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MULTISCALE MODELLING OF SHORT CRACKS IN RANDOM POLYCRYSTALLINE AGGREGATES

VEČNIVOJSKO MODELIRANJE KRATKIH RAZPOK V NAKLJUČNIH VEČKRISTALNIH SKUPKIH

Leon Cizelj, Igor Simonovski
"Jožef Stefan" Institute, Reactor Engineering Division, Jamova 39, 1000 Ljubljana, Slovenia
Leon.Cizelj@ijs.si, Igor.Simonovski@ijs.si

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The identification and explanation of processes potentially responsible for the initiation and development of intergranular cracks are topics of wide concern. Especially the early phase of the development of cracks seems to be beyond the present state-of-the-art explanations. An effort was therefore made by the authors to construct a computational model of the crack growth kinetics at the grain-size scale. The main idea is to divide continuum (e.g., polycrystalline aggregate) into a set of subcontinua (grains). Random grain structure is modelled using Voronoi-Dirichlet tessellation. Each grain is assumed to be a monocrystal with random orientation of crystal lattice. Elastic behaviour of grains is assumed to be anisotropic. Crystal plasticity is used to describe (small to moderate) plastic deformation of monocrystal grains, caused mainly by the strains along the "incompatible" grain boundaries and at triple points. Finite element method is used to obtain numerical solutions of strain and stress fields. The analysis is currently limited to two-dimensional models. The paper focuses on the dependence of crack tip loading (J-integral) on the random orientation of neighbouring grains. The limited number of calculations indicate that the incompatibility strains, which develop along the boundaries of randomly oriented grains, influence the local stress fields (J-integrals) at crack tips significantly.

Key words: short cracks, random polycrystalline aggregates, multiscale modelling

Spoznavanju in pojasnjevanju procesov, ki bi lahko povzročili nastanek in razvoj medkristalnih razpok, namenjajo raziskovalci po svetu veliko pozornost. Še najmanj raziskane in pojasnjene so zgodnje faze razvoja razpok. Avtorja sta zato sestavila računalniški model napredovanja razpok na nivoju kristalnih zrn. Ključna ideja je razdelitev kontinuuma (večkristalni skupek) na množico med sabo povezanih manjših kontinuumov (kristalno zrno) z uporabo Voronojevega oz. Dirichletovega mozaika. Vsako izmed kristalnih zrn nato opišemo kot monokristal z naključno orientirano kristalno rešetko. Predpostavimo anizotropno elastično vedenje, zmerne plastične deformacije pa opišemo s kristalno plastičnostjo. Veliko plastičnih deformacij povzročijo že nekompatibilnosti specifičnih deformacij ob kristalnih mejah in v trojnih točkah. Deformacijska in napetostna polja računsko ocenimo z metodo končnih elementov. Analize so sedaj omejene na ravninske primere. V članku smo se osredinili na odvisnost vrednosti J-integrala od naključne orientacije okoliških kristalnih zrn. Omejeno število izračunov nakazuje močan vpliv nekompatibilnih deformacij vzdolž kristalnih mej na porazdelitev napetosti ter specifičnih deformacij v okolici razpoke, s tem pa tudi na vrednosti J-integrala.

Ključne besede: kratke razpoke, naključni večkristalni skupki, večnivojsko modeliranje

1 INTRODUCTION

The identification and explanation of processes potentially responsible for the initiation and development of intergranular cracks are topics of wide concern. Despite significant research performed in the past decades, the root mechanisms of intergranular (stress corrosion) cracking (IGC, IGSCC) are still not understood completely. Recent research shows that the intergranular cracking is strongly dominated by the microstructural features, especially those on the grain boundaries.

Computational algorithms aiming at modelling and visualization of the IGSCC initiation and growth on the grain-size scale have already been proposed [1]. Randomness of the grain structure and of the crack initiation and growth processes were assumed. The random crack growth was simulated with algorithms allowing for crack branching, coalescence and interference. The method yielded patterns of cracks with shapes and structure comparable to those observed in experiments. However, a number of potentially important microscopic features (e.g., random orientation and anisotropy of grains, grain boundary mismatch etc.) were not taken into account. A convenient approximation with isotropically elastic continuum was implemented instead, allowing for simplified but efficient estimation of stress intensity factors.

In this paper, the dependence of crack tip loading (J-integral) on the random orientation of neighbouring grains under anisotropic elasto-plastic material response is numerically investigated. The simulation framework [2] relies on explicit models of a random grain structure and finite element solution of the boundary value problem using standard crystal plasticity models. Similar approach has been followed by Simonovski et al [3] while analyzing a transgranular crack emanating from the surface of a polycrystal. A very detailed study of the crack tip opening displacements of short crack in mono- and bi-crystals modelled using standard crystal plasticity models is available in [4].

The results obtained are discussed and compared with solutions for homogeneous isotropic and anisotropic plates. The results obtained are important for the future developments of the already proposed modelling and visualization of the IGSCC initiation and growth at the grain-size scale [1].

2 MODEL

The essential features of the proposed multiscale simulation model are briefly described in this section. Further details are available in [2].

The random grain structure is modelled as a planar Voronoi tessellation representing a cell structure constructed from a Poisson point process by introducing planar cell walls perpendicular to lines connecting neighbouring points. This results in a set of convex polygons embedding the points and their domains of attraction, which completely fill up the underlying space. The concept of Voronoi tessellation has recently been extensively used in materials science, especially to model random microstructures like aggregates of grains in polycrystals, patterns of intergranular cracks and composites.

All tessellations used in this paper were generated using the code VorTESS [5]. Only a subset of Voronoi tessellations is considered suitable for the finite element meshing with quadrilaterals [6].

Constitutive modelling. Each grain (as formed randomly by the Voronoi tessellation) is assumed to be anisotropically elasto-plastic with randomly oriented crystallographic directions. The utilized crystal plasticity model assumes that plastic deformation takes place by simple shear on a specific set of slip planes. A further constitutive assumption is that the shear rate depends on the stress only through the Schmid resolved shear stress.

Detailed description of the constitutive models and algorithmic framework used is given in [7].

Homogenisation. Volume averaging of mesoscopic strain and stress tensors is used to estimate the effective macroscopic stress and strain tensors.

The crack tip loading. The loading of the crack tips is achieved through the prescribed remote macroscopic biaxial stress field. The J-integrals are then calculated for each crack tip using the built–in features of ABAQUS [8], which rely on the Virtual Crack Extension method combined with the divergence theorem, transforming the integration domain onto the area enclosed by the chosen contour.

The scatter caused by the randomly shaped isoparametric finite element meshes at crack tips randomly positioned within Voronoi tessellations has been studied in isotropic continuum and reported as reasonable (e.g., up to about 10 %) elsewhere [9,10]. The accuracy of the J-integral estimates in randomly oriented anisotropically elastic media has been found reasonable in [10].

3 NUMERICAL EXAMPLE

The planar structure with 101 grains is depicted in **Figure 1** with blue lines representing the intact grain boundaries. The red line between points A and B represents cracked grain boundary – a simple straight inclined crack.

The finite element mesh (isoparametric 8-noded quadrilaterals with reduced integration) used in subsequent calculations is depicted in **Figure 1**, too. The loading of the mesh is prescribed by tensile macrostress with magnitudes 600 MPa and 300 MPa in directions X and Y, respectively. The size of the model studied was significantly smaller than the size of a representative volume element (RVE), which has been estimated for a similar non-cracked case to be about 350 grains in elastic and 800 grains in plastic deformation modes [2]. Both essential types of macroscopic boundary conditions were therefore simulated: (1) prescribed macroscopic stress and (2) prescribed macroscopic strain.

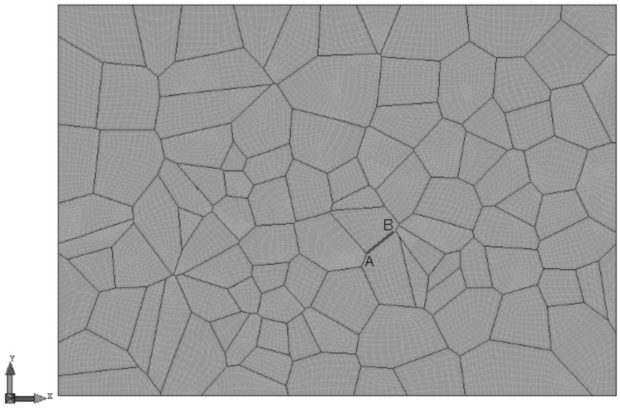

Figure 1: FE Model of a inclined crack in polycrystal

Slika 1: Mreža končnih elementov s poševno razpoko v večkristalnem skupku

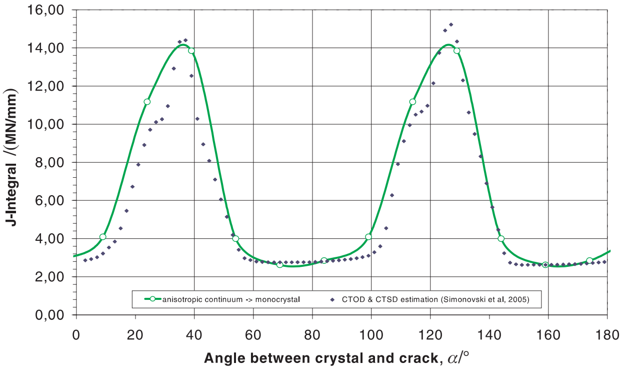

Figure 2: J-integrals and CTOD for an inclined crack in an anisotropic monocrystal (macroscopic equivalent strain of 0.2 %)

Slika 2: Vrednosti J-integrala in CTOD za poševno razpoko v anizotropnem monokristalu (makroskopska ekvivalentna specifična deformacija 0,2 %)

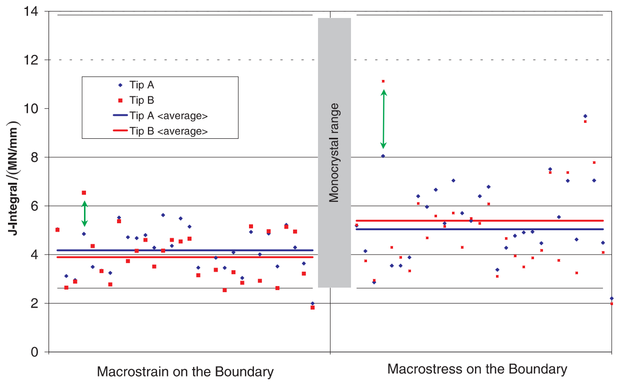

Figure 3: J-integrals and CTOD for an inclined crack in a polycrystal (macroscopic equivalent strain of 0.2 %)

Slika 3: Vrednosti J-integrala in CTOD za poševno razpoko v večkristalnem skupku (makroskopska ekvivalentna specifična deformacija 0,2 %)

Two distinct cases are studied: (1) anisotropic continuum representing a monocrystal and (2) polycrystalline aggregate with grains modelled as randomly oriented anisotropic continua. In both cases, the influence of grain orientations on the magnitude and orientation of the crack tip loading are sought under the assumption of plane strain and both macroscopic boundary conditions.

Reasonably constant estimates of J-Integral were obtained for three different contours. The average value of those three estimates is consistently used in subsequent discussion. The scatter of J-integral in plain strain is presumably governed by the random orientations of grains in the simulated system. It is therefore useful to compare such scatter by the variability of J-integral estimates obtained by assuming an inclined crack in a homogenous anisotropic plate. For this reason, all grains in **Figure 2** were identically oriented (= monocrystal), and material orientations were systematically varied in increments of 15 degrees. Results are given as a function of crack orientation. Additionally, the J integral estimates obtained from scaled Crack Tip Opening and Crack Tip Sliding Displacements (CTOD and CTSD, resp.) in a similar case [3] are also plotted for comparison. Qualitative agreement between J and CTOD&CTSD estimated is deemed reasonable. It should however be noted, that [3] analyzed a surface crack, which might well explain the quantitative differences in the response.

The scatter of J-integral in a polycrystal was studied using 30 realizations of random grain orientations within the fixed grain structure (**Figure 3**). The results are presented for macrostress and macrostrain boundary conditions. Two data points (Tip B and Tip A) are plotted for each realization of random grain orientations and each type of boundary conditions. A rather large difference between J integrals in both crack tips (extremes indicated by green arrows) is found in some cases. This significantly exceeds the finite element numerical error and therefore clearly indicates existence of a preferential crack growth direction as opposed to the well-known symmetric behaviour of such crack in isotopic conditions. The observed scatter seems to be generally consistent with the angular variations of J-integrals in monocrystal.

The total strain of about 0.2 % indicates that the calculations were performed in the neighbourhood of the macroscopic yield strength, with only a subset of grains experiencing plastic deformation. This particular choice is expected to maximize the scatter of J-integrals due to highly scattered microscopic stress and strain fields.

4 CONCLUSIONS

The influence of randomly oriented anisotropic elasto-plastic grains on the microscopic stress fields at crack tips is studied numerically in this paper using Voronoi tessellation and finite element method. The limited number of calculations indicates that the incompatibility strains, which develop along the boundaries of randomly oriented grains, influence the local stress fields (J-integrals) at crack tips significantly.

Results clearly indicate significant difference between the J-integrals at both crack tips. This supports existence of a preferential crack growth direction as opposed to the well-known symmetric behaviour of the same crack in isotopic conditions. It is also a clear indication that mode II represents a significant part of the total crack tip loading. Purely elastic estimates of J integral at the onset of global yielding (0.2% strain) may be more than one order of magnitude lower than those calculated with account for the incompatibility strains along the grain boundaries. The influence of the macroscopic boundary conditions seems to be pronounced at the onset of global plastification.

The results obtained are especially important for the future developments of the modelling and visualization of the initiation and growth of intergranular and transgranular cracks on the grain-size scale.

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