

NUMERICAL ANALYSIS OF STRESS DISTRIBUTION IN POLYCRYSTALLINE MICROSTRUCTURE

NUMERIČKA ANALIZA RASPODELE NAPONA U POLIKRISTALNOJ MIKROSTRUKTURI

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Keywords

- grain orientation
- microcrack
- stress distribution
- tessellation

Abstract

The paper presents a numerical analysis of stress distribution in micromechanical models in order to simulate microstructural mechanisms of microcrack initiation and propagation in polycrystalline metals. The analysis is based on plane-strain finite element crystal elasticity models. The microstructure is generated using Voronoi tessellation, encompassing random crystallographic orientation and position of grains that have different shapes and sizes. Since the correlation between the physical mechanisms of deformation and the microstructure is essential for sound understanding of crack initiation and propagation, the paper considers development of microstructural models of behaviour of anisotropic linear-elastic and elastic-plastic polycrystalline metals. The results indicate that the key factor for good agreement with the data obtained from polycrystalline microstructure, is the correct and proper interpretation of material heterogeneity between grains. The attention should be placed on proper material characterization, crystallographic slip mechanism representation and orientation.

INTRODUCTION

One of the major concerns in maintaining the integrity of structures is the appearance of damage, such as fracture resulting from defects, present on microstructural level during exploitation. The material microstructure plays an important role in dictating the modes of fracture and the macroscopic response of real materials. The fracture from the macroscopic point of view can be divided into two phases: crack initiation and crack propagation, /1/. The macroscopic crack initiation is related to microstructural short cracks that can appear due to accumulation of persistent slip bands at the peaks of surface roughness or inhomogeneities in polycrystalline materials, /2/. In polycrystalline materials the grain morphology strongly affects mechanical properties and failure mechanisms, /3, 4/. Grain boundaries can hinder dislocation movements that controls the spreading of elastic and plastic deformation. Due to dislocation

Ključne reči

- orijentacija zrna
- mikroprslina
- raspodela napona
- teselacija

Izvod

Data je numerička raspodela napona u mikro-mehaničkom modelu sa ciljem da se simuliraju mikrostrukturni mehanizmi inicijacije mikroprslina i njenog širenja u polikristalnim metalima. Analiza je zasnovana na modeliranju elastičnosti kristala konačnim elementima u slučaju ravnog stanja deformacija. Mikrostruktura je generisana primenom Voronoi mozaika, kojim su obuhvaćene proizvoljne kristalografske orijentacije i pozicije zrna različitih oblika i veličina. S obzirom da je korelacija između fizičkih mehanizama deformacije i mikrostrukture od suštinskog značaja za temeljno razumevanje inicijacije i širenja prslina, ovaj rad je značajno doprineo razvoju mikrostrukturnih modela ponašanja anizotropnih linearno-elastičnih i elasto-plastičnih polikristalnih metala. Rezultati su pokazali da je ključni faktor za dobro slaganje sa podacima dobijenim iz polikristalne mikrostrukture, tačno i pravilno tumačenje heterogenosti materijala između zrna. Pažnju bi trebalo obratiti na pravilnu karakterizaciju materijala, i na kristalografsko predstavljanje mehanizma klizanja i orijentacije.

pile-ups at grain boundaries, the stress is locally raised and this might induce dislocation movement of existing dislocations in the next grain or even cause nucleation of new dislocations in the adjacent grain. The microstructure of polycrystalline materials is composed of many grain boundaries and grains with different shapes, sizes and components. The complexity of the microstructure increases the difficulty in investigating the relationship between microstructural morphologies and mechanical properties. In order to investigate this relationship, a proper numerical approach should be established which can be used to characterize the microstructure and stress behaviour when subjected under loading.

Many researchers have been investigating the influence of grain size, shape and crystallographic orientation on different parameters regarding to cracks in different materials, using experimental and numerical models to verify their results, /5-8/. Some were focused on investigating the

numerical representation of microstructural aspects of different metals, thus certain corrections and recommendations are provided for further investigation on implementing proposed numerical techniques, /9-10/. The differences between mechanical properties obtained for fine-grained and coarse-grained microstructures, /11/, have led to conclusions that grain boundaries greatly affect stress and deformation distributions in heterogenic materials. A perfect example for this is the heterogeneity in welded joints. Microstructural differences in different parts of welded joints can influence the overall properties of a structure. Experimental investigation in specific sections of the welded joint is very difficult because sizes of these sections are very small and make it almost impossible to be achieved. Numerical investigation can certainly alter this specific problem. In the field of structural mechanics, the scientific community has been developing models of material behaviour in a lesser time and at smaller space scales, trying to tackle phenomena, such as the representation of materials' constitutive behaviour and fracture.

In this paper, the effect of grain size, shape and orientation of a polycrystalline material is analysed in terms of numerical representation and stress distribution. The material is linear elastic and is considered to be subjected to tension loading. Several two-dimensional numerical models are constructed in order to simulate different grain structures, from coarse-grained to fine-grained small segments, extracted from a bulk metal material. The Voronoi tessellation is used to represent the microstructure; finite element calculation is conducted using ABAQUS. The construction of representative volume elements (RVE), material characterization, meshing techniques and boundary conditions used in numerical models are described in the following text, together with the interpretation of results.

NUMERICAL SIMULATION

Many researchers have shown that the microstructure of polycrystalline material can be numerically represented by using the Voronoi tessellation algorithm, /14/. This algorithm divides space randomly into regions that are convex polygons with various numbers of edges on a two-dimensional plane completely filling up the space without overlapping. The polygons obtained with this process are very similar to real austenite grains in polycrystalline materials. Each grain in the aggregate has its own orientation that corresponds to crystallographic axes. This is defined with the assigned local coordinate system of each polygon. The simulated grains have random size, shape and orientation as presented in Fig. 1.

The classical approach in modelling the mechanical response of a structure that is subjected under tensile loading is to use continuum mechanics theory, assuming that constituent materials are homogeneous and in most cases isotropic, without considering microstructural features of the materials. This is applicable and valid for structures that have dimensions much larger than microstructural features such as grains. This approach breaks down if the characteristic dimensions of the structure are of the same order of magnitude as characteristic microstructural scales. If the

RVE is large enough it can be macroscopically described as an isotropic linear elastic material characterized by a set of two independent material parameters such as Young's modulus E and Poisson's ratio ν .

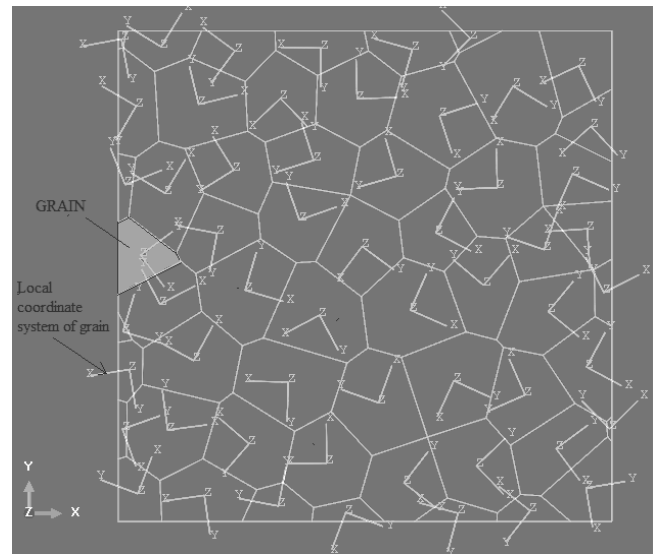


Figure 1. Numerically simulated grains.

When the volume of the material is small, so that it consists of a limited number of grains, the overall elastic behaviour may be highly dependent on specific elastic properties of individual grains. This means that all individual grains will microscopically show anisotropic material behaviour that is dependent on the crystal structure and orientation. In this paper the linear elastic behaviour of the martensitic tetragonal crystal structure, exhibiting orthotropic behaviour, is analysed. The material is defined in the property module through the stiffness matrix D_{ijkl} : $D_{1111} = D_{2222} = D_{3333} = 233$ MPa, $D_{1122} = D_{1133} = D_{2233} = 135$ MPa, $D_{1212} = D_{1313} = D_{2323} = 118$ MPa. The finite element models are quadratic planer plates of dimension 1×1 mm². Microstructures A–D established for numerical calculations are shown in Fig. 2. Microstructures in Fig. 2a and b (denoted as microstructure A and B, respectively) are considered to be coarse grained structures. The microstructure A consists of 58 grains ($N = 58$) and the average grain size of the grain in this model is 0.01 mm². Microstructure B contains 119 grains ($N = 119$) with an average size of 0.008 mm². Microstructures in Fig. 2c (denoted as microstructure C) consist of 261 grains ($N = 261$) with an average grain size of 0.0038 mm² and Fig. 2d (denoted as microstructure D) consists of 471 grains ($N = 471$) with an average grain size of 0.0021 mm².

In each model there is a variation in the average value of the area, size and orientation of the grain. Each grain is subdivided into 8-noded quadratic strain finite elements of type CPE8R, according to the recommendations in article /15/. The finite element meshing of the grains in all four models is automatic and mainly depends on the size and shape of grains. Details on the mesh specifications for each model are given in Table 1.

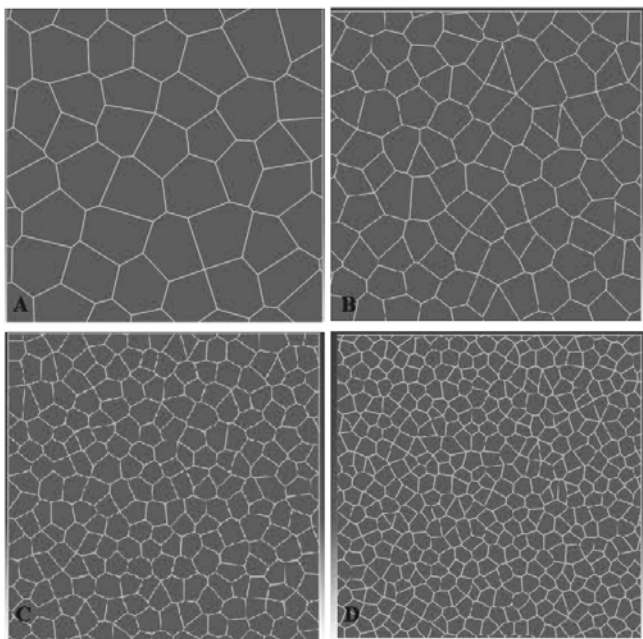


Figure 2. Coarse grained structures (A and B) and fine grained microstructures (C and D).

Table 1. Microstructure and mesh specifications.

Structure	N	Average grain (mm ²)	Elements	Approximate element size
A	58	0.01	3915	0.02
B	119	0.08	9992	0.02
C	261	0.003	4097	0.02
D	471	0.002	4568	0.02

The boundary condition is chosen so that the edges of the domain remain straight. At the upper and lower side the displacements are fixed in *y* direction, as well as the rotation of the nodes. The left-hand side is constrained in *x* direction, that means that the *x* values for all nodes on this side of the RVE are zero. Rotations are also constrained. The right-hand side of the RVE is free to move in *x* direction. On this side of the aggregate, the tensile loading is applied by imposing displacement of 1 mm.

RESULTS AND DISCUSSIONS

Martensite laths share the {110} slip planes which lie along the axis of the lath. The slip plane in martensite laths is assumed to be 110, meaning that martensite laths are 45° inclined to the grain orientations, /16/. The potential microcrack will initiate along these persistent slip bends which in this case would be the martensite lath. This slip band can be numerically simulated as shown in /17-18/. When an individual grain reaches a critical value of shear stress on the slip band, the movement of the slip can cause stress in neighbouring grains which can result in micro-cracking or propagation of the already existing crack. The orientation angle of the potential crack is determined through $\alpha = \varphi + 45^\circ$, where φ determines the orientation of slip according to the global coordinate system, /19/. The primary goal here is to estimate the influence of random grain structure on the overall stress distribution. Investigation is focused on the randomness of orientation while keeping a constant size of the numerically modelled aggregate. The obtained results are shown in Figs. 3 and 4.

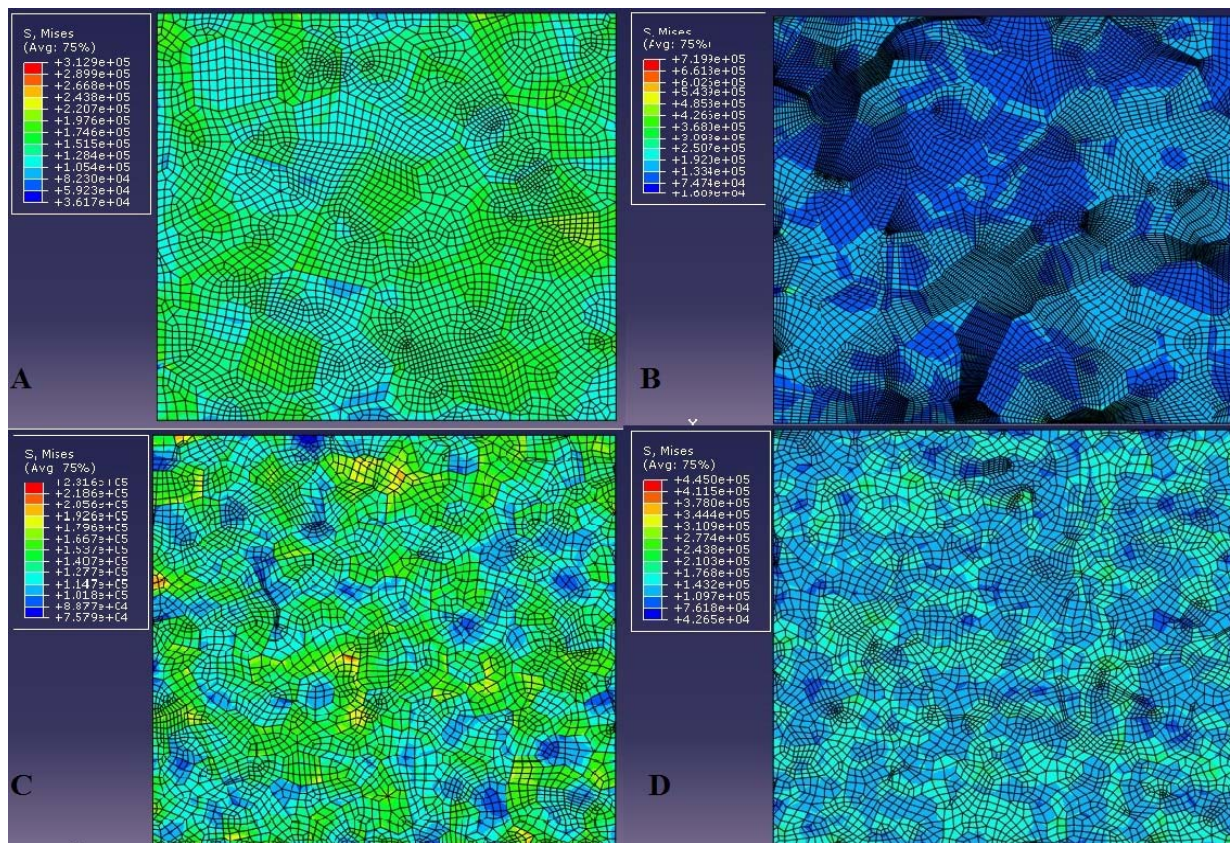


Figure 3. Von Misses stress distribution in microstructures A, B, C and D.

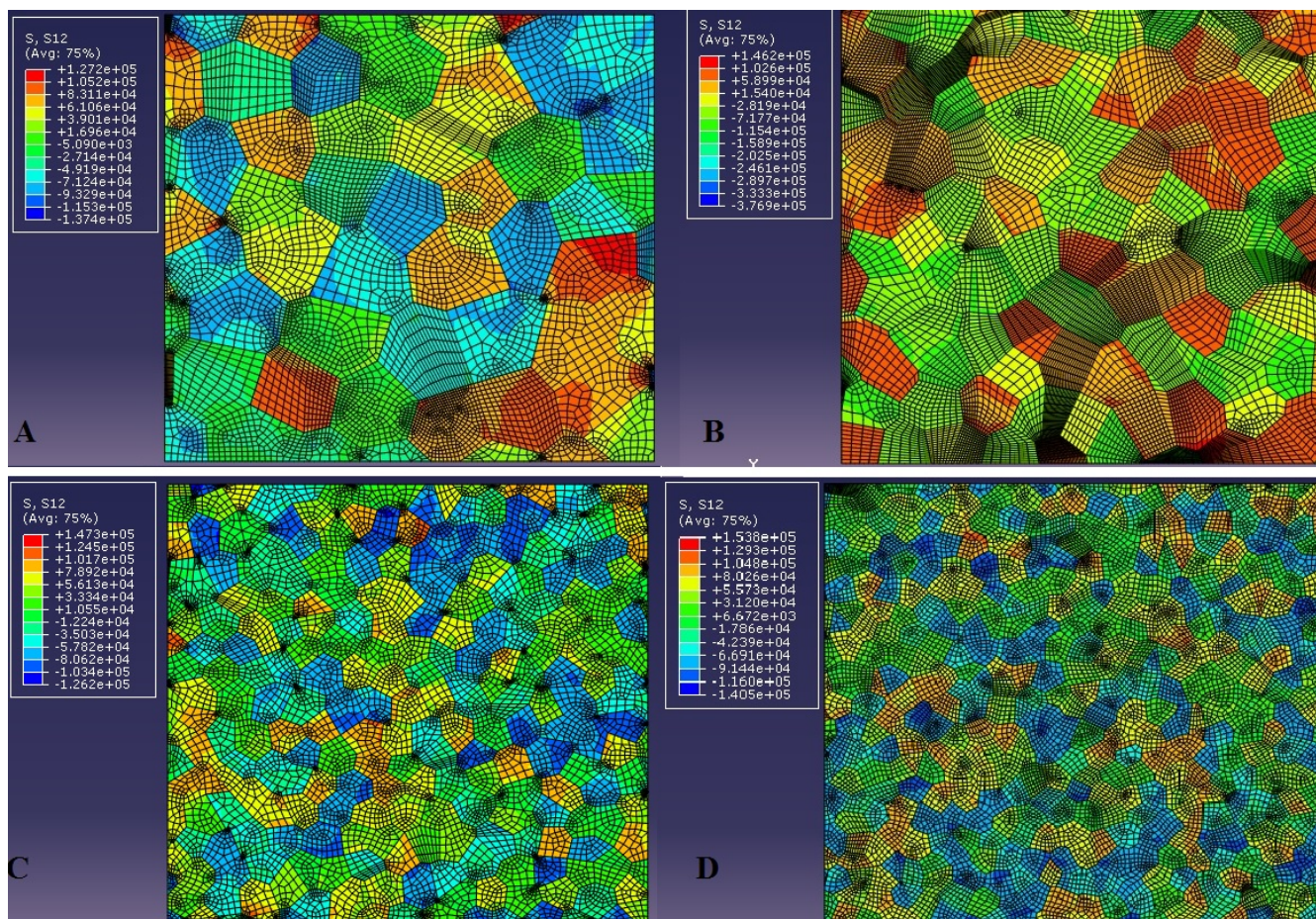


Figure 4. Von Mises shear stress distribution in microstructures A, B, C and D.

From the results shown in Figs. 3 and 4 it can be easily concluded that there is an eminent influence of grain density over Von Mises stress distribution. In Fig. 3, there is a severe difference that is characteristic for so-called coarse-grained quadratic plates A and B which conforms to the assumption that when the volume of the material is small, so that it consists of a limited number of grains, the overall elastic behaviour may be highly dependent on the specific elastic properties of individual grains. This means that their influence on the effective elastic properties of the material may not be averaged out, so that the previous theory is not applicable. On the other hand, structures C and D, or the fine-grained microstructure shows a more even and similar distribution of stress which can imply that the material can be considered as isotropic when RVE is large enough.

CONCLUSIONS

For different numerical calculations with distinct sets of orientation, the effective linear elastic behaviour of the simulated microstructures shows substantial scatter. The effective properties are determined by exact orientations, and hence the specific properties of microstructures determine the mechanical behaviour at the scale considered. The most important conclusion from computations, therefore, is that for relatively small polycrystalline aggregates the microstructure must be explicitly taken into account in

mechanical studies, and the use of effective isotropic elastic properties is not correct. The results here obtained encourage further investigation of possibilities to predict two-dimensional crack propagation numerically accounting for real microstructure data. Stress concentrations, which certainly can arise from second phase precipitates or pores, cause local plastic deformation to an extent that depends on local slip geometry with respect to the local direction of maximum shear stresses. The models show that stress value and distribution within grains is related to the orientation of the grain and the orientation of its neighbouring grains.

The preliminary motivation for this numerical investigation is analysis of characteristic zones in welded joints that are microstructurally distinguished as fine-grained and coarse-grained structures. The stress distribution that could potentially effect crack initiation and propagation is substantial in welded joints. Therefore, further investigations should be considered with distinct focus on microstructural aspects of materials in the heat affected zones of a welded joint and correct definition of material characteristics. This investigation should also include definition of plastic behaviour at grain level with the crystal plasticity theory.

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