Development of digital material representation model for porous metallic microstructures

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Abstract. The overall goal of the research is development of the integrated method for determining the formability characteristics of porous materials for application in computer simulation of metal forming processes. Particular attention is put on implementation of digital material representation model replicating complex morphology of sintered porous microstructures for subsequent micro scale analysis of deformation. Image processing and discrete modelling approaches namely cellular automata method will be used within the work to develop digital representation of sintered porous microstructure morphologies.

1 Introduction

The sintered porous materials become increasingly popular in various practical applications (e.g. sintered tool materials, super hard cutting materials etc.) because they provide desired physical and chemical properties of products [**Erreur ! Source du renvoi introuvable.**]. However, to improve and control material properties e.g. tensile strength, a detailed knowledge on influence of porous microstructure on material behavior under deformation conditions is off importance. In that case application of numerical modelling techniques can support and extend experimental investigation performed on this group of materials [**Erreur ! Source du renvoi introuvable.**].

In the present research the Digital Material Representation (DMR) concept will be used to numerically evaluate porous material behavior under loading conditions.

2 Digital Material Representation concept

The DMR concept was proposed a decade ago and is constantly evolving [1,4]. The definition according to [3] states that Digital Material Representation is a material description based on measurable quantities that provides the necessary link between simulation and experiment. Thus, the main objective of the DMR is to design and create the digital representation of investigated microstructure with its features represented explicitly to match real microstructure morphology [4].

The DMR can be used during simulation as a Unit Cell (UC) or Representative Volume Element (RVE), depending on what kind of information is required, either local or global [5].

For the purpose of numerical calculations digital microstructures are often created as exact replicas of real microstructures. In this case an image of real microstructure is required, what always employs series of experimental analysis. This procedure is becoming quite complex when 3D digital microstructures are required. In this case advanced experimental procedures have to be used e.g. near-field high-energy X-ray diffraction microscopy (nf-HEDM) or X-ray diffraction contrast tomography. The other solution is to use a statistically equivalent microstructures created using only numerical methods. That way a 2D and 3D digital microstructures can be obtained in a fast and efficient way. Both of these approaches are used within the present research.

3 Image processing

The algorithm responsible for transferring light optical microscopy image of sintered porous microstructure into the DMR form consists of three steps. During the first, the image of investigated microstructure is subjected to digital treatment with the defined threshold function [6], what results in the simple binarization. During the second step, any noise present at the image after binarization is eliminated by the filtering algorithm The third and the last step, involves application of the erosion and dilation algorithms to improve quality of complex shapes, which are typical for pores. Example of application of the image processing algorithm to the image of sintered porous microstructure with the porosity level ρ_w=0.75 [7] is presented in Fig. 1.

Approaches based on real microstructure images are very efficient and commonly used for two dimensional investigations. However, in 3D case the DMR is usually created based on the reconstructed 2D slices obtained using a destructive method [8]. Such a procedure is based

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on series of costly and time consuming experimental research and metallographic analysis.

As mentioned, the solution is development of numerical methods based on discrete cellular automata technique, that among other algorithms e.g. Monte Carlo, Voronoi tessellation, can provide statistically representative morphology of investigated microstructure both in 2D and 3D computational domains.

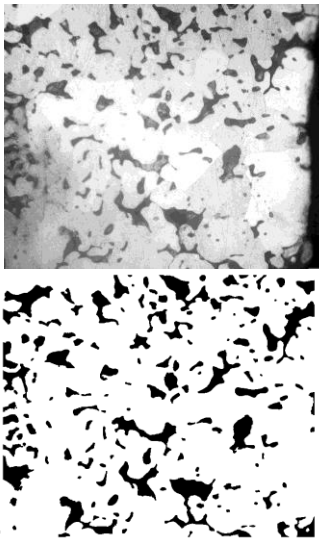
a)

b)

Figure 1. Illustration of the a) real and b) digital representation of sintered porous microstructure.

4 Cellular Automata

The simplified unconstrained grain growth Cellular Automata model was used during the present research [9]. The 2D and 3D versions, of stochastic hexagonal CA neighborhoods were used during the investigation to obtain reliable grain shapes. In this type of the neighborhood, each CA cell in each time step can select one of six (in 3D, Fig. 2) or one of two (in 2D) available neighborhoods with a probability *p*. As a result of the unconstrained CA grain growth model, the 2D or 3D representation of microstructure morphology without pores is created where each grain is described by a unique identifier as seen in Fig. 3.

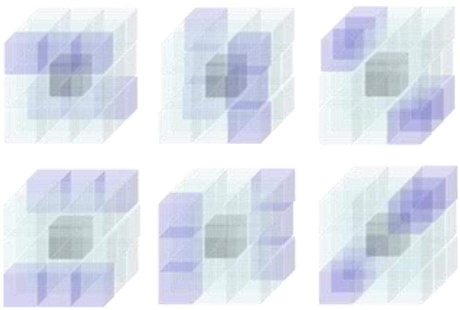


Figure 2. Illustration of six possible neighborhoods in the 3D stochastic hexagonal CA neighborhood type.

Obtained digital microstructures are then modified by implemented algorithm responsible for generation of features representing pores. The algorithm operates in a discrete cellular automata space, and is used to identify CA cells that will represent pores in the microstructure.

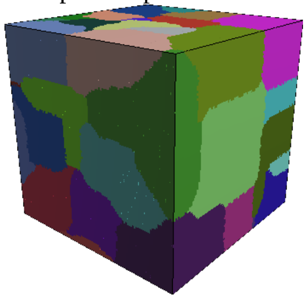


Figure 3. Three dimensional representation of microstructure morphology obtained from unconstrained CA grain growth algorithm in 3D.

First, a central cell is selected that is located in the triple point junctions or along the grain boundaries. Then CA cells within the specified region are being associated with the central cell according to different mathematical formula, what can be schematically illustrated for spherical pore shape in Fig. 4. As a result, identified cells located within the defined radii, will change the state and will be considered as cell representing pores in the microstructure.

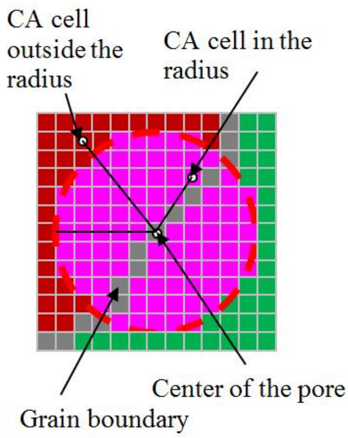


Figure 4. Illustration of modification of the CA space, by selecting CA cells representing porous feature.

At present stage of the research, pores can be characterized by different shapes namely: spheres, cubes and ellipsoids in 3D space. Analogous two dimensional microstructures with pores can also be created. During the generation stage size, position and volume fraction of pores can be controlled to provide required microstructure morphology. Examples of simple pore geometries both in 2D and 3D spaces are presented in Fig. 5 and Fig 6, respectively. In the three dimensional cases only pores are visualized within the microstructure. Additionally in 2D space, the algorithm based on Bezier curves [10] was implemented in order to obtain more complex description of pores morphologies as seen in Fig. 7.

Obtained digital microstructures with features representing pores, can be then incorporated into the finite element software and digital material representation model can be established.

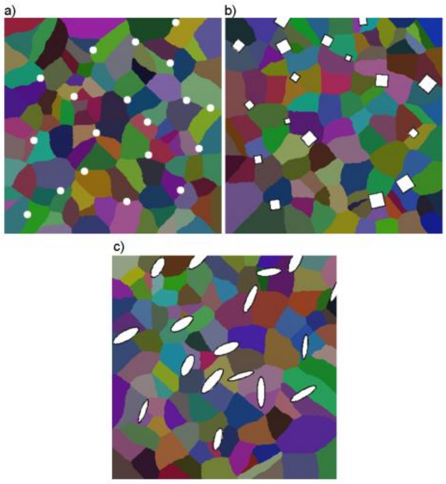


Figure 5. Examples of two dimensional digital microstructures with pores with a) circular, b) square and c) ellipse shapes.

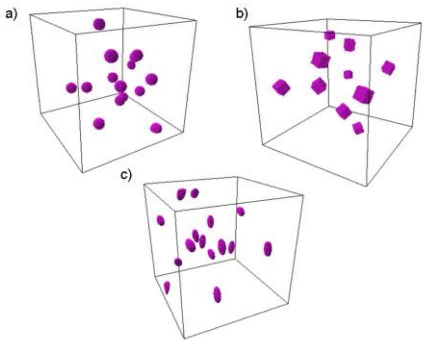


Figure 6. Examples of three dimensional digital microstructures with pores with a) spherical, b) cubic and c) ellipsoid shapes.

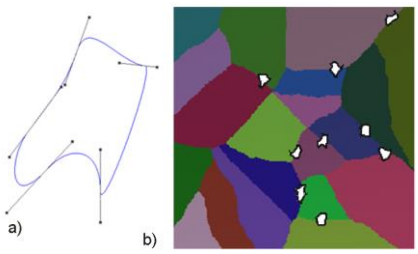


Figure 7. Illustration of the a) Bezier curve and b) digital microstructure with complex pore shapes.

As a result, microstructure behavior under various loading conditions can be evaluated. Details on the procedure can be found in [5, 10]. Example of numerical results that can be obtained during e.g. simulation of compaction process are presented in Fig. 8. Conventional J2 plasticity was used during the investigation. Flow stress characteristic was obtained from uniaxial compression of a solid material without porosity and incorporated into the finite element software. As seen in Fig. 8, detailed information on material inhomogeneous behavior at the microstructure level can be obtained from such an investigation. Besides that other information on e.g. level of compactness or failure initiation regions can also be provided.

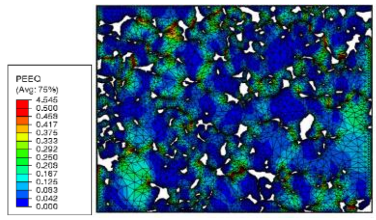


Figure 8. Illustration of digital material representation model, of microstructure from Figure 1 after compression.

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