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Boundary element analysis of crack problems in polycrystalline materials

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Abstract

This work analyses the mechanical behaviour of polycrystalline structures with intergranular cracks, leading to a reduction of stiffness and material strength. The 2D polycrystalline structure is generated using an average grain size through the Voronoi tessellation method and simulated with random crystalline orientation. Polycrystalline materials demand fracture mechanics analysis in the grain interfaces. This paper presents this analysis using the multi-domain Boundary Element Method (BEM) with anisotropic fundamental solution and applying the Multiscale Cohesive Zone Model (MCZM) to characterize the onset and growth of cracks in the grain interfaces, considering the atomistic behaviour inside the interfaces. Comparisons of the results of BEM are performed through simulations in ABAQUS in order to validate the response of the method and comparisons of results with the literature are made to validate the present technique.

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Keywords: Boundary element method, Polycrystalline materials, Interface crack growth, Multiscale Analysis;

1. Introduction

Over recent year the study of failure and behaviour of polycrystalline materials have been growing specially due to the multiple number of industrial applications of these materials. Due to the characteristic of the crystalline structures, the failure generally is presented in the microscale such as free zones, voids, cracks and impurity particles, that will affect the effective mechanical properties in the macroscale. The BEM has the ability to model high gradients problems, as those found in fracture mechanics applications. BEM has been applied to computer modeling in micromechanics by Czyz et al. (2013). Sfantos and Aliabadi (2007a), used the BEM for polycrystalline structure analysis. The authors investigated 2D crack propagation along grain boundaries using a linear cohesive law, and mixed mode failure condition. Sfantos and Aliabadi (2007b), proposed a multi-scale BEM modeling for material and degradation fracture using a conventional cohesive zone model. Turon et al. (2007). They proposed a methodology to determine the constitutive parameters for the simulation of progressive delamination using cohesive zone models for mixed-mode of fracture.

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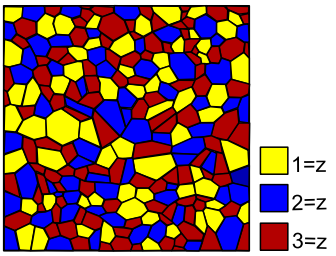

Fig. 1. Artificial structure generated with randomly distributed material orientation for each grain

Benedetti and Aliabadi (2013), analyzed a 3D micro-mechanical failure and degradation using cohesive zone model in polycrystallyne material. These works mentioned are based in conventional cohesive zone models. The MCZM was developed by Zeng and Li (2010) for the analysis of fracture and damage problems, that take into account the atomistic scale in order to obtain the cohesive forces as a fracture criterion using colloidal physics and micromechanics homogenization techniques. In this paper is proposed the (MCZM) using the implementation of multidomain formulation of BEM by Kane (1994) with anisotropic fundamental solution Sollero and Aliabadi (1993) performed over polycrystalline structure generated in order to simulated and predict the crack propagation. Finally, conclusions are pointed out.

2. Polycrystalline Structure Modeling

The material modeling technique used in this work is the generation of a random artificial structure with the Voronoi tessellation method as in Sfantos and Aliabadi (2007a) and Okabe et al. (2000). This approach defines the behavior of the structure with random orthotropic material and crystalline orientation.

Due to the formulation used in this paper, the material orientation coordinated axes 123 coincides with the geometrical coordinate system xyz, that means $\theta = 0$. Different cases are taken into consideration when each axis coincides with the axis z of the geometry coordinated system; thus case $1 \equiv z$, case $2 \equiv z$ and case $3 \equiv z$. These cases are presented in three different colors in Fig. 1.

Grain material properties are modeled for plain strain and plain stress analyses with the following constitutive relations, Eq. 1.

$$\sigma_{ij} = c_{ijkl}\varepsilon_{kl}, \qquad \varepsilon_{ij} = s_{ijkl}\sigma_{kl} \tag{1}$$

where c_{ijkl} is the stiffness tensor and s_{ijkl} is the compliance tensor using the Voigt notation as presented by Sfantos and Aliabadi (2007a) and Rousselier et al. (2009), given by

$$\mathbf{s} = \left[s_{ij}\right], (i, j = 1, 2, ..., 6) \tag{2}$$

In this work the formulation was adapted to implemented the material constants in the plane $z = 3$, Galvis et al. (2013).

3. Multiscale Cohesive Zone Model

To develop the implementation of the MCZM it is proposed a new approach: the use of the BEM to model the behaviour of polycrystalline materials. In order to analyse intergranular cracks, a modification over the boundary element mesh is necessary, the MCZM requires the creation of an additional grain boundary zone or the cohesive zone, Qian and Li (2011), as shown in Fig. 2.

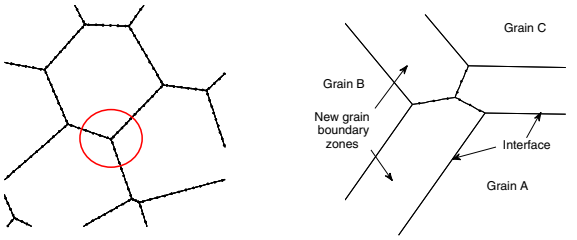

Fig. 2. Cohesive interface zone in the (BEM) mesh

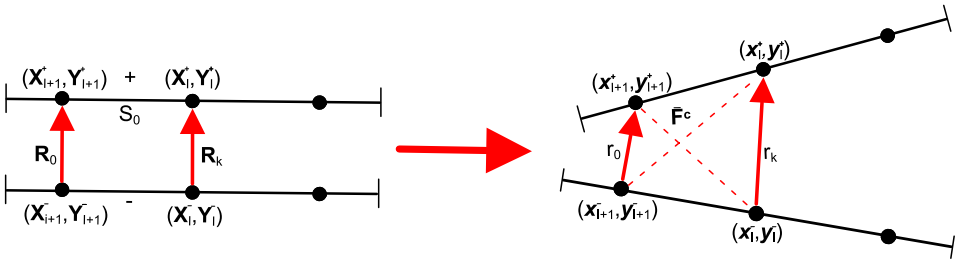

Fig. 3. Deformation gradient in cohesive zone

The cohesive zone has a finite thickness R_o related to the characteristic length scale of specific defects, Qian and Li (2011). In this work the value of R_o is among $S_o \times 10^{-3} \leq R_o \leq S_o \times 10^{-1}$ where S_o is the length between two nodes of the boundary element.

By constructing the finite width cohesive zone and computing the deformation gradient using the displacement information from the BEM, it is possible to use the Cauchy-Born rule in order to get a simplification of the deformation in the cohesive zone and finally apply the interfacial potential theory, Zeng and Li (2012).

3.1. Effective Deformation Gradient in Cohesive zone

The global non-uniform deformation field can be represented as a piecewise uniform deformation in each boundary element and they are connected to each other by the interface cohesive zone with highly non-uniform deformations, Zeng and Li (2012) and Qian and Li (2011). The deformation field inside the cohesive zone, is used the Eq. 3, Zeng and Li (2012), that represents the efective deformation gradient, that will be used in the Cauchy-Born rule, see Fig. 3.

$$\begin{bmatrix} \bar{\mathbf{F}}^c_{11} \\ \bar{\mathbf{F}}^c_{12} \\ \bar{\mathbf{F}}^c_{21} \\ \bar{\mathbf{F}}^c_{22} \end{bmatrix} = \begin{bmatrix} d & 0 & -b & 0 \\ -c & 0 & a & 0 \\ 0 & d & 0 & -b \\ 0 & -c & 0 & a \end{bmatrix} \begin{bmatrix} x^+_{l+1} - x^-_l \\ y^+_{l+1} - y^-_l \\ x^+_l - x^-_{l+1} \\ y^+_l - y^-_{l+1} \end{bmatrix} \tag{3}$$

where $a = X^+_{l+1} - X^-_l$, $b = Y^+_{l+1} - Y^-_l$, $c = X^+_l - X^-_{l+1}$ and $d = Y^+_l - Y^-_{l+1}$, following the scheme in Fig. 3.

3.2. Interfacial Atomistic Potential

Recently, Qian and Li (2011) implemented the MCZM using the Finite Element Method. The authors adopted two different magnitudes for the potential, the first is the bulk potential, that are inside the bulk element used to trangranular fracture and the second is called the depletion or cohesive potential, that is employee inside the cohesive zones for intergranular fracture. In this work, only the depletion potential will be used due to the nature of the BEM

mesh. Zeng and Li (2010) and Li et al. (2012) proposed the bulk potential, based on the Lennard-Jones (LJ) atomistic potencial, as

$$\phi(r) = 4 \in \left(\frac{1}{45} \left(\frac{\sigma}{r} \right)^{12} - \frac{1}{3} \left(\frac{\sigma}{r} \right)^{6} \right) \tag{4}$$

The expression of the cohesive potential is given by the Eq. 19 that results from the integration of the LJ potential over a rigid half space with several assumptions, see Sauer and Li (2007).

$$\phi_{cohe}(r) = \frac{\pi \in}{\sqrt{2}} \left(\frac{1}{45} \left(\frac{r_0}{\bar{r}} \right)^{9} - \frac{1}{3} \left(\frac{r_0}{\bar{r}} \right)^{3} \right) \tag{5}$$

where $\in$ is the depth of the potential, σ is the finite distance at which the LJ atomistic potential is zero and $r_0 = \sigma 2^{1/6}$, is the equilibrium bond distance. The cohesive potential is considered weaker than the potential inside the grains, Zeng and Li (2012), because different bonds presented in the microstructure may have been degenerated to non-covalent bonds, and are presented inside the cohesive zone intermolecular interactions by the van der Waals forces, Callister (1997).

3.3. Cauchy-born Rule

In the proposed Multiscale Cohesive Zone Model, in order to reduce the computational cost, the Cauchy-Born rule has been adopted Zeng and Li (2010) to evaluate the elastic energy in each element. The Cauchy-Born rule says that when the deformation in an element of the region is uniform, the gradient deformation in the element will be constant Li et al. (2012). Then, it is possible to use the same deformation gradient, evaluated by Eq. 3 inside the cohesive zone, in the fine scale.

In order to evaluate the potential energy for a crystalline solid it is used the same atomistic potential of a hexagonal lattice structure found Zeng and Li (2010). This potential is used to deform the structure applying the deformation gradient, Weinan and Pingbing (2007), as expressed by Eq. 6.

$$\bar{\mathbf{r}}_i = \bar{\mathbf{F}}^c \mathbf{R}_i \tag{6}$$

where $\bar{\mathbf{r}}_i$ is the deformed bond vector, $\mathbf{R}_i$ is de undeformed bond vector and $1, 2, ..., n_c$ are the number of total bonds in the unit cell.

Since the deformation in the boundary elements are considered uniform, it is possible to use the Cauchy-Born rule applying the average deformation gradient to simplify the computation of the non-uniform deformation field inside the cohesive zone. The effective first Piola-Kirchhoff stress, Qian and Li (2011) tensor in each cohesive zone, is written as

$$\bar{\mathbf{P}} = \frac{\partial W}{\partial \bar{\mathbf{F}}^c} = \frac{1}{\Omega_0^c} \sum_{i=1}^{n_c} \frac{\partial \phi_{cohe}}{\partial \bar{r}_i} \frac{\bar{\mathbf{r}}_i \otimes \mathbf{R}_i}{\bar{r}_i} \tag{7}$$

The effective deformation field and the atomistic stress tensor in the cohesive zone can be evaluated by the nodal displacement response from the BEM. To evaluate the cohesive traction along the boundary interface element, which is the same boundary element with opposite normal, it is just required to compute the stress tensor by the out-normal vector, as shown in Eq. 8.

$$\mathbf{T}^{cohe} = \bar{\mathbf{P}} \left(\bar{\mathbf{F}}^c \right) \cdot \mathbf{n} \tag{8}$$

4. Numerical Results

Simulations performed in this work are for 7075-T7351 aluminum alloy, according to ASM (1990). Material is generated with a virtual polycrystalline structure as abovementioned with the same plane ($z \equiv 3$), in Fig. 1, to use

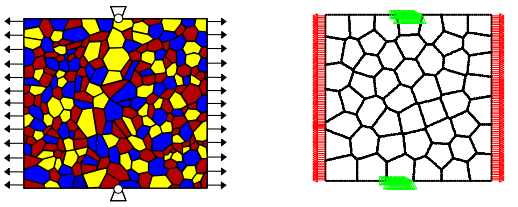

Fig. 4. Boundary conditions for polycrystalline structure

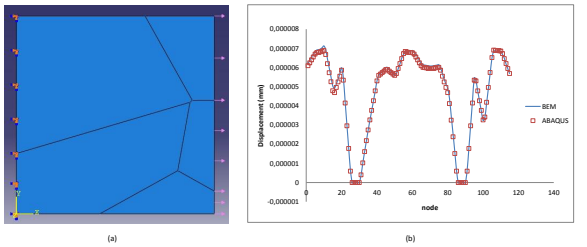

Fig. 5. (a) Model in ABAQUS; (b) Displacement response.

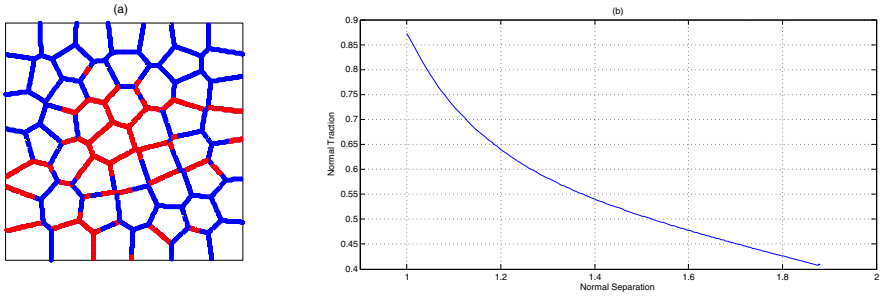

Fig. 6. (a) Fracture map; (b) Cohesive normal traction vs Normal separation

this material with the anisotropic BEM formulation. The mechanical properties are calculated as a quasi-isotropic material, see Sollero (1994). The boundary conditions of the analyzed numerical example are shown in Fig. 4.

In this paper discontinuous quadratic boundary elements and anisotropic fundamental solution were applied to model a polycrystalline structure generated with 60 grains. An incremental load is applied, with an initial value of 160 N.

To validate the BEM displacement response a simulation in ABAQUS was performed for a five grain anisotropic polycrystalline structure, as shown in Fig. 6. The results show good approximation.

With the correct displacement response, the MCZM can be applied. In this work the multiscale analysis begins when the Von Mises stress in the interface reaches the material strength. Results are presented in Fig. 6(a), where the fracture interfaces zones are shown in red and in blue color the cohesive zones. Fig 6(b) shows the relationship between cohesive normal traction and relative normal separation.

In Fig. 6(b) it is possible to see the reduction of the normalize separation force when unit increments of load are applied over the specimen, that can be compared to the figure presented by Li et al. (2012) where the shape of the curve is similar after the maximum separation force. If the separation force becomes zero the real separation between atoms will take place and the propagation fracture is initiated in the material. In Fig. 6(a) it is shown the crack propagation prediction for a set of applied load, see Fig. 4. The first set of elements that reached a zero cohesive

separation force are in the center of the specimen. Due to the displacement restriction in the boundary conditions, the fracture propagation are not totally perpendicular to the applied load.

5. Conclusions

In this work the Multiscale Cohesive Zone Model was applied in conjunction with the multidomain boundary element method to model polycrystalline structure materials. Due to the fine discretization and the mesh structure, see Fig. 2, new solvers are require to solve more efficiently the final BEM equations.

The developed method presents the ability to evaluate the cohesion forces without demand of internal interpolation or high computational cost inside the cohesive zone.

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