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Review

Digital/virtual microstructures in application to metals engineering – A review

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ABSTRACT

Recent progress in application of digital/virtual microstructure models in the area of metals engineering science is presented within the paper. First, various approaches to digital reconstruction of microstructure morphology of investigated materials is presented. Possibilities of generation of both: exact replicas of morphology, as well as, synthetic microstructures are discussed. Advantages and limitations in the case of two and three-dimensional problems are highlighted in that section. Then, the state of the art in the evaluation of material properties at the microstructure scale is addressed. Various experimental techniques, characterized by different levels of complexity, which are capable of providing information on materials hardening behavior at the micro scale level are presented. Finally, possibilities of introduction of microstructure morphology with specific properties into the finite element solution are described. The work is complemented by series of practical applications of the digital/virtual microstructure models to show their capabilities and present directions for further development.

1. Introduction

Most of numerical simulations of elasto-plastic material deformation conditions are carried out by means of the finite element (FE) method, which can be successfully used in modeling of standard plastometric tests (e.g. compression, tension, torsion) as well as complicated metalforming operations (e.g. closed die forging, porthole extrusion, shape rolling) [1]. However, the accuracy of a finite element solution, among finite element mesh density or initial and boundary condition definitions, is particularly related to proper description of material hardening behavior.

Plastometric tests at different deformation conditions are often used to provide information on material response during loading. To improve mathematical description of obtained results, interpretation of these data can be efficiently carried by means of the inverse analysis technique [2,3]. That way influence of heterogeneities related e.g. to friction or deformation heating, can be taken into account and eliminated from the solution. Eventually, set of homogenized flow stress data in the investigated range of process conditions is provided. These data are then usually described by a single flow stress equation representing behavior of the entire material, implicitly including influence of local morphological

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heterogeneities during FE analysis such as different phases, inclusions, precipitations, etc. Advantages provided by the approach are widely appreciated and used in scientific as well as practical industrial investigations of large scale metalforming processes.

However, it seems that since the beginning of new millennium the approach not always provide satisfactory description of material behavior. This is mainly related to two issues that an industry is presently facing:

- Fast development of modern metallic materials like complex multi-phase steels, aluminum, magnesium or copper alloys, which are characterized by elevated material properties that are directly related to sophisticated microstructures. Interaction between different phases, inclusions or precipitations directly influence microstructure response to processing and exploitation conditions [4–7] and should not be described by a single homogenized flow stress model.
- Development of micro forming technologies, where sample is no longer an aggregate of billions of microstructural features but contains significantly limited number e.g. hundreds of them [8,9]. Like in the previous case, interactions between particular features cannot be neglected and described by a single flow stress model.

To address presented issues, different approaches capable of detailed, local investigation of material behavior has recently been developed such as image based modeling, virtual microstructure modeling, explicit microstructure modeling, etc. Their common feature is representation of morphology of investigated microstructures, where each morphological feature is presented explicitly. The approach in the present work will be called by a unified term – the Digital Material Representation (DMR). Presentation of its recent progress, advantages and limitations as well as possibilities of practical applications is the main goal of the paper.

2. Algorithms for generation of digital material representations

First attempts to include a simplified polycrystalline structure during a finite element simulation appeared at the end of 80 s of the last century [10]. However, fast development in this field is clearly visible for last 10–15 years as researchers were trying to incorporate microstructure into various numerical models [11–26]. At the beginning, a microstructure in its explicit manner was usually considered only as a support to better understand material behavior at the micro scale level. Thus, the microstructure was rather an addition to the model, and little attention was put on crucial aspects of its accurate reconstruction prior simulation or evaluation of material properties at the appropriate length scale.

However, that research and fast progress in the multi scale modeling capabilities gave an invaluable input into development of the Digital Material Representation concept. The first and crucial step in development of a DMR model is digital reconstruction of a microstructure morphology, with investigated features represented explicitly to match experimentally observed microstructure morphologies. The more detailed the reconstructed morphology is, the higher quality of calculation results is expected. Consequently two major groups of approaches based on an exact reconstruction or synthetic generation have been proposed.

2.1. *Methods of exact reconstruction of microstructures*

DMR models are most often created as exact replicas of microstructures based on post-processing of metallography images acquired from light (LM) or electron (EM) microscopy in 2D or 3D spaces. Image processing procedures, which are then applied, are usually based on several stages [27]. The first is preprocessing focused on improving quality of an input image by application of denoising, filtering, sharpening, etc. operations. Then, segmentation algorithms are applied to differentiated subsequent microstructural features from an input image. Solutions with different levels of complexity can be used during the stage like thresholding, clustering, graph partitioning, etc. Finally, feature identification and evaluation (e.g. shape coefficients calculations, skeletonization) operations are frequently performed [27]. An image processing has successfully been applied to analyze single [28] and multiphase [29] microstructures in order to reconstruct their digital form as presented for example in Fig. 1. Sometimes, to obtain required results, image processing is also combined with other numerical solutions like a cellular automata (CA) grain growth model [30].

Obtaining three-dimensional digital representations based on experimental data is more demanding and requires application of advanced experimental procedures, such as X-ray diffraction contrast tomography or near-field high-energy X-ray diffraction microscopy (nf-HEDM) [31]. Techniques based on high energy X-ray diffraction can provide large set of 3D information on morphological features of investigated metallic microstructures and they are also classified as non-destructive approaches. In the case, a microstructure can be investigated prior and after deformation or even under in situ conditions [31]. However, these methods in application to metals are still expensive and not easily accessible. Also the volume of investigated sample is limited by required image resolution, that directly affects quality of further digital reconstruction.

That is why, digital microstructures in three-dimensional space are usually created based on a reconstructed set of 2D images obtained by a destructive method – the serial sectioning (Fig. 2).

Again, a light or an electron microscopy can be used during the serial sectioning procedure to provide input data for subsequent image processing and reconstruction algorithms.

The conventional approach to serial sectioning, based on manual labor, is extremely time consuming and requires series of steps:

- Precise grinding/polishing. The sample is polished for a required time to remove desired amount of material and reveal the underlying microstructure. This is followed by rinsing to eliminate any polishing residue. To help identify the investigated zone and evaluate amount of removed material, usually a set of pyramidal micro indentation markers is induced into the sample.