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Effect of number of grains and boundary conditions on digital material representation deformation under plane strain

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ABSTRACT

The main goal of this paper is to investigate the digital material representation of a single-phase polycrystalline unit cell. Particular attention is put on the amount of grains in the microstructure, which can be considered as the representative volume element of a sample subjected to plastic deformation conditions. Additionally, the influences of the periodic and non-periodic boundary conditions on deformation behavior of the unit cells are evaluated. Possibility of the application of periodic boundary conditions on the non-periodic unit cells using a buffer zone approach is also discussed. Obtained results of equivalent strains and reaction force on case studies are presented.

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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 standard stress–strain relationship. Due to the fact that large scale samples with 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. Such a procedure is usually used to solve problems occurring in metal forming processing during rolling, forging, stamping, etc. However, the fast development of modern steel grades (TRIP, CP, DP, etc.) is one of the main challenges leading to significant changes to this commonly used approach. Mentioned materials are characterized by highly elevated material properties, which are the results of sophisticated and complex 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. The Digital Material Representation (DMR), which is the subject of the present work, is one of the possible solutions. The concept of the DMR was proposed recently and is constantly evolving. The definition according to [1] states that Digital Material Representation is a material description based on measurable quantities that provides the necessary link between simulation and experiment. The DMR is expected to create a possibility for analyzing material behavior in the

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conditions, which are difficult or even impossible to be monitored experimentally at the present state of equipment. The main objective of the DMR is creation of the digital representation of microstructure with its features represented explicitly to match real microstructure morphology. The DMR is used for calculations related to a unit cell or Representative Volume Element (RVE), depending on what kind of information is required either local or global. The RVE is a model of the material to be used to determine the corresponding effective properties for the homogenized macroscopic model. The RVE should be large enough to contain sufficient information about the microstructure in order to be representative, however it should be much smaller than the macroscopic body [2,3]. The unit cell is a part of RVE that enables obtaining results for particular part of the material. Thus the unit cell is not representative for the whole numerical model. Application of the unit cell idea, enables analyzing material behavior in particular location, e.g. crack initiation along the inclusion, without focusing on the rest of the material. As a result the unit cell provides data only for local analysis, not for whole material behavior (unlike the RVE). Usually several unit cells can be considered as the RVE. However, both of the presented approaches can have a detailed or simplified geometry of microstructure features. In the simplified model e.g. only volume fraction of particular phase is considered while shape of this phase is not regarded. Such model can provide representative global response, while morphology is significantly simplified and only statistically similar to real materials [4–6]. In the present paper, a detailed representation of morphology of real microstructure is investigated. To highlight this assumption the DMR approach is used.

It can be summarized that the DMR approach makes it possible to obtain a completely virtual description of the deformation process and provides better quality of numerical simulations to material scientists. Additionally this leads to a reduction in research costs and simplifies design of new materials. The use of advantages provided by the DMR is becoming increasingly popular as can be seen in many research works focused on different modern practical materials, e.g. heterogeneous or composite structures [7–17]. A description of recent developments in the DMR concept of polycrystalline metallic materials in various research laboratories located mainly in the United States [18–20] and Europe [21,22] is described in another work of one of the co-authors [23]. From that study it can be concluded that the more accurate the DMR is, the more reliable are the results of calculations regarding material behavior.

However, there is still a relatively small amount of exploration work on the representativeness aspects of the digital microstructures in polycrystalline metallic materials. One of these studies is focused on identification of the size of the representative volume element in linear elastic randomly structured polycrystals made up of cubic single crystals [24]. In this case a stochastic Dirichlet and Neumann boundary value problems consistent with the Hill(-Mandel) macrohomogeneity conditions were analyzed. Another similar research was undertaken in [25], where a micromechanical model of ductile damage was made, and its effects on the plastic behavior of FCC polycrystalline metallic materials were investigated. Also research related with discrete element simulations of shocked

wave propagation in polycrystalline copper can be found in [22].

Thus, the main purpose of the present study is focused on determination of the amount of grains in the digital single-phase microstructure unit cell, which can be representative for a larger volume of material. To achieve that a series of compression tests with non-periodic and periodic boundary conditions was conducted. Previously developed DMR methodology was used and the obtained results are then compared and summarized below.

2. Digital material representation model

As mentioned, the generation of microstructure morphology with its specific features and properties is one of the most important algorithmic parts of systems based on DMR. There are several experimental and numerical methods that can provide accurate representation of microstructure morphology e.g., Voronoi tessellation, voxel method, serial sectioning, cellular automata, sphere growth, inverse analysis or Monte Carlo. The problem of generating accurate DMRs with various algorithms was extensively studied by one of the co-authors in [26,27] and is not addressed in the present work.

In the DMR approach, the obtained representation of microstructure morphology is further used in numerical simulations of processing or simulation of material behavior under exploitation conditions. For that reason, the obtained digital microstructures have to be incorporated into commercial FE software by application of user defined subroutines. The algorithm is as follows:

a) Based on the obtained morphology of the DMR, the generation of the non-uniform triangular mesh is performed using the DMR mesh software developed in [28] (Fig. 1). In this solution, size of the finite elements decreases along the grain boundary in order to obtain a refined mesh for precise modeling of strain gradients. A coarse mesh is used for modeling the grain interior.

b) Selected flow curves describing behavior of particular grains in the investigated microstructure are assigned to FE elements that represent microstructure features.

c) The possibility to capture differences in grain flow due to various crystallographic orientations is the advantage of the presented approach. That is why diversification in the flow curves for each grain is introduced by application of the random Gauss distribution to the K coefficient in the following equation (Fig. 2):

$$\sigma_p = K(\varepsilon_i + E_{bp})^n \tag{1}$$

where σ_p – flow stress value, ε_i – equivalent strain, K and E_{bp}, n – model coefficients.

d) Starting the FE simulation is the final step.

The described procedure was applied in the present research to investigate representativeness aspects of the unit cell DMR in single-phase polycrystalline metallic materials. Numerical simulations of the compression test with specified deformation conditions were carried out in the commercial finite element program Abaqus. The triangular mesh with