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2D NUMERICAL ANALYSIS OF MICRO-CRACKS

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Abstract:
In this paper, 2D numerical models are developed in order to investigate the micro-cracks initiation caused by the persistent slip bands formation inside the grains of polycrystalline materials. The structure is artificially generated and should be similar to the grain structure present in real materials. Considering the crystallographic orientation of each grain through which the distribution of stress and deformation can be observed, initiated micro-cracks tend to propagate in certain manner. The results from the analysis are describing the impact of grains density, shape and orientation on micro-cracks propagation, theoretically and numerically. The results obtained are compared with various experiments and conclusions by different authors and are presented in order to get a good overview of the problem and to propose a different approach in representing the cracks numerically.

Keywords: *Micro crack; Crystal grains; Voronoi tessellation; Persistent slip bands; Shear stress*

1. INTRODUCTION

Crack initiation and propagation in polycrystal materials strongly depends on local microstructure of the material, the loading conditions and the internal stress concentrations and distributions [1]. Stress concentrations can be attributed to a variety of micro-structural inhomogeneties in engineering materials, but the mechanism of propagation is still not fully understood. Many experiments and tests are required for investigating the possibilities of micro-crack coalescence. The costs of these investigations are very high so the development of numerically based models can represent a useful tool in the process.

Grain and phase boundaries are one of the most prominent micro-structural characteristics that can cause local stress-strain concentration, because of the elastic and plastic anisotropy of the microstructure of polycrystalline materials [2]. The grains within a polycrystalline material are randomly oriented. The difference in crystallographic orientation causes stress peaks and triple lines at grain boundaries that may exceed the local yield strength and cause local plastic deformation [2].Correlation between the physical mechanisms of deformation and the material's microstructure, is substantial for sound understanding of crack initiation and propagation behavior.

The relationship between orientation, stress distribution and deformation in grains can be analyzed through numerical models that are developed in this paper. The models are two-dimensional and are simulating a microstructure similar to the one in a real poly-crystal material. The Voronoi algorithm is used for generating grain structure with random orientation in each grain. The elastic anisotropy is important factor for determining local deviations that arise from remote stresses, therefore the stiffness matrix Dijkl is introduced in the models [2]. The methodology used for constructing the representative volume elements (RVE), the assignment of the material properties and formation of the slip systems that are causing stress concentration near grain boundaries, are fully described in this paper and results from several numerical investigations are graphically displayed and analyzed.

2.DESCRIPTION OF NUMERICAL MODELS

Polycrystalline materials have random orientation of grains and this leads to macroscopically isotropic properties, but if each grain is considered separately on a microscopic level each grain is anisotropic and this leads to inhomogeneous stress states even if the applied stress is uniform [3]. The Voronoi tessellation process is the most suitable method used to simulate randomly divided regions that are convex polygons. Each of these polygons is created in a two-dimensional rectangular plate completely filling the space without overlapping and has various numbers of edges. The polygons represent austenite grains and each grain has its own orientation. The orientations correspond to the crystallographic axes and are defined through local coordinate systems that are generated. An example is shown in Figure 1.

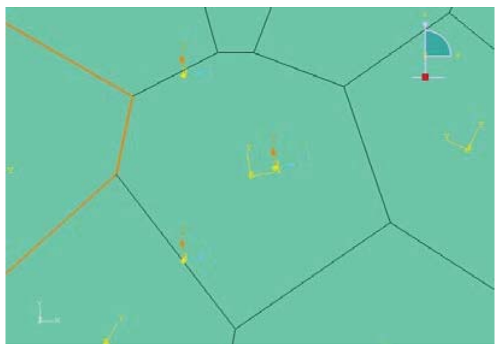

Figure 1: Local coordinate system in grain

In this work we analyze the behavior of martensit structure, therefore the material properties in the models are elastic orthotropic and the stiffness matrix of the assigned material are as follows: D1111 = D2222 = D3333 = 233000Pa, D1122 = D1133 = D2233 = 135000Pa, D1212 = 1313 = D2323 = 118000Pa. The laths share the {110} slip planes, which lie along the axis of laths [4]. The slip plane in martensitic laths is assumed to be$1\bar{1}0$, which are 45 degrees inclined to the grain orientations [2]. The potential micro-crack is expected to initiate along persistent slip bands. The slip band can be numerically simulated if the nodes that lie on the slip band are constrained to permit the sliding movement during deformation parallel to the line that is dividing the grain [4]. The displacement of each couple of nodes is constrained by$V_u - V_l = tg\alpha\,(U_u - U_l)$, that allows movements only in the direction of the partition. The models that are analyzed differ in grains shape and density. For plane stress analysis it is recommended to use 4-node linear elements [5], so the present models mainly consist of 4-node linear elements (CPS4R). There are also 3-node elements (CPS3) present in some areas of the mesh, because of the complex geometry of the randomly obtained grains. Several meshes were tested in order to find the most suitable one for the purpose of this investigation. The numbers of elements that are used vary in each grain from 50 to100. The boundary conditions of each model assigned, are such that all nodes located on the left side of the plate are free to move in y direction but not in x direction, except the node located at the lower left corner which is constrained ($x = 0$,$y = 0$).The loading is static and is assigned through displacement at the nodes on the right side of the plates.

3. RESULTS AND ANALYSIS

At the beginning each model has one initiated micro-crack. Each of the models gave different stress values for each loading. The maximum value of shear stress for each analysis was concentrated in grains that are located near the grain with the initiated crack. The results that are graphically given in Figure 2 and 3 represent the Von Misses stress distribution for two selected cases for observation (Model with rectangular plate containing 50 grains and rectangular plate with 100 grains).

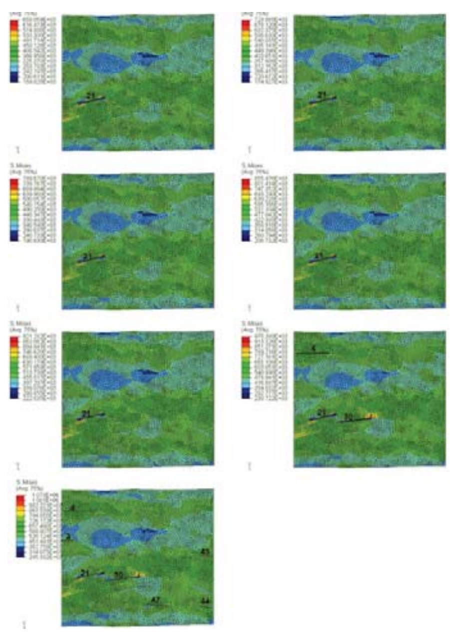

Figure 2: Numerical model of a rectangular with 50 grains, showing the trend of crack initiation in different grains

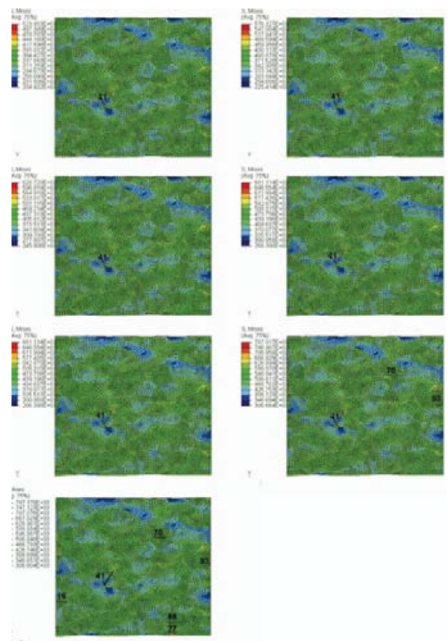

Figure 3: Model of rectangular plate with 100 plate grains, showing the trend of crack initiation in different grains

The micro-cracks are initiated in the grains where the maximum shear stress is calculated according to the local coordinate system. In all of the simulated models micro-cracks are initiated along the potential crack paths according to a defined failure criteria. The initiated crack is introduced into the representative volume element by separation, with length identical to the crack path, and this simulates one-segment crack as it is observed in experiments [6]. The grain that has a high level of stress and is oriented at about +/- 45^{o} to the loading axis is the next grain where crack can occur. From the results it can be easily detected that after each initiated crack the stress is redistributed. These micro-cracks are one-segment cracks initiated on the maximum shear stresses failure criteria and they are likely to form a macro crack by coalescence. The expected coalescence and formation of macro-cracks is different in each model.

3. CONCLUSIONS

There is no doubt that it is impossible to describe the complex interactions between microstructure, load and crack propagation rate by simple mathematical equations and numerical interpretations. The results here obtained encourage further investigation of the possibilities to predict two-dimensional crack propagation numerically accounting for real microstructural data. The models show that stress value and distribution within grains is related to the orientation of the grains and the misorientation of its neighboring grains.

The present work arouses the existence of unifying aspects and facts that the integrity of a structure is strongly dependent from the microstructure and the interactions between the crack tip and the crystallographic orientation and shape of the adjacent grains. There are also important quantitative information that can be extracted from the models about the direction of the crack propagation and the possible coalescence. The models are very close to introduce the phenomenon of stress concentration in triple points and along neighboring grain boundaries and can certainly be used as a tool that will assist in further understanding and investigating the materials microstructure and crack propagation.

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