Computational Materials Science 96 (2015) 200–213

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Numerical analysis of the influence of number of grains, FE mesh density and friction coefficient on representativeness aspects of the polycrystalline digital material representation – Plane strain deformation case study

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ARTICLE INFO

Article history:
Received 19 May 2014
Received in revised form 19 August 2014
Accepted 22 August 2014

Keywords:
Digital material representation
Single phase polycrystalline microstructure
Representativeness
Finite element method
Plane strain

ABSTRACT

Investigation of the influence of digital material representation model parameters of a single phase polycrystalline unit cell on its behavior under loading conditions is the subject of the present paper. Firstly, investigation of the impact of the finite element mesh density on the quality of obtained results is conducted. However, the particular attention is put on the selection of the minimum amount of grains in the microstructure with periodic boundary conditions that can be considered as the representative volume element of a sample subjected to plastic deformation under plane strain. Finally, the influence of different friction coefficient values between tools and the sample, on deformation behavior of the unit cells is evaluated. Obtained data in the form of equivalent strain distributions and homogenized stress–strain curves for the analyzed case studies are presented and discussed within the paper.

1. Introduction

Application of advanced numerical modelling techniques on development of modern macro and micro metal forming operations or designing of new innovative materials is presently very common in industrial practice. Computer aided design is cheaper and less time consuming than the traditional trial and error approach based on a series of experimental and industrial tests/trials. Unfortunately, most of industrially made numerical simulations are based on a conventional approach to modelling that usually describes material behavior as a continuum, and are based on a general constitutive law in the form of the relationship between stresses and strains or strain rates [1–3]. This flow stress model plays a crucial role in the constitutive law as it describes material response to loading. Thus a series of plastometric tests in various deformation conditions (e.g., temperatures, strain rates) is performed to obtain realistic flow stress information for a particular material. Additionally, interpretation of results of these tests must eliminate the influence of heterogeneities of strains, stresses and temperatures caused by such variables as friction and deformation heating. An inverse analysis can be applied to determine a strain–stress relationship that is insensitive to these heterogeneities [4]. In large-scale problems involving billions of grains, the behavior and interaction between particular grains can be averaged in the form of a single flow stress model. This procedure is widely used to solve problems occurring during material deformation as well as to develop novel technologies for materials processing (e.g., [5–8]). The morphology of a microstructure is not explicitly taken into account in this case.

However, modern market demand for innovative products drives significant changes to this commonly used approach. The first need is for the development of modern engineering materials (e.g., advanced high strength steels, aluminum, magnesium, titanium, copper alloys, metallic foams, asphalt, graphene) where elevated properties are obtained by the creation of sophisticated multiphase microstructures [9,10]. Interaction at the nano and micro scale levels between microstructure features and the surrounding material under processing or exploitation conditions directly results in excellent properties at the macro scale level. The second need is related to a symbol of our times, which is omnipresent miniaturization that requires the development of new micro forming technologies such as micro forging or micro extrusion [11–13]. In this case the sample is no longer a large aggregate of billions of grains, but it contains only hundreds of grains. Thus, behavior and interaction between each particular grain become important as these grains can be characterized by different crystallographic orientations or significantly different properties. Finally,

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http://dx.doi.org/10.1016/j.commatsci.2014.08.037
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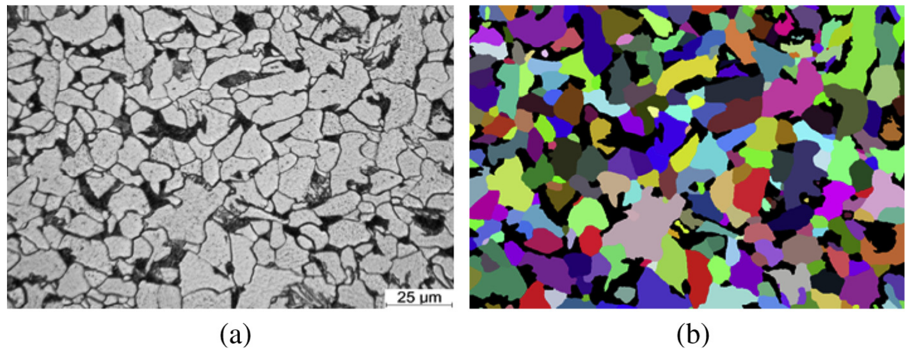

Fig. 1. Concept of DMR generation: (a) Light Optical Microscopy (LOM) image and (b) DMR based on LOM image [34].

it should also be mentioned that improvement in experimental techniques broadening the fundamental knowledge on deformation mechanisms (e.g., electron microscopy, micro tomography, nano deformation/indentation) is another factor stimulating research and introducing changes to the above-mentioned commonly used numerical approaches.

To meet these market pressures and support experimental research, modern numerical methodologies are being developed [14–16]. One of the perspective approaches is based on the digital material representation (DMR) concept that is the subject of this paper.

2. Digital material representation concept

The DMR approach enables a precise description of real material morphology, where different micro scale features are directly included (e.g., precipitates, inclusions, big and small grains, grain boundaries, crystallographic grains orientations, phases boundaries). Digital material representation can be defined as a material description, based on measurable quantities, which provides the necessary link between simulation and experiment [17]. The DMR enables analysis of material behavior in conditions that are very difficult or even impossible to be supervised experimentally at the present state of research equipment. The more precisely DMR is applied, the more realistic results of calculations regarding material behavior are obtained, which has been proven by research groups from the United States [18–20], Europe [21–23] and Australia [9,10]. The DMR approach enables a detailed virtual analysis of real material behavior, while errors of calculations are minimized. Numerical models based on the DMR give more detailed results than those based on previously mentioned conventional approaches because they take complex microstructure morphologies into account in an explicit manner during simulation.

Thus, generation of microstructure morphology with its specific features and properties is one of the most important algorithmic parts of systems based on the DMR. There are several experimental and numerical methods that can provide accurate representation of microstructure morphology, such as those based on microscopy imaging (e.g., Optical Microscopy, Scanning Electron Microscopy) [24–26] or those based on less time consuming computer methods (e.g., Voronoi tessellation, voxel method, cellular automata, sphere growth or Monte Carlo methods) [30,31]. The problem of proper generation of the DMR with various algorithms was extensively studied in [32,33]. The concept of DMR generation for metallic materials is presented in Fig. 1.

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 developed by the

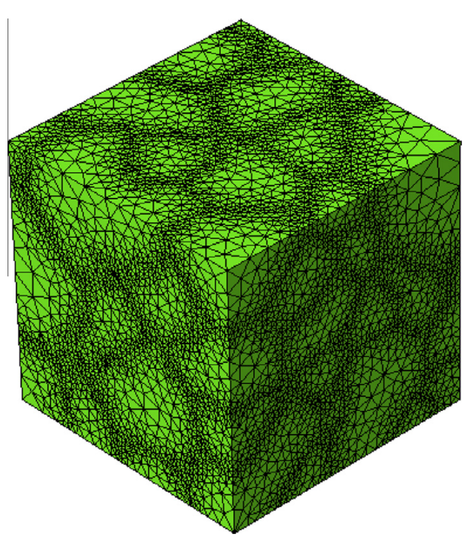

Fig. 2. Digital microstructure with non-uniform FE mesh obtained using DMRmesh software [35].

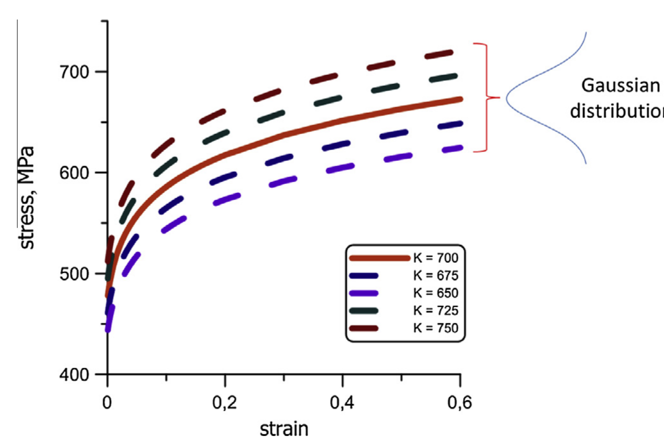

Fig. 3. Concept of diversification in flow curves using the Gauss distribution function, where an expected material response is for parameter $K = 700$ used in the conventional flow stress equation.