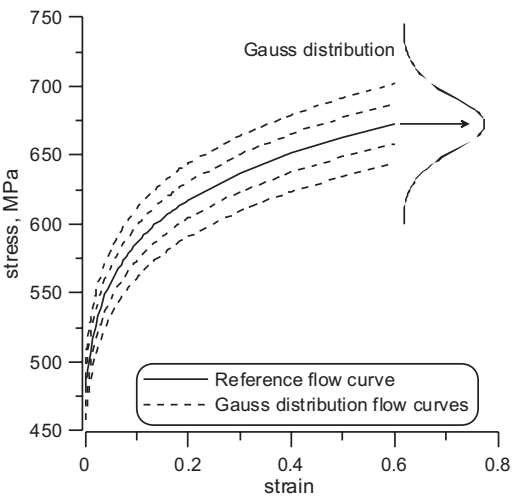

Fig. 3. Idea of diversification in flow curves for the ferrite phase using the Gauss distribution function

- Starting the FE simulation is the final step.

This procedure was applied in another authors work [14] and it revealed some limitations of this approach. Due to the fact that a homogenous mesh is used to describe behaviour of grains that are characterized by different properties, strain gradient occurs along the grain boundaries as presented in Figure 4. In this example a behaviour of the three grains with different crystallographic orientation was analysed.

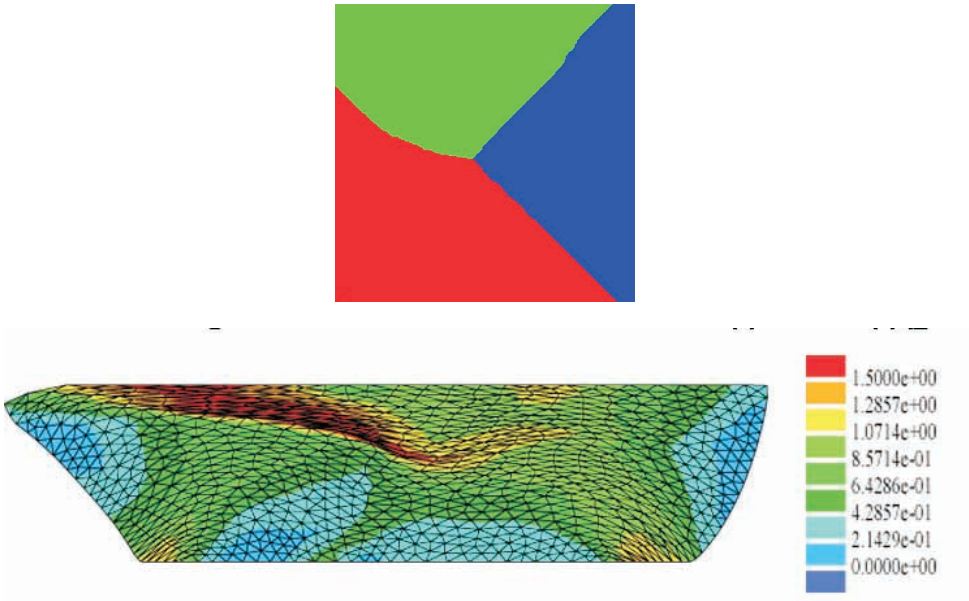

Fig. 4. Plane strain compression with unconstrained vertical edges of the triple point junction

To properly capture material behaviour along the grain boundaries a specific heterogenic FE meshes have to be used. Due to the fact that this kind of functionality is not available in the commercial FE mesh generators Authors decided to use an in-house code. This code was adapted to generate FE meshes on the basis of the DMR, as presented in Figure 5.

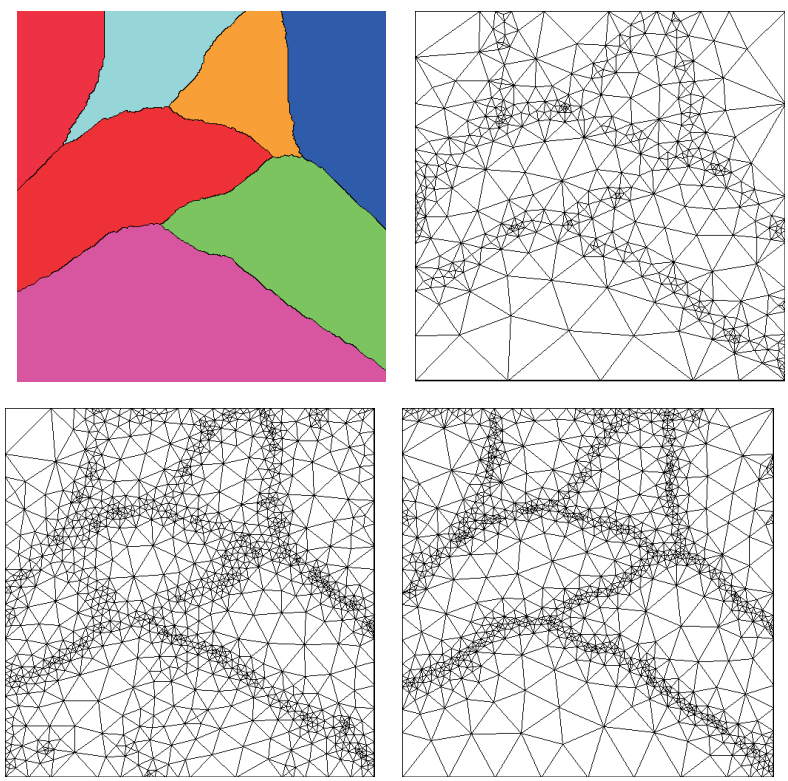

Fig. 5. Digital material representation and subsequent steps of FE mesh refinement along the grain boundaries

As seen in Figure 5 the size of the finite elements decreases along the grain boundary, to obtain refined mesh for accurate modeling of strain gradients and coarse mesh for modeling grain interior. These refined meshes with assigned different material properties were than an input data for the finite element simulation. Examples of results of simple compression test performed at micro scale level are shown in Figure 6. To describe the different character of grain flow due to crystallographic orientation a flow stress model for the ferrite phase was differentiated as in the example presented in Figure 3.

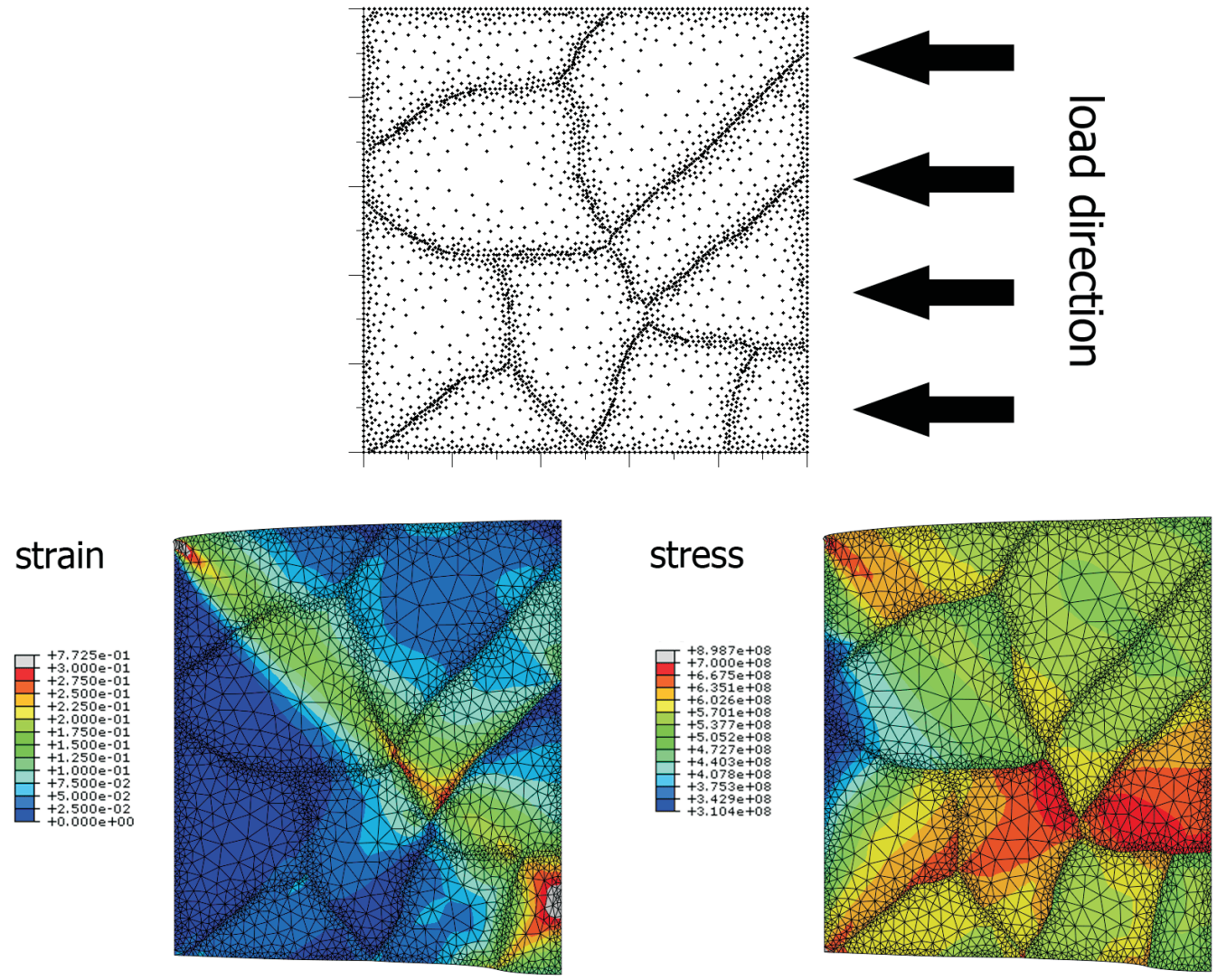

Fig. 6. Initial shape of microstructure containing 10 ferrite grains with slightly diversified flow stress models

Despite that fact that it is one phase material, strain distribution is highly non-uniform and it can be assumed that strain localization occurs through the grains with proper crystallographic orientation. Similar analysis was performed for the two phase material. Most of the grains where assumed to be austenite grains while some of the grains were selected to be ferrite grains. Differences in strain and stress distribution obtained for two different alignments of the ferrite grains within austenite matrix are shown in Figure 7.

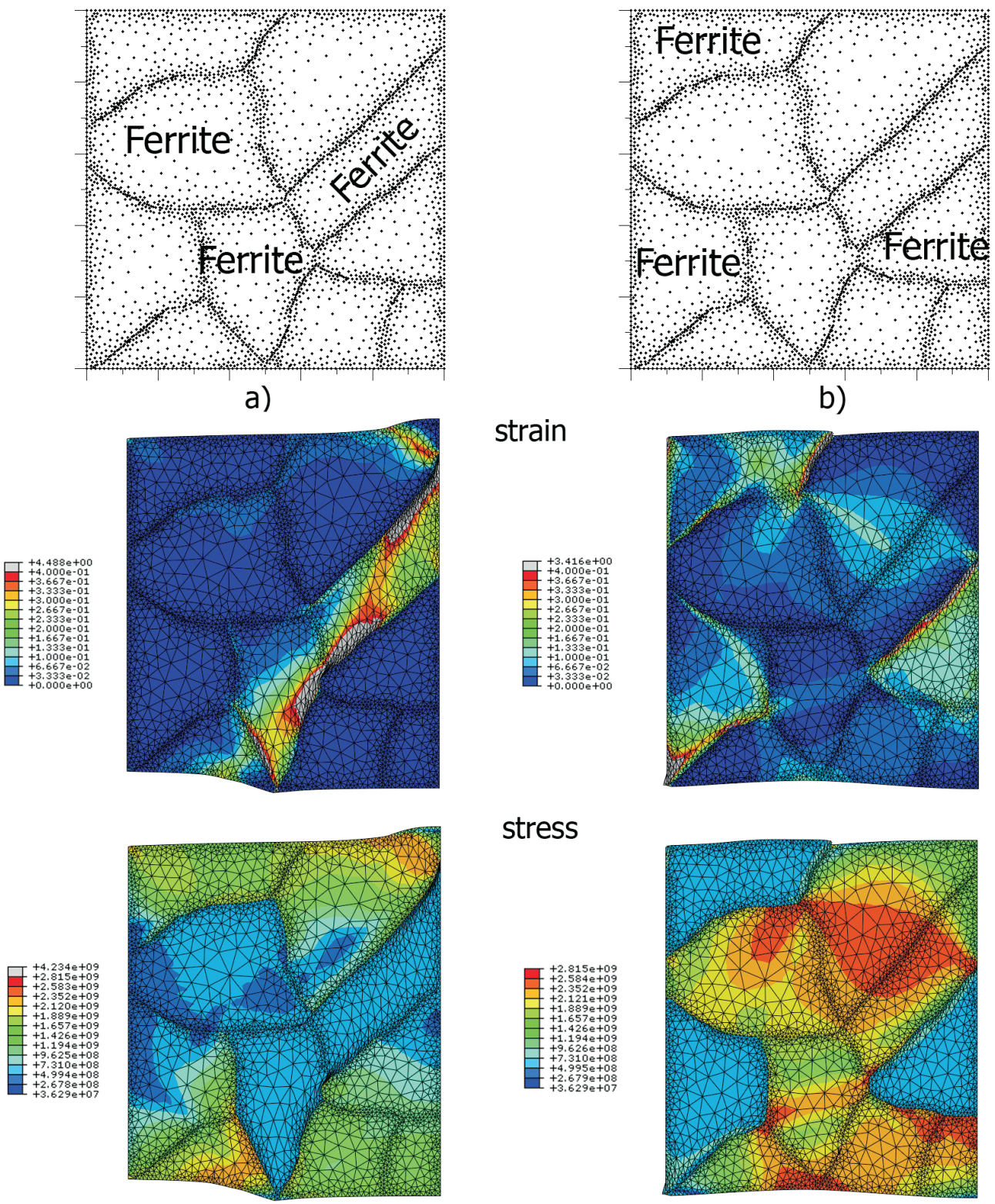

Fig. 7. Initial shape of microstructure containing 7 austenite grains with slightly diversified flow stress models and 3 ferrite grains with different alignment a) and b)

As can be seen in Figure 7 volume of ferrite phases in the two cases is similar and despite that differences in strain and stress distributions are significant. Refined meshes along the grain boundary provide a very detailed information regarding strain localization what can be clearly seen in Figure 7b. These results show how important is to take into account local material behavior when one is interested in simulation of the micro forming processes. The same initial microstructure in the geometrical sense with different arrangement of the ferrite grains can provide completely different properties of the final part.

5. Discussion

The results of research on development of digital representation of microstructure and the advantages provided by this technique are presented in ,paper. Particular attention is put on development of the cellular automata algorithm. This algorithm gives the possibility to obtain a realistic digital microstructure for further FE mesh generation. The FE mesh is refined along the grain boundaries to capture the large strain gradients occurring during material deformation. Based on this digital representation the FE simulation of the compression test were performed to show the capabilities of the developed methodology in interpretation of material behaviour. The developed methodology is performed with user friendly software which can be easily continued by scientists not familiar with details of numerical simulations. This is one of the main advantages of this approach.

Presented approach combined with sophisticated optimization methods can provide a powerful tool able to support the designing process of initial microstructure, which will be the main subject of the future work. The goal functions in such case should be based on specific macro scale features of material after deformation, while input data should be composed of microstructural characteristics, e.g. size of second phase grains, their special location or distribution, etc. Despite that, developed approach can be easily coupled with other material models describing for example dynamic recrystallization, phase transformation or crack growth. To obtain this aim an efficient remeshing algorithm that is capable to work with the DMR structures has to be designed.

Beyond this: during future works the inverse; analysis method will be applied to obtain desired initial microstructure, as well as more accurate crystal plasticity based approaches will be added to properly describe rotation of the grains during deformation.

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