Intergranular crack propagation in brittle polycrystals using topological procedures and accurate finite element analyses

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To my parents
Acknowledgements

The road has been rather long — not to mention somewhat winding.

Journeying through the dim realm of research requires more than personal effort and firm conviction. The extending hands of the following people have been my recourse in encountering numerous periods of disillusionment and anxiety.

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I shall express my deepest gratitude to my parents without whose unconditional, selfless and perpetual supports I would not be even close to where I am now. Words would not be able to convey the true degree of my appreciations and thanks for their dedications and surpassing the paternal responsibilities.

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Ehsan Nasresfahani
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Chapter 1

Introduction

1.1 Crack path in polycrystals

Understanding the deformation and failure of polycrystalline aggregates is vital for further advance development of structural materials. A substantial body of research exists which addresses the crack propagation in heterogeneous materials such as ceramics as a structural material. Poor fracture resistant and brittle behavior of these materials not only lead to catastrophic failure but also have prevented the vast structural use of them.

On the other hand, reliability of brittle polycrystalline materials can be determined only by true understanding of failure behavior and hence, for instance its crack path. One of the important fields of Solid Mechanics is linked to fractography which is concerned with the study of surfaces produced by crack propagation. The work is motivated by a cutting edge observation that the crack path in a specific grain arrangement is insensitive to material properties (cohesive law parameters) \cite{36}. However, the effects of polycrystals microstructure (i.e. grains arrangement, mixed mode fracture at micro-level, relative energy of grain boundaries vs. energy across grain interior, etc.) on mode-I crack path is not fully explored yet.

The primary contribution of this project is aimed at finding any possible geometrical procedure to describe crack propagation. Crack paths based on accurate description of the stress field in a polycrystal compared to those based on the topology when considering intergranular crack propagation. It turns out that the material microstructure plays a crucial role in dictating the modes of fracture and consequently on the crack propagation and its crack path and grain boundaries are the most important micro-structural elements of polycrystals \cite{32}.

The project is divided into two main parts. In the first part, mode-I fracture and its characteristics for brittle polycrystals will be investigated. To this end, GFEM for polycrystals is used. Investigations will be continued in order to shed some more light on the fracture localization phenomena and optimized mesh refinement for crack propagation.

This work represents a model, as its second main part, in which a method will be described for crack path prediction. The crack path is defined just based on the topological procedure. The model will be validated by GFEM analyses.
1.2 Thesis Context and Overview

This thesis constitutes a part of ongoing research project at the Computational Mechanic group of Civil Engineering And Geoscience faculty, Delft University of Technology, The Netherlands. The project deals with better understanding of deformation and failure of brittle structural polycrystalline materials.

The thesis is outlined as follows:

Chapter 2 gives a brief Introduction to GFEM for polycrystals, the methodology for modeling and describing random polycrystalline microstructure, etc. In this chapter the result of a literature review will be presented.

In chapter 3, we will show that in the framework of linear elastic fracture mechanics (LEFM), the crack path growth is dominated by the Griffith energy criterion \[ 9 \]. Through this study and in line with studies of Shabir et al. \[ 36 \], it will be shown that mode-I crack path and fracture surface obtained from fracture of brittle polycrystalline materials are insensitive to material properties (cohesive law parameter), test setups and boundary conditions. The Generalized Finite Element Method (GFEM) for polycrystalline \[ 39 \] is used in order to find the crack paths and prove the above points.

In the last main chapter 4, we will investigate the localization of crack propagation at the micro-level. This study will show that arrangement of grain junctions are mainly governing for determination of mode-I crack path. As a result, a mesh refinement optimization for GFEM of polycrystalline will be developed which makes simulations extremely faster than old method. Further development of this investigation will show that only some parts of grain boundaries which are located in small area in the vicinity of crack tip, are playing a pivotal role in dictating the crack path and other grains can be ignored and replaced by a linear homogeneous material. Finally a topological model is constructed. The described model allows the crack path and hence surface roughness to be computed at a low cost. As it will be shown, due to the fact that the crack path is dictated solely by grain arrangement, the only input for this method is the material topology.

Chapter 5 (Conclusion) closes the thesis with a summary and discussion of the presented research topics, concluding with some suggestions for future research.
Chapter 2

Literature Study and Methodology

2.1 Analysis of Polycrystals by Generalized Finite Element Method

Quasi-static intergranular crack propagation in disordered (heterogeneous) materials such as ceramics has received wide attention. In order to simulate this brittle fracture, many approaches have been developed. Fracture and damage in polycrystals which have been modeled by various methods such as Lattice spring models \[13, 17\], fuse model \[42\], Boundary element method \[35\], etc. are expensive or mainly lacking enough quality. On the other hand, alternatively fracture phenomena can be modeled by use of cohesive surface within a Finite Element formulation in an arbitrary microstructure \[47\]. By taking advantage of FEM and cohesive zone models, a detailed description of the stress field, stress-strain curve and crack path can be reliably obtained. However, generation of satisfactory mesh is cumbersome and needs human intervention.

In this study, we determine the intergranular crack path with a Generalized Finite Element Method for polycrystals \[39\]. This method which is based on concept of partition of unity of finite element shape functions \[7, 15\], does not need a mesh generator to mimic the polycrystalline topology (Figure 2.1). The polycrystalline topology will be superimposed on a basic background mesh in order to obtain GFEM discretization. Noteworthy, the grain boundaries can cut the elements and grain junctions are arbitrarily located within elements. Accuracy of solution can be improved by automatic mesh refinement of boundaries, junctions and even grains interior. In this approach a simple assumption on the form of the displacement field has been used. Grain boundaries and junctions are described by means of discontinuous enrichment functions. This approach makes use of a displacement decomposition where \( \hat{u} \) is the standard displacement field.
and $\tilde{u}$ is the enrichment to $\hat{u}$ as following

$$u = \hat{u} + \sum_{i=1}^{N_0} \mathcal{H}_i \tilde{u}_i,$$

(2.1)

where the generalized $\mathcal{H}$ function is equal to 1 in grain $i$ and 0 otherwise. Note that this displacement decomposition is directly linked, via the constitutive equations, to the definition of discrete surfaces in correspondence of the boundary of each grain. These grains can communicate with each other by means of cohesive laws of any type. The model is then completed by employing any constitutive relationship describing the behavior within the grain. For more details see [39].

2.2 Test Setups

The geometry and boundary conditions of “Single-Edge-Notched Tension” or SENT specimen are shown by Figure 2.3. A uniform quasi-static tensile stress $\sigma$ is incrementally applied at both ends of notched specimen. The SENT setup which is employed in our simulations has a length of $L = 360 \mu m$ and width of $w = 240 \mu m$. The initial notch has length of $a = 120 \mu m$. According to [20] for $\frac{a}{w} = 0.5$ (crack length to specimen width ratio), ratio of beam length to width ($\frac{L}{w}$) should be at least 1.5 or more to be sure that there is no interference of boundary condition on the fracture procedure. The process zone which is the region in which grains and grain boundaries are represented explicitly, has dimensions of $170 \times 150 \mu m$ in order to contain
2.3 TEST SETUPS

80 grains. The outside of this zone represents homogeneous continuum which works as a loading device.

The second test setup is four point-bend test setup which is reported in Figure 2.4 in which two point loads $P$ are applied incrementally on a notched specimen, subjecting middle part of the beam pure bending $M = PL/5$. The process zone dimensions, crack length and width of the beam are the same with SENT setup, but length of the beam is $L = 2400 \mu m$. Effect of boundary conditions on process window is negligible, for $\frac{a}{W} = 0.5$ (crack length to specimen width ratio), if ratio of beam length to width $\frac{L}{W}$ exceeds 2 [19].

Both test setups are subjected to a quasi-static loading. The uniform tensile stress, $\sigma$ is incrementally applied on SENT specimen, while point loads, $P$ are applied on 4PB specimen. The failure of brittle polycrystals are characterized by the frequent snap-back behaviors which is associated with opening of each individual grain boundary. A dissipation-based arc-length method is employed [21] in order to trace the complex stress-strain path.
2.3 Topologies

Modeling of random polycrystalline microstructures gets lots of researchers attention. Several techniques have been used for modeling of two-dimensional grain geometries such as deterministic grain geometry with random material properties for grain boundaries (Harlow et al. [22]; Rice and Anderson [5]; Wilkinson [44]). In our study we take advantages of two different methods for modeling of random realizations explicitly. Polycrystalline micro-structures are modeled with help of two sets of different topology generation techniques. The first method is based on perturbation of a regular hexagonal geometry as it could be seen in Figure 2.5. In order to generate a random realization, each grain junction of a regular hexagonal topologies is randomly perturbed. The process window has dimensions of $165 \times 150 \, \mu m$ and contains 80 grains in which average grain length differs slightly for different realizations in range of $12 \, \mu m$.

![Figure 2.5: Three different realizations of 80 grains in the process zone. Figures above show a regular realization (a), medium perturbed realization (b) and fully perturbed realization (c) of one deterministic hexagonal geometry.](image1)

The second technique is Centroidal Voronoi Tessellation (CVT). It is a special type of Voronoi Tessellation whose generating point of each cell is its centroid. In our simulations—with help of our developed code—we generate hundreds of random Centroidal Voronoi tessellations. Figure 2.6 shows some example of CVT’s. It should be noted that, in the same size of process window ($165 \times 150 \, \mu m$), 106 grains have been generated with average grain boundary length of $11.5 \sim 12 \, \mu m$.

![Figure 2.6: Three example of different random Centroidal Voronoi tessellations in the process zone.](image2)
2.6 RANDOMNESS PARAMETER

2.4 Randomness parameter

In order to identify the randomness of grain arrangement, an empirical dimensionless randomness parameter $\bar{\rho}$ will be used [30]. The minimum value of this parameter is obtained for a regular hexagonal topology which is equal to 0.289. $\bar{\rho}$ is the average randomness over the whole system of grains where for each grain cell

$$\rho = \frac{1}{K A_{G}} \sum_{k=1}^{K} L^{(k)^2} \left[ 1 + \sin \left( 2\psi^{(k)} \right) \right]$$

(2.2)

is a geometrical parameter at the grain level which is defined in Figure 2.7. In the above formula $K$ is the number of grain boundary facets, $A_{G}$ is the grain area, $L^{(k)}$ is the part of vector $L^{(k)}$ within the grain area adjacent to facet $k$ and $\psi^{(k)}$ is the angle between the normal $n^{(n)}$ to the facet $k$ and $L^{(k)}$, see Figure 2.7

![Figure 2.7: Definition of quantity $\rho$ (adapted from [30])](image)

2.5 Bulk behavior

The models are constructed such that they are representative of an average polycrystalline alumina, $\text{Al}_2\text{O}_3$. According to observations by [31], grain boundaries of polycrystalline alumina compared to grain interiors have low interfacial energies and also different atomic structures. Spychalski et al. [32] proved that crack path becomes insensitive to relative energy of fracture along grain boundaries when there is less than 60% of the fracture energy along grain boundaries compared across grain interiors. Molinari et al. [26, 43] observed that elastic anisotropy of polycrystalline alumina does not have a considerable effect on an intergranular fracture. Based on above mentioned, we assume an intergranular crack propagation in our simulations.

In this study, regarding to the behavior of brittle polycrystalline aggregates, several general assumption are made, namely:

- The crack remains intergranular, i.e. the crack only propagates along grain boundaries;
- There is neither crack branching nor crack bridging; and
- The plain strain analysis will be performed under small scale strain assumption.
2.6 Cohesive law for grains boundary behavior

In this study, the only non-linearity in the materials is defined by means of Xu-Needleman cohesive law \[45\]. Cohesive model describes the cohesive force along grain boundaries when the grains are being pulled apart. Therefore cohesive zone boundaries which do not have any physical material are put alongside of grain boundaries as shown in Figure 2.8. Grain boundaries will face traction in normal and tangential directions in a two dimensional system.

There are variety of descriptions for traction-separation (Chandra et al. \[12\]) but they all explain the same global behavior. Xu-Needleman is an exponential model to describe traction-separation in both normal and tangential directions as the following:

\[
T_n = \frac{\phi_n}{\delta_n} \left( -\frac{\Delta_n}{\delta_n} \right) \left\{ \frac{\Delta_n}{\delta_n} \exp \left( -\frac{\Delta_n^2}{\delta_n^2} \right) + \frac{1}{r-1} \left[ 1 - \exp \left( -\frac{\Delta_t^2}{\delta_t^2} \right) \right] \left[ r - \frac{\Delta_n}{\delta_n} \right] \right\} \tag{2.3}
\]

and

\[
T_t = 2 \left( \frac{\phi_t \Delta_t}{\delta_t^2} \right) \left\{ q + \frac{r-q}{r-1} \frac{\Delta_n}{\delta_n} \right\} \exp \left( -\frac{\Delta_n}{\delta_n} \right) \exp \left( -\frac{\Delta_t^2}{\delta_t^2} \right). \tag{2.4}
\]

In the above equations, \( \phi_n \) and \( \phi_t \) are the work of normal and tangential separation( area under normal traction-separation curve and shear traction curve), \( \Delta_n \) and \( \Delta_t \) are the normal and tangential openinng, while \( \delta_n \) and \( \delta_t \) are respectively characteristic separations, in which \( T_n(\delta_n) = \sigma_{\text{max}} \) and \( T_t(\delta_t / \sqrt{2}) = \tau_{\text{max}} \). \( \sigma_{\text{max}} \) and \( \tau_{\text{max}} \) represent the cohesive strength in normal and tangential directions. Furthermore, \( q = \phi_t / \phi_n \) and \( r = \Delta_t^* / \delta_n \) are coupling parameters where \( \Delta_t^* \) is normal opening after a complete shear separation at \( T_n = 0 \). \( \Delta_n / \delta_n \) and \( \Delta_t / \delta_t \) are dimensionless normal and tangential openings while \( T_n / \sigma_{\text{max}} \) and \( T_t / \tau_{\text{max}} \) represent the dimensionless traction. Figures 2.9 and 2.10 illustrate normalized traction curve for uncoupled normal separation and shear separation. Normal traction-separation graph clearly shows that during crack propagation, as grain boundary is opening, the traction increases until that its maximum value \( (\sigma_{\text{max}}) \) reaches at characteristic opening \( (\delta_n) \). Then, subsequently the traction will drop to zero until the time that cohesive boundary no longer has any stiffness.

In this numerical simulation, a crack will grow when crack openings \( \Delta_n \) or \( \Delta_t \) are bigger than corresponding characteristic openings \( \delta_n \) or \( \delta_t \). Characteristic openings \( \delta_n \) and \( \delta_t \) are set to be equal and for any values of cohesive strength \( \sigma_{\text{max}} \) and fracture energy \( \phi_n = G_{\text{Ic}} \), they can be computed by Xu and Needleman relations \[45\]:

\[
\phi_n = \sigma_{\text{max}} \exp (1) \delta_n, \quad \phi_t = \tau_{\text{max}} \sqrt{\frac{\exp (1)}{2}} \delta_t. \tag{2.5}
\]
Bosch et al. [41] found out that normal and tangential coupling is only well-described by taking the value of $q$ equal to one. This is shown, also by works on mesoscopic failure analysis of alumina [28, 46]. By keeping $q = 1$, it could be observed in 2.3 and 2.4 that the value $r$ no longer has any influence in the cohesive law.

Xu-Needleman model [45] accepts a reversible cohesive zone. Zavattieri et al. [46] considered secant unloading in mesoscopic failure of polycrystalline materials. Shabir et al. [36] performed numerical analysis, using both reversible behavior and Secant unloading, compared the material response and showed that there is an insignificant difference in some part of loading/reloading branches of load-displacement curve. In line with their studies, Secant unloading has been considered in the numerical analysis of polycrystalline aggregates.

By the end of this section, it should be clear that the only important parameters for cohesive law are cohesive strength $\sigma_{\text{max}}$ and Fracture energy $G_{\text{IC}}$ (Griffith criterion) where the shape of cohesive law does not matter [4, 40].

### 2.7 Length Scale

In the simulation there are some characteristic lengths employed. First of all $L$ employed as macroscopic scale which is equal to specimen length. $l_e$ is the longest side of mesh element (Figure 2.11) and $l_z$ is the characteristic cohesive length over which constitutive cohesive relations play a role. For potential-based cohesive law this parameter at zero velocity is approximated as [16]

$$l_z = \frac{9\pi E}{32 \left(1 - \nu^2\right)} \frac{G_{\text{IC}}}{\sigma_{\text{max}}^2}$$  \hspace{1cm} (2.6)

where $G_{\text{IC}}$ is the fracture toughness and $\sigma_{\text{max}}$ is the cohesive strength and hold for plain strain analysis.

To resolve the cohesive zone truly -which is considered as discontinuity in GFEM- each discontinuity segment length $l_d$ should be at least smaller than cohesive length as it can be seen in Figure 2.11. In the literature, one can find various suggestions for the minimum number of elements varying from two elements to fifteen [11, 16, 23, 29, 35]. In line with mesh refinement studies by Shabir et al. [36], we use a mesh size such that length of the longest side of all the elements intersected by grain boundaries $l_e \leq \min(l_z/3, l_{gb}/2)$ with at least four intersecting
elements along each grain boundary [36]. In the previous inequality $l_{gb}$ is the average grain boundary length.

2.8 Britteness

In the literature, it is common to characterize material response by a brittleness index. For ceramic material such as concrete, Hillerborg et al. [24] has defined a ratio between fracture ligament length $b$ and cohesive length $l_z$ to describe the response of material. Carpinteri et al. [10, 11] proposed a closely related quantity. This quantity is structural-shape independent and thus it is not possible to define an absolute domain to use the advantages of LEFM. This problem was addressed by Bazant and Pfeiffer [8] who defined the structural shape independent brittleness parameter based on microstructure of concrete (aggregate size).

The same procedure has been done for polycrystalline material. Abdel-Tawab and Rodin [3] proposed a brittleness parameter $GB$ as a ratio of grain diameter $d$ to the plastic radius $r_p$ ($GB = d/r_p$). Shabir et al. [37] developed this concept by taking advantage of cohesive law. They proposed a non-dimensional grain boundary brittleness number as

$$\beta_{GB} = \frac{l_{gb}}{l_z}$$  \hspace{1cm} (2.7)

where $l_{gb}$ is the average grain boundary lengths and $l_z$ is the cohesive length. In both brittleness parameters, the high values of the number indicates a brittle structural response such that a fully brittle material is defined by $\beta_{GB} = \infty$ where the plastic zone shrinks to a point.

2.9 Material parameters

The following material parameters are used in our simulations:

- **Mechanical properties**: as we mentioned before, all parameters are taken to be representative of $\mathrm{Al}_2\mathrm{O}_3$. Young’s modulus $E = 384.6$ GPa and Poisson’s ratio $\nu = 0.237$.

- **grains size**: in line with studies of Kraft and Molinari [26] and Zavattieri et al. [46], we have chosen an average grain size of 21 $\mu$m which corresponds to average grain boundary length $l_{gb} \approx 12\mu$m.
• **Micromechanical properties**: a broad range for values of grain boundary cohesive strength, $\sigma_{\text{max}}$ and critical fracture energy, $G_{\text{IC}}$ for polycrystals can be found on literature [26, 34, 46]. In our simulations we consider a broad range for cohesive strength, $\sigma_{\text{max}}$ between 0.6 and 3.0 Gpa and for $G_{\text{IC}}$ from 7.09 to 39.9 J/m$^2$.

Various sets of material parameters which will be employed in the fracture of polycrystals are listed in Table 2.1.

<table>
<thead>
<tr>
<th>$\beta_{gb}$</th>
<th>$K_{IC}$ [MPa√m]</th>
<th>$G_{IC}$ [J/m$^2$]</th>
<th>$\sigma_{\text{max}}$ [GPa]</th>
<th>$\delta_n$ [µm]</th>
<th>$l_0$ [µm]</th>
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<td>1.03</td>
</tr>
</tbody>
</table>

**Table 2.1**: Different sets of material properties used in our simulations
3.1 Introduction

3.1.1 The Stress at a crack tip

Different ways of loading a solid cause different crack types:

- **Mode-I crack** (Opening mode): tensile stress normal to crack opening gives rise to mode-I crack. See Figure 3.1(a)

- **Mode-II crack** (Sliding mode): shear stress working on plane of crack. See Figure 3.1(b)

- **Mode-III crack** (Tearing mode): caused by out of plane shear stress. See Figure 3.1(c)

Now, consider the example shown in Figure 3.2. In the sheet with an initial crack length $a$ under mode-I of loading, the stress ahead of crack tip with help of linear elastic fracture mechanics (LEFM) can be expressed as

$$\sigma_{ij} = \frac{K_1}{\sqrt{2\pi r}} f_{ij}(\theta).$$  \hspace{1cm} (3.1)

![Figure 3.1: The three modes of loading, (a) Mode-I crack or tensile-mode crack; (b) mode-II or sliding crack (shear mode crack); (c) mode-III or tearing crack (shear-mode crack)](image)
With respect to polar coordinates, at distance $r$ and angle $\theta$ from the crack plane, $\sigma_{ij}$ are the Cauchy stresses acting on element $dxdy$ and $f_{ij}(\theta)$ are known as universal functions of $\theta$. All external boundary conditions, shape of body, etc are reflected in $K_1$ known as “mode-I stress intensity factor”. Indeed, it seems that the entire stress field at crack tip is described by means of $K_1$ in a linear elastic material.

As it can be seen from eq. 3.1, infinite stress can be expected in immediate vicinity of the crack tip. However, it is not the case in reality: linear elasticity breaks down, irreversible and plastic deformations take place in an area called “plastic zone” or “process zone”, which avoid large stresses and keep them finite. In other words, the $\frac{1}{\sqrt{r}}$ singular field is invalid in the fracture plastic zone, where inelasticity prevails or when its size is not small enough in comparison with external boundary. This invalidity (square-root singularity of $r$) is a universal fact independent of external boundary conditions. Moreover, far away from the crack tip, on the scale compared to crack length $a$, eq. 3.1 gives an invalid result. This area is working as loading device and depends on external boundary.

Equation 3.1 should hold for every arbitrary body such as an infinite plate with a central crack $2a$ under a stress $\sigma$, known as Griffith crack [18]. Stress intensity factor can be derived in form of

$$K_1 = \sigma_{yy} \sqrt{\pi a}$$  \hspace{1cm} (3.2)

with help of linearity and dimensional considerations. For a finite size plate, stress intensity factor is

$$K_1 = Y_1(a/L)\sigma \sqrt{a}$$  \hspace{1cm} (3.3)

where $L$ is the generalized size parameter, $\sigma$ is the remote stress and $Y_1(a/L)$ is the dimensionless number(shape factor) depending on load distribution and body shape.

### 3.1.2 $K$ dominance

The size of plastic zone $r_p$ at the crack tip could be derived using FEM and for case of plane strain is approximately

$$r_p = \frac{1}{3\pi} \left( \frac{K_1}{\sigma_{yy}} \right)^2$$  \hspace{1cm} (3.4)
and for plane stress is given by

\[ r_p = \frac{1}{\pi} \left( \frac{K_1}{\sigma_{ys}} \right)^2. \]  

(3.5)

Here \( \sigma_{ys} \) is the yield strength of material and \( r_p \) is size of zone around the crack tip which inelastic deformations occur. The shape of plastic zone is illustrated by Figure 3.3 for both plane stress and plane strain for ductile material. For the case of polycrystalline materials, Figure 3.3(b) shows contours of equivalent stresses at the crack tip for plane stress obtained from generalized finite element method.

![Figure 3.3: (a) Shape of plastic zone around crack tip for plane stress and plane strain cases; (b) Scaled plastic zone around crack tip obtained from our GFEM analysis.](image)

As discussed earlier, very close to the crack tip and also far away, \( \sigma_{ij} \) is not well-approximated by equation 3.1. Thus, \( K \) solution is only valid in a region with dimensions of \( r > r_p \) and \( r \ll a \), which is called \( K \)-dominant zone or \( K \)-annulus. If the size of plastic zone is small relative to \( a \) (crack length) and \( K \)-dominant zone is much smaller than specimen size, mode-I solution of LEFM should hold for \( K \)-annulus and indeed, \( K \)-field is valid in this region. This is known as “small scale yielding” (SSY) assumption.

Rice [33] explains the SSY assumption as:

The utility of elastic stress analysis lies in the similarity of near crack tip stress distributions for all configurations. Presuming deviations from linearity to occur only over a region that is small compared to geometrical dimensions (small scale yielding), the elastic stress-intensity factor controls the local deformation field. This is in the sense that two bodies with cracks of different size and with different manners of load application, but which are otherwise identical, will have identical near crack tip deformation fields if the stress intensity factors are equal. Thus, the stress intensity factor uniquely characterizes the load sensed at the crack tip in situations of small scale yielding, and criteria governing crack extension for a given local load rate, temperature, environments, sheet thickness (where plane stress fracture modes are possible) and history of prior deformation may be expressed in terms of stress intensity factors.

Further details and conditions of this assumption will be discussed in the next section.
**3.1.3 Fracture Criteria**

As it was discussed in section 3.1, boundary conditions reflect in the stress intensity factor $K_I$. For instance, with increasing the load, $K_I$ will be increased until the time that material can not undergo the load and fracture starts. Thus, this characteristic resistance to fracture or so called “fracture toughness” $K_{IC}$ could be a criterion for propagation of an exciting flaw (crack) if the applied load is such that

$$K_I \geq K_{IC},$$  \hspace{1cm} (3.6)

then the crack will propagate. Indeed, “fracture toughness” is an indication for amount of stress which crack needs to propagate.

This criterion is known as “stress based” criterion however, it is possible to develop an “energy based” criterion. Griffith [18] states that to propagate a crack, available energy dissipated per unit area of new fracture surface should be more than a required amount of energy

$$G \geq G_{IC},$$  \hspace{1cm} (3.7)

where $G$ is “energy release rate” which is provided from external loading and strain energy stored in material and $G_{IC}$ is toughness of material or a minimum required amount of energy needed for crack propagation. Energy dissipation includes e.g. surface energy in all materials, energy for plastic deformation at the crack tip for metals, micro-cracking for ceramics, etc.

By taking advantages of SSY assumption, stress criterion and energy criterion are fulfilled simultaneously and it could be shown that $G$ scales with $K_I$ as

$$G = \frac{K_I^2}{E} \quad \text{and} \quad G_{IC} = \frac{K_{IC}^2}{E} \quad (3.8)$$

in case of plane stress and

$$G = (1 - \nu^2) \frac{K_I^2}{E} \quad \text{and} \quad G_{IC} = (1 - \nu^2) \frac{K_{IC}^2}{E} \quad (3.9)$$

in plane strain situation, where $\nu$ is “Poisson’s ratio”.

**3.1.4 Goals of this chapter**

The goal of this study is considering the effect of boundary conditions on failure of brittle polycrystalline materials and specially on its intergranular crack path. As it is discussed in chapter 2, fracture occurs when crack starts growing along grains boundaries. In this brittle intergranular fracture, dissipation of energy due to plastic deformation is negligible in comparison with surface energy. Thus, Griffith criterion still holds and in this case, if the criteria for mode-I of fracture is met, it could be concluded that the crack path is independent of the boundary conditions.

An important point in this study is to compare GFEM crack path with a pure geometrical model in which the crack path obtained based on the topological procedure. The main aim of this chapter is to show that effects of boundary condition on the mode-I fracture can be excluded. It will be shown that under mode-I loading, the crack path is independent of the loading conditions, specimen size, different mode-I test setups and material properties. This will be proved by numerical analyses using generalized finite element method (GFEM) for hundreds of different realizations considering different topologies and with different test setups using different material properties.
3.2 Mode-I of fracture and its characteristics in intergranular fracture

In this section, the necessary conditions for mode-I fracture of perfectly brittle polycrystalline will be discussed. It is noted in section 3.1.2 that three different zones around crack tip could be identified. The characteristics of each zone for brittle polycrystalline such as alumina is explained in the following.

- **Process zone**: Very close to the crack tip in which $K$-filed is invalid. In this region the physical field strongly depends on elastic constants and crystallographic orientations of individual grains [Abdel-Tawab] [2]. The size of plastic zone is dependent on fracture toughness and yield strength. Generally, the more ductile material, the bigger the plastic zone. This will be defined in our model with help of cohesive law in which low values of cohesive length $l_z$ is related to ductile material by means of high $\sigma_{\text{max}}$ and low $G_{\text{inc}}$. In ceramics at ambient temperature it is assumed that plastic zone ahead of crack tip is much smaller than grain sizes [27].

- **$K$-annulus**: This region should contain enough grains of ceramic in order to be treated as homogeneous and isotropic material and also much smaller than specimen size. According to [1], this condition is realized in specimens whose minimum dimension is:

$$a, B, W/2 \geq L_y = 2.5\left(\frac{K_{\text{inc}}}{\sigma_y}\right)^2$$

(3.10)

i.e. each specimen dimension should be at least 25 times larger than $r_p$ if $r_p \approx 0.1\left(\frac{K_{\text{inc}}}{\sigma_y}\right)^2$ in plane strain situation. This restriction is even more crucial in case of plane strain as the body should be thick enough for triaxial stress state.

- **External boundary**: External boundary should be far away from crack tip (comparable and larger than crack length, $a$). It should be noted that load application should be in such a way that local stress due to load application do not interfere with process window as the crack propagates. It has been investigated by doing a mode-I three point-bend test (Figure 3.4) that due to application of point load at the mid-span, high local stress could be expected in this region which can affect the fracture procedure and naturally the crack path. Figure 3.5 shows the result for analysis of a three point-bend specimen using GFEM and contours of equivalent stress at the crack tip and load application point. High amount of stress can be seen in vicinity of load application point, which could even causes crack growth in that region. Although 3PB test is one of the popular mode-I tests, because of its unreliable results is not employed in our simulations.

$K$-dominance is guaranteed under specific conditions and limitations. It should be noted that as it is mentioned in section 2.6, in our model the only non-linearity in material response defines by means of cohesive law across the grain boundaries. Thus, there is no plastic deformation or non-linearity inside the grains. it could be concluded that for a brittle polycrystalline material two restrictions should be met:

1. process zone at the crack tip should remain small during the test.
2. the specimen should be large enough to contain sufficient number of grains

These requirements are necessary in order to promote mode-I loading, but only at specimen size order. There are more considerations at the grain boundary level to control the microscopic mode-I failure. In a brittle polycrystalline aggregate with a stationary crack, asymptotic linear
Figure 3.4: Three point-bend specimen

Figure 3.5: The point load effects on the plastic zone and crack propagation procedure. Equivalent stress contour obtained via GFE analysis of 3PB specimen.
stress field at the crack tip could be characterized by the stress intensity factor $K_I$. If we assume a mode-I loading at micro-level, the grain boundary should merely open in the normal direction (no energy consumption in tangential direction). However, intergranular failure of brittle polycrystalline aggregates is quite different rather than the situation for pure mode-I. In this case, in different test setups a crack starts to propagate from an initial notch tip under a quasi-static load. This means there is no stationary crack and also the stress field is changing during the crack propagation. Thus, in our simulation the relative contribution of dissipated energy in normal direction should be checked in order to be sure that mode-I fracture is happening along the grains. It will be shown by results of numerical analyses in the next section (3.3).

Once all conditions above hold, one can assume pure mode-I loading i.e. $K_{Ic}$ is a material parameter which is not sensitive to specimen details \[3\]. In other words fracture process is not controlled by test setup if above conditions hold. Furthermore, it can be concluded that the shape of process window is insensitive to specimen geometry or loading conditions. Thus, every test setup for mode-I loading should result in an identical crack path for each of realizations.

### 3.3 Results

In this section, it will be proved that mode-I crack path in brittle polycrystalline is independent of test setups. For this aim, hundreds of different realizations are analyzed using GFEM in different topologies with two test setups: SENT and 4PB.

#### 3.3.1 Results and Discussion

According to our hypothesis, the crack path should remain identical in every mode-I test setup. To prove this fact, we have performed more than 2000 of GFEM analyses for both SENT and 4PB specimens and compared the crack path from the same realization but different mode-I test setups (SENT and 4PB). This comparison has been done twice, for both hexagonal and CVT Topologies. In each phase, series of CVT or Hexagonal realizations have been analyzed and the crack path have been studied.

Various series of random hexagonal realizations have been sorted in the descending order with respect to the randomness of grains. The randomness parameter explained in section 2.4. Special codes and scripts have been developed in order to systematize the failure simulation of polycrystals. After performing analyses for both SENT and 4PB specimens, from a set of 100 realizations, we found 82 identical crack paths. One example of this analyses will be illustrated in the Figure 3.6. As it can be seen from the Figures, the obtained crack paths in both test setups are identical.

The remaining 18 cases have been studied extensively, to find out why the crack paths are different. In majority of cases, the crack paths are partially overlapped and at a junction, one of the crack paths changes its direction. This is shown in the Figure 3.7.

As it is mentioned before, there are several restrictions for mode-I loading tests. The specimen dimensions are one of the restrictions which one needs to be sure that there is no interference of boundary conditions on the process window which is known as size effect. On the other hand, for the most convenient and fastest simulations, the minimum allowed dimensions have been used. Therefore, for some of the cases, we performed analyses with double sized specimen but the same process window and we found the same results. Analyses of specific realizations with different specimen sizes clearly show that if the size effect limitation meet, the crack path for a specific realization is unique regardless of how big is the specimen.

The other possible problem could be the problem of equal angle or Y-like configuration (Figure 3.8), as it has been noted also by Shabir et al. \[36\]. In these cases, when the crack tip reaches
at a junction, there are two grain boundaries with the same angles in which numerically there are the same solutions for both of them unless a superfine mesh density and also grain interior refinement are considered. Therefore these are cases which it is cumbersome to obtain reliable results. Shabir et al. [36] proposed a method to solve this problem. For this aim, a special code has been developed in order to find the Y-configurations in the realizations and perturb the junction randomly. The grains geometry which was shown in Figure 3.7 has been modified and can be seen in the Figure 3.9. Note that After perturbation, analysis of both specimens will result in an identical crack path 3.9(c). However, it is hard to state that which test setups is preferable in the scene that it gives more reliable results.

It is important to note that regular and semi-regular hexagonal geometries because of high amount Y-like configurations are the most difficult cases to analyze. The results of analyses also prove this fact as the most non-identical crack paths can be seen in regular hexagonal geometries. Also the real polycrystalline microstructure such as alumina microstructure is more random and could have more than six sides. That is why that Centroidal Voronoi Tessellations(CVT) are employed in modeling of polycrystalline aggregates.

One of the big advantages of CVT’s is that tessellations are in such a way that in principle the equal angle and Y-like configurations rarely happen. For instance, considering SENT and 4PB test setups, analyses of 89 out of 100 realizations resulted in identical crack paths 3.10. In the remaining 11 cases, Y-like configurations can be clearly seen. This problem solved using the previous technique. Results are reported in the Figure 3.11.

So far, it has been shown by all the results above that for every realization of brittle polycrystalline aggregates, the crack paths obtained from every mode-I of loading test setups is unique.

Figure 3.6: Crack paths obtained from analysis of 4PB and SENT specimens: (a) original grains arrangement. Thick black line indicates traction-free notch; (b) Pink line indicates crack path obtained from 4PB specimen; (c) blue line indicates crack path obtained from SENT specimen; (d) superimposed crack paths.
3.3 RESULTS

Figure 3.7: Non-identical Crack paths obtained from same realization in analysis of different test setups. (a) original grain arrangement; (b) and (c) crack paths obtained from analysis of SENT and 4PB specimens; (d) superimposed crack paths.

Figure 3.8: Y-like configuration causes different crack paths

and identical. These results strongly proved mode-I cracking at grain boundary level, also (see 3.2). According to the result of GFEM, relative contribution of energy dissipated in tangential direction along the grain boundaries is between 8 and 12 percent for a set of hundred realization in 4PB specimen and 10 and 14 percent for the same realizations in SENT specimens. Respectively, contribution of normal separation is between 88 and 92 % for 4PB specimen and 86 and 90 % for SENT specimen which is shown in Figure 3.12 for SENT and 4PB analyses of 100 hexagonal realizations with different randomnesses. The results show practically the same relative contribution of mode-I fracture energy which also prove a mode-I dominated cracking behavior.
Figure 3.9: Influence of Y-configuration on the crack path. (a) Perturbed realization (black lines) vs. original grain geometry 3.7; (b) the modified grain geometry; (c) identical crack paths obtained from analysis of modified geometry in different specimens.

Figure 3.10: One example of identical crack paths obtained via analysis of CVT realizations. (a) Original grain arrangement; (b) superimposed crack paths obtained via analysis of 4PB and SENT specimens.
Figure 3.11: Equal angle configuration has caused different crack paths obtained via analysis of CVT realizations. (a) Original grain arrangement; (b) crack path obtained from SENT specimen analysis; (c) crack path obtained from 4PB specimen analysis; (d) superimposed crack paths obtained via analysis of 4PB and SENT specimens; (e) perturbed realization (black lines) vs. original grain geometry shown in (a) (blue lines); (f) the modified grain geometry; (g) identical crack paths obtained from analysis of different specimens.
Figure 3.12: Relative contribution of normal separation for 100 hexagonal realizations in different test setups.
3.4 Summary and conclusion

Intergranular fracture of brittle polycrystalline aggregates have been studied using different type of topologies and test setups. Brittle polycrystalline aggregates have been modeled using Centroidal Voronoi tessellations and also various random realizations of 80 regular hexagonal grains. Crack propagation starts under quasi-static loading and the crack paths obtained from different test setups have been compared. It has been observed in this study that for every mode-I test setup, for a specific material properties which is defined by means of cohesive law, intergranular crack path is insensitive to all boundary conditions and specimen size. Shabir et al. [36] have discovered that with special refinement rules, the intergranular crack path is insensitive to cohesive law parameters such as maximum cohesive strength or fracture toughness. Merging the result of their work with our investigations could be resulted in the following: mode-I intergranular cracking of brittle polycrystalline aggregates solely depends on its microstructure.

Some other findings of this study will be stated as following:

1. Y-like configurations in the grains arrangement should be avoided as these are fallible and uncertain cases in which it is cumbersome to find a proper result. It observed that after perturbing the Y-like Junctions, crack paths obtained from every mode-I test setup are reliably identical.

2. Studies have been performed to find proper mode-I test setups. With help of our investigations, we found an appropriate specimen and initial traction-free notch sizes in which minimum allowed dimensions are used for modeling of mode-I test setups. The results of our simulations strongly showed a mode-I failure not only at specimen-size level but also at grain-boundary level. It has been shown that relative energy dissipation for opening the grains in a normal direction(opening-mode or mode-I crack) is somewhat between 86 and 92 percent for 200 different realizations obtained from different test setups.

Although we have simulated the crack propagation of polycrystalline aggregates by considering Hexagonal and CVT topologies and using limited number of grains inside the process window(between 80 and 110), we expect the conclusions above to be valid for intergranular fracture of any brittle polycrystalline aggregates.
Chapter 4

Localization of crack propagation

In the previous chapter, it became clear that crack path obtained from fracture of brittle polycrystalline materials is neither sensitive to material properties (cohesive law parameters) nor to boundary conditions. It was shown that the crack path is solely dependent on grain geometry. However, it is still unclear to us that how many grains around the crack path could play a role in the fracture.

4.1 Different randomness, same crack propagation procedure

For this aim, we tried to perturb the grains far from crack path in some of the realizations. As it could be seen in Figure 4.1, 80 percent of grains at right and left sides of process window have been perturbed several times with different offset lengths. At each step a new realization has been created which has different randomness parameter. It can be seen that the randomness parameter $\rho$ varies between 0.32 and 0.38 (note that $\rho$ is $\sim 0.29$ for a regular hexagonal realization and $0.40$ for a highly randomized realization).

The same procedure has been done for 5 centroidal Voronoi tessellations and 4 more hexagonal realizations and two following observations are made:

- The crack path is not dependent on entire grains but just on some of them close to the crack path; and,
- The randomness parameter $\rho$ is not a good indicator for crack propagation. Indeed, it gives a global overview of geometry while the crack propagation is a local phenomena which needs a local indicator, also, to be described.

It could be summarized as following: Inter-granular crack propagation in brittle polycrystalline aggregates is dependent on grains arrangement merely in the small vicinity around crack tip.

4.2 Different Brittleness number

As the brittleness of material increases, the crack propagation getting more localized but still the crack path is identical. For the high values of brittleness number, Small Scale Yielding assumption (section 3.1.2) can be used. Employing SSY assumption means that large portion of specimen deforms elastically and only a plastic region around crack tip will undergo a plastic...
deformation. Thus LEFM can be used in $K$ dominant zone and nonlinearities will be limited to a small area.

To investigate geometrical effects on crack propagation, we modify our GFEM program such that cohesive law is only defined in a specific region around crack tip, so called “nonlinear window”, in which always nonlinear window is growing with crack growth, simultaneously, responsible for all nonlinearities in model as it is illustrated by Figure 4.2.

Two different hexagonal realizations and one centroidal Voronoi tessellation (shown by Figure 4.3), have been analyzed using ten different sets of material properties when nonlinearities have been confined only to nonlinear window with certain dimension (the same order of magnitude compared to average grain size). The minimum dimension of nonlinear window $a$ which allows us to finish the simulation and obtain the crack path is the matter of interest.

Results of this study have been summarized in table 4.1. First of all, The result verified, once again, that crack path in a specific realization is not dependent on material properties (cohesive law parameter) as it was shown by Shabir et al [36]. In each realization, all ten crack paths obtained from different material properties were identical. Second, the results strongly prove that crack localization is merely controlled by brittleness parameter. It can be stated that for realizations with the same average aggregate size $l_{gb}$, the localization only depends on cohesive length $l_z$.

From theoretical point of view and also according to the numerical results, high values of $\beta_{gb}$ allow us to use a smaller nonlinear window. It is obvious by these results that minimum allowable dimension of nonlinear window $a$ is much smaller than specimen dimension ($a \ll L$) and even further it is smaller than an average grain boundary length ($a \ll l_{gb}$). According to
4.2 DIFFERENT BRITTLINESS NUMBER

Figure 4.2: Definition of nonlinear window size, a based on the crack tip.

(a)  
(b)  
(c)  

Figure 4.3: Identical crack paths obtained in (a) highly-randomized hexagonal realization ($\rho = 0.40$); (b) randomized hexagonal topology ($\rho = 0.36$); (c) Voronoi topology ($\rho = 0.40$).

SSY assumption, by taking advantage of metal plasticity and use it for fracture of polycrystals, the size of plastic zone ($r_p$) around crack tip could be estimated for a plain strain condition (see section 3.1.2)

$$r_p = \frac{1}{3\pi} \left( \frac{K_{lc}}{\sigma_{max}} \right)^2.$$  \hspace{1cm} (4.1)

Despite the fact that there is no plasticity around crack tip like metallic materials and nonlinearities defined only along grains boundaries, diffusion of this nonlinearity could be estimated by borrowing this concept. The theoretical plastic radios and the the minimum allowable size of nonlinear window $a$ are compared in the table 4.2. Although the results show relatively big difference between two dimensions, we expect to have almost the same sizes by super-refinement of mesh which is not possible at the time being.

The force displacement curves are given in Figure 4.4. It has been observed that using a very small area of nonlinearity around the crack tip does not change the structural response of material (Figure 4.5). It has been shown by Figure 4.4, once again, that crack propagation in brittle polycrystalline material is only controlled by fracture energy. According to Shabir et al. [37], for brittleness number two and higher, load-displacement curves can be univocally scaled using the following relations:

$$F = \frac{K_{lc}}{K_{lc}} \bar{F} \quad \text{and} \quad \Delta = \frac{K_{lc}}{K_{lc}} \bar{\Delta}$$  \hspace{1cm} (4.2)

such that for a specimen with fracture toughness $K_{lc}$ every point $(F, \Delta)$ on load displacement
curve can be scaled from every point $(\bar{F}, \bar{\Delta})$ of the master curve related to the same specimen with fracture toughness $K_{IC}$.

Traction-separation curves (normal components) are reported in Figure 4.6. It could be intelligibly observed in Figures 4.6 and 4.4 that the stress localization, is not proportional by peak load nor on Traction force and characteristic opening. Here, in line with Shabir et al. [37] investigation, we verified that stress localization in brittle polycrystalline aggregates is only characterized by brittleness number, i.e. cohesive length.

For resolving the cohesive law, we have to provide enough elements inside the cohesive zone in which each part of any grain boundary inside the nonlinear window has at least 10 intersecting elements. Using inadequate elements in the nonlinear window can result in obtaining a wrong crack path or missing some parts of loading/unloading of force-displacement curve. This phenomenon observed specially in Y-like configuration when at the junction, one of boundaries opens first and then should be unloaded, so the other boundary will be opened. Lack of mesh refinement may affect the process, thus simulation software may not find a solution in such a case. One of the cases reported in Figure 4.7, where at a junction the opened boundary which was supposed to be closed, can not unload and then as the simulation software can not find a solution, it increases the load and then it stops.

Moreover, there is a huge difference for computational costs of crack propagation analysis in the same realization with different cohesive law parameters. As it can be seen in the table 4.3, by increasing the brittleness, there is a need for finer mesh, which results in more degrees of freedom and consequently takes more time.

In summary, we have shown in this section that brittle fracture of polycrystals is a localized procedure in which we can reduce the the nonlinearities to close vicinity of crack tip.

### 4.3 Sequential Analysis

Results of previous section clearly showed that crack formation is mainly controlled at micro-level. It turned out by the last results that for forming a crack in brittle polycrystals only a small area around the crack tip is crucial. In this section we are going to show that not only the nonlinearities, but also mesh-refinement can be confined to the close vicinity of crack tip.
4.3 Optimization of Mesh-refinement

As it is already discussed in section 2.7, studies by Shabir et al. [36] suggest to use a mesh size such that length of longest side of all the elements intersected by grain boundaries $l_e \leq \min(l_z/3, \frac{t_{gb}}{2})$, with at least four intersecting elements along each grain boundary for the whole process window. However, as the most of nonlinearities are arising around the crack tip, it could be concluded that there is no need to the suggested mesh-refinement in the entire process window (fig. 4.8(a)) but only to a mesh-refinement around the crack tip (fig. 4.8(b)). Nonlinearities are happening alongside the grain boundaries in a small vicinity surrounding the crack tip. Adequate refinement level in this area is necessary to resolve the cohesive law truly. For the elsewhere, As the LEFM holds, four intersecting elements along each grain boundary can insure the quality of numerical analysis.

Therefore, a new code has been developed that allows the simulation to automatically have a mesh-refinement just around the crack tip. The background mesh always will be the same and mesh-refinement is updated as the crack grows (area around crack tip refined, elsewhere de-refined). Thus, the number of degrees of freedom will be decreased enormously as well as the computation costs and consequently we are able to find the crack path faster. Figure 4.9 depicts an example how this code works.

This code has been examined for different geometries, different sets of materials and variety of specimen sizes and the following messages have been observed:

- Crack path is not affected if the size of mesh-refinement window is chosen appropriately;

<table>
<thead>
<tr>
<th>$\beta_{gb}$</th>
<th>$r_p [\mu m]$</th>
<th>$a [\mu m]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.05</td>
<td>1.38</td>
<td>15</td>
</tr>
<tr>
<td>1.77</td>
<td>0.818</td>
<td>11</td>
</tr>
<tr>
<td>1.95</td>
<td>0.736</td>
<td>10.2</td>
</tr>
<tr>
<td>2.28</td>
<td>0.631</td>
<td>9.6</td>
</tr>
<tr>
<td>2.31</td>
<td>0.625</td>
<td>8.8</td>
</tr>
<tr>
<td>3.1</td>
<td>0.456</td>
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<td>0.355</td>
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</tr>
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<td>0.230</td>
<td>4</td>
</tr>
<tr>
<td>11.6</td>
<td>0.124</td>
<td>4</td>
</tr>
</tbody>
</table>

Table 4.2: Theoretical Plastic Radii vs. minimum allowable dimension of nonlinear window

<table>
<thead>
<tr>
<th>$\beta_{gb}$</th>
<th>Simulation time [hr]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.77</td>
<td>0.9</td>
</tr>
<tr>
<td>3.1</td>
<td>2.45</td>
</tr>
<tr>
<td>6</td>
<td>24.5</td>
</tr>
<tr>
<td>12</td>
<td>45</td>
</tr>
</tbody>
</table>

Table 4.3: Simulation time for analyses of same realization with different material properties showed in Figure 4.3(a). Each simulation has been run on an Intel 2916 MHz CPU.
4.3.2 Effect of participant grains on the fracture

Furthermore, based on above results and the results of section 4.2 we concluded that for the crack propagation only a small system of grains around the crack tip is governing and far grains from the crack tip can be trimmed and ignored by converting to homogeneous elastic material ($K -$ dominance zone). As it is illustrated by Figure 4.11, one full analysis is divided to smaller simulations and in each of the divided simulations only the local grains and local mesh-refinement around the crack tip is considered (sequential polycrystalline analysis by Shabir et al. [38]). In each new step, the last obtained crack path is considered as traction-free crack line. Therefore, at every step, there are limited number of grains around the crack tip in which they are highly refined. Thus in this sequential analysis, due to less number of degrees of freedom, we have a fast analysis in which the quality of numerical analysis is ensured by high local mesh-refinement.

All of this procedure is automated using the new developed code. Using this optimized method for mesh refinement and use of local grains and ignoring other ones in fracture of brittle polycrystals, have extremely decreased the time of computation. Table 4.4 shows the computation time for different material properties using different methods of analysis.

As it can be seen from this table the computation time for previous method (employing all the grains through entire process window) is increasing as the brittleness increases. This is of course due to the fact that for more brittle material there is a need to finer mesh in order to resolve the cohesive properties of grain boundaries and Naturally number of degrees of freedom is increased.
4.3 SEQUENTIAL ANALYSIS

Figure 4.5: Same structural response obtained via different non linear windows sizes. Analysis performed on realization given by Figure 4.3(b) with $\sigma_{max} = 890$[Mpa] and $K_{IC} = 2.165$.

Table 4.4: Comparison between simulation times for two methods of analysis and various material properties. Each simulation has been run on an Intel 2916 MHz CPU.

As we showed in this section, there is no need to mesh-refinement everywhere and also as the material is getting more brittle the diffusion of nonlinearities decreased (see section 4.2). Then, it can be stated that, for more brittle material although there is need for higher level of refinement, but only in a smaller area.

Consider two sets of materials, one with high number of brittleness and one with a low value. For the more brittle one, there should be higher refinement to insure the quality of numerical analysis. However, we have found that this refinement can be allocated in smaller area as the brittleness increases. In other words, only the scale of these two problems are different and costs of computation should not increase proportionally by the brittleness.

However, table 4.4 shows that still as the materials get more brittle , the computation cost increases. That is due to the fact that the background mesh size is the same always and also we use finer mesh than necessary one in order to ensure the results of computation.
σ_{max} = 0.6, K_{lc} = 2.165, \beta = 1.05
σ_{max} = 1.08, K_{lc} = 3.0, \beta = 1.77
σ_{max} = 0.82, K_{lc} = 2.16, \beta = 1.95
σ_{max} = 0.82, K_{lc} = 2.0, \beta = 2.28
σ_{max} = 0.89, K_{lc} = 2.16, \beta = 2.31
σ_{max} = 0.82, K_{lc} = 1.7, \beta = 3.1
σ_{max} = 0.82, K_{lc} = 1.5, \beta = 4.05
σ_{max} = 0.82, K_{lc} = 1.25, \beta = 5.85
σ_{max} = 2.0, K_{lc} = 3.0, \beta = 6.0
σ_{max} = 2.0, K_{lc} = 2.165, \beta = 11.6

Figure 4.6: Traction-separation curves for ten different sets of material properties

Figure 4.7: Inadequate mesh refinement level causes a wrong structural response.

This method has been examined, also, for variety of different simulations and the following observations are observed:
4.4 Crack Path Determination based on Grain Geometry

In previous sections, we showed that only a small number of grains participates in the fracture process of brittle polycrystalline aggregates. That strongly proved that crack formation is mostly dependent only on the geometry of those grain boundaries inside process window. It is worth again noting that mode-I crack path is not dependent on material properties (Shabir et al. [36] and previous chapter of this work), nor on the boundary conditions and test setups (see chapter 3).

Based on all the above findings, it seems that there should be an easy geometrical approach to find the crack path just based on arrangement of grain boundaries in front of crack tip.

Figure 4.8: Example of different mesh-refinement. Figure (a) shows: the background mesh (red lines), mesh-refinement through whole process window (blue lines) and the system of grains (black lines); Figure (b) shows: traction-free crack path (thick black lines), a background mesh and mesh-refinement just around the crack tip (blue lines) and the system of grains (black lines).

- Crack path is not affected if the number of surrounding grains and consequently size of mesh-refinement window is chosen appropriately;
- Structural response is not affected. Figure 4.12 shows an example of using both methods;
- Appropriate size of mesh-refinement window is only dependent on cohesive length $l_c$. 

4.4 Crack Path Determination based on grain geometry

In previous sections, we showed that only a small number of grains participates in the fracture process of brittle polycrystalline aggregates. That strongly proved that crack formation is mostly dependent only on the geometry of those grain boundaries inside process window. It is worth again noting that mode-I crack path is not dependent on material properties (Shabir et al. [36] and previous chapter of this work), nor on the boundary conditions and test setups (see chapter 3).

Based on all the above findings, it seems that there should be an easy geometrical approach to find the crack path just based on arrangement of grain boundaries in front of crack tip.
Figure 4.9: Example of optimized mesh-refinement around the crack tip. Figures (a) to (h) show mesh-refinement at some of the steps.

In the following we are going to investigate some geometrical algorithms in order to predict statistical crack prediction and compare both crack paths obtained from GFEM and the geometrical approach.
4.4 CRACK PATH DETERMINATION BASED ON GRAIN GEOMETRY

Figure 4.10: Load-displacement response obtained from sequential analysis for the realization given by Figure 4.9

4.4.1 Dijkstra’s Algorithm

“For a given source vertex (node) in the graph, Dijkstra’s algorithm finds the path with lowest cost (i.e. the shortest path) between that vertex and every other vertex.”[14] We have employed Dijkstra’s algorithm such that it gives the shortest path from the edge-notch tip to the opposite specimen edge (Figure 4.13). Indeed, Dijkstra’s path determines the minimum fracture energy crack path at the specimen-size level.

On the other hand, the Finite Element Method also obtains its solution by minimizing the energy functional. As both methods minimize the fracture energy consumption, one can conclude that under certain conditions these two methods can predict the same crack paths. We are expecting that if the microstructural randomness parameter $\bar{\rho}$ is beyond a specific value, both crack paths are identical and therefore expensive GFEM simulations are avoided.

In order to shed more light to this procedure, we performed sets of series of simulations to compare the obtained crack paths from a method which allows a precise description of the stress field (GFEM) and a network algorithm (Dijkstra’s path).

In one set of simulations, we performed GFEM analysis and Network analysis on 750 different hexagonal realizations with 80 grains (average grain size of 12 $\mu$m) inside the process window ($170 \times 120 \mu m^2$). Out of these 750 crack paths, 123 crack paths obtained from Dijkstra’s algorithm and GFEM were identical (17%). Some of those realizations are shown in Figure 4.14 with superimposed crack paths obtained from both methods. The length of cracks obtained from both methods are plotted versus non-dimensional randomness parameter $\bar{\rho}$ in Figure 4.15. The identical crack paths have been observed in variety of randomness values (from 0.29 to 0.40) and it does not seem that identical crack paths are clustered in a specific domain of randomness value. Figure 4.15 clearly illustrates that variations of randomness parameter $\bar{\rho}$ for the same
number of grains do not have a considerable effect on the path length. This is a verification, once again, that $\bar{\rho}$ is not an appropriate indicator for prediction of crack path.

The same study on Centroidal Voronoi tessellations (the size of process window is the same as the previous analysis) gave identical crack paths in 46% of cases. Result of this study is reported in Figure 4.16 where the length of cracks obtained from both methods is plotted versus non-dimensional randomness parameter $\bar{\rho}$. Two main comments can be observed from graph 4.16 are as the followings:

- Randomness parameter $\bar{\rho}$ [30] can not faithfully describe microstructural variations of Voronoi tessellations. It is very likely that two CVT’s with very different grain arrangement have the same values of $\bar{\rho}$.

- Variations of randomness parameter $\bar{\rho}$ do not have significant effect on the crack path length.

Nevertheless, increasing the height of specimen will result in decreasing the chance of obtained crack path from Dijkstra’s algorithm to be identical with the equilibrium path (GFEM path). Our studies on 130 different Voronoi Tessellations with 380 grains inside the process window ($170 \times 480 \ \mu m^2$) finds no identical crack path from both methods. Concerning the correctness of results, more sets of analysis with more precise solutions (finer mesh, smaller time step, etc.) have been accomplished and the same trend has been observed.
4.4 CRACK PATH DETERMINATION BASED ON GRAIN GEOMETRY

Figure 4.12: Load-displacement response for the realization given by Figure 4.11(a). In each step, a new analysis started considering the last obtained crack path as a traction-free notch line.

Figure 4.13: Crack path obtained with Dijkstra’s algorithm (red line) in CVT (thin black line). The algorithm finds the shortest path from the notch tip (Thick black line) to the top of Specimen.

Study on this phenomena consists a big part of this project. At the end, it seems that Dijkstra’s path is unable to explain local effects of microstructure. Our investigation showed that the crack path is mostly dependent on the geometry of grain boundaries at each of junctions in a micro-level.
Figure 4.14: Some examples for analysis of different hexagonal realizations. Superimposed crack paths obtained with the GFEM (blue lines) and Dijkstra’s algorithm (red lines) are shown in each realization.

Figure 4.15: Correlation of crack length with microstructural randomness $\bar{\rho}$ in analysis of hexagonal realizations. Best fits have been obtained with a least squares fit.
4.4 CRACK PATH DETERMINATION BASED ON GRAIN GEOMETRY

Figure 4.16: Correlation of crack length with microstructural randomness $\bar{\rho}$ in analysis of CVT’s. Best fits have been obtained with a least squares fit.

sense while Dijkstra’s crack path is defined based on global arrangement of grains.

In brittle polycrystalline materials the crack propagates by satisfying Griffith criterion. However, as the crack meets heterogeneity (junctions), the microstructure of junction itself has the great influence on the crack propagation. This fact is not included in the Dijkstra’s model and thus it fails to predict the true crack path [25].

4.4.2 Minimum Deviation Method (MDM)

So far, it has been observed that Dijkstra’s algorithm failed to predict crack propagation in brittle polycrystalline materials. Indeed, Dijkstra’s algorithm minimize the energy consumption globally (at specimen-size level) while this crack propagation is highly localized and there is a need to consider local minimization of mode-I energy consumption, as well.

Considering identical crack paths obtained from analysis of models with different material properties and same grain arrangement (e.g. see Figure 4.4) raises this question that why the crack paths are the same, although the number of participant grains (grains and grain boundaries which are located inside the nonlinear window) and distribution of nonlinearities are different.

To address this question, dozens of GFEM analysis have been performed for materials with very high brittleness number. Increasing the brittleness although make the simulation exceedingly expensive, but allows us to consider a small area of grains around crack tip and ignore all other grains. More brittle materials allow us to limit this area more and more until we attain a dimension for this window that is much less than grain size. Indeed, we are just considering a junction instead of system of grains. Our attempts to answer this question showed that no matter how many grains surrounded by nonlinearities diffusion but only the geometrical structure of junction is mainly decisive as the crack arrives at a heterogeneity.
In consequence of that, a new method has been developed just based on geometry of grain segments at every junction. We predict the crack path based on minimum deviation of segments with respect to normal direction of loading. At a junction we consider all of the grain boundaries and the crack propagates along grain boundary which lies closest to the homogeneous trajectory. [6]

As we mentioned before, we use two different techniques for modeling material microstructures. Variation of material microstructure has been modeled by means of random perturbed hexagonal topologies in the first method. In the second method, The Centroidal Voronoi tessellations have been used as a model for grain geometry of polycrystals. In the following, we are going to study the crack propagation in polycrystals modeled by both techniques.

**Hexagonal topologies**

Different hexagonal topologies i.e. various specimen sizes, different material properties and variety of grain arrangement (different randomness) have been analyzed, GFEM and MDM crack paths for each realization have been obtained (Figure 4.17).

Studies and analyses on brittle polycrystalline aggregates which are modeled by hexagonal realizations, showed that Minimum Deviation Method always predict the same crack path as the GFEM one. More than 300 realizations of different size of hexagonal topologies have been analyzed and it turned out that in case of hexagonal topologies, the GFEM and MDM crack paths are always identical.

**Centroidal Voronoi tessellations**

Unlike the hexagonal topologies, the MDM’s crack path is not always reliable in case of Voronoi tessellations. Studies on different size of Voronoi tessellations show different rate of success. Analysis of 260 different tessellations with 80 grains inside the process window show 73 % of identical crack paths from MDM and GFEM analysis. The same analysis for 140 case of Voronoi Tessellations with 180 grains inside the process window show 61 % of identical crack paths.

A massive study has been performed on non-identical cases. Figure 4.18 shows an example of such case in which at one of junctions GFEM crack path does not take the minimum deviated segment but the smaller segment. Such a case seems to be the typical situation where non-identical cases have been observed (Y-like configuration ignored).

Employing MDM in crack propagation is meant to minimize the local mode-I fracture energy. Nevertheless, we have shown that crack forms mostly at each junction based on the geometry of that junction. However, it does not mean that if we minimize the mode-I energy in each junction (local minimization), the global energy consumption will be minimized.

**4.5 Geometrical Model**

In this section, we are going to determine the suspicious junctions without performing an expensive GFEM analysis. Then, we will define an index in order to describe the presence of suspicious junctions. It is already clear to us that in absence of suspicious junctions the MDM and GFEM both will compute the same crack path. If we are able to recognize the suspicious junctions, we are able to predict a topological model to predict the crack path. In other words, we will describe a model in which it is possible to predict the crack path just based on topology of polycrystalline aggregates.

It is shown that MDM’s crack paths obtained from analysis of hexagonal realizations were always identical with the equilibrium paths while it is not the case for Voronoi tessellations.
Figure 4.17: Examples of different hexagonal microstructures used in the computations. GFEM crack paths (blue lines) are shown in the top Figures while crack paths obtained from MDM method (pink lines) are shown in the bottom Figures. Note that all crack paths obtained from both methods are identical.
Figure 4.18: Example of Voronoi tessellation (thin black line) with initial edge notch (thick black line). Non-identical crack paths obtained via GFEM analysis (blue line) and MDM (pink line).

Figure 4.19: Definition of quantities for the computation of parameter $\zeta$.

Understanding the reason of this phenomena may help us to define our index. In hexagonal realizations, the length of the grain facets are more or less in the same range. Thus, the length of each segment in front of the crack tip is approximately the same. Naturally, the length effect is neglected and That is why that a crack path based on MDM is always identical with the GFEM one. The comment can be observed in the previous work is: in order to define a suspicious junction not only the deviation of the segment is an important factor but also the length of segment is not uninfluential. we propose an index for each segment such as following:

$$\zeta_i = [\cos(\theta_i)]^\alpha \times [l_i]^\beta$$  \hspace{1cm} (4.3)

where segment $i$ make an angle $\theta_i$ with the normal to assumed direction of the applied load ($\theta_i$ is the angle between segment $i$ and macroscopic direction of crack growth) and has the length $l_i$, see Figure 4.19. $\alpha$ and $\beta$ should define such that $\zeta_i$ is the maximum for the segment which takes the crack path.

Through lots of try and errors for the known suspicious junctions, we could find the appropriate amount of $\alpha$ and $\beta$. Values of $\alpha = 2$ and $\beta = -0.5$ seem the best fit to predict the suspicious junctions. Our empirical formula for this index is determined as follows;

$$\zeta_i = \frac{\cos^2(\theta_i)}{\sqrt{l_i}}$$  \hspace{1cm} (4.4)

From physical point of view, the above formula can be explained as following: in the nominator $\cos^2(\theta_i)$ is responsible to choose a segment based on MDM (maximizing mode-I fracture
energy), power two is used in order to avoid a negative amount. In the dominator, \( \sqrt{l} \) is responsible for minimization of global energy in the sense that if a segment has the minimum deviation but it is too long the crack path will not take that segment. If at a junction, MDM’s crack path take the segment \( j \) and \( \zeta_j \) is not the maximum amount among all \( \zeta_i \) of that junction, then we can assume that the junction is suspicious and MDM’ crack path is not reliable.

In this way, it would be possible that for every given topology, a MDM’s crack path is computed and then if no suspicious junction is found, we can make sure that the inexpensive MDM’s crack path is identical with the GFEM crack path. To do so, the following algorithm has been coded and used in our simulations.

- MDM’s crack path is computed.
- We go through the computed crack path, starting from the notch tip. As soon as we meet an heterogeneity (a junction), \( \zeta_i \) is computed as followings:

\[
\zeta_i = \frac{\cos^2(\theta_i)}{\sqrt{l_i}}, \quad i = 1..n
\] (4.5)

where \( n \) is the number of present segments at the junction.
- The maximum amount of \( \zeta_i \) is computed. The segment which has the maximum amount should take the crack path. If it is the case, junction is not suspicious and we go through crack to the next junction. Otherwise, we have a suspicious junction;
- In case of suspicious junction, the ratio of maximum to minimum \( \zeta_i \) is computed:

\[
\zeta = \frac{\max(\sum_{i=1}^{n} \zeta_i)}{\min(\sum_{i=1}^{n} \zeta_i)}
\] (4.6)

and the minimum amount of \( \zeta \) is equal to one;
- We move to the next junction and repeat the above mentioned; and
- if no suspicious junction is found, \( \zeta = 0 \)

In order to test the above method, more than two thousand GFEM analyses with various type of material properties and topologies have been performed. Some of the results are visualized here. The results are visualized by depicting the difference of obtained crack length \( \delta l \) from both methods in vertical axes versus our index \( \zeta \) in the horizontal axes. We have done this analyses for different number of grains inside the process window and a few results of this work are illustrated by Figure 4.20, Figure 4.21 and Figure 4.22.

In all graphs, a threshold can be seen on \( \zeta = 1 \). In fact, we have proposed a simple geometrical model that nevertheless retains enough realism to make its predictions relevant in applications. In cases that \( \zeta \) is set to 0, we can expect the MDM to have an identical crack path with GFEM one, while for \( \zeta \geq 1 \), a topological procedure is not helpful to find the crack path.

Four different zones can be distinguished in Figure 4.20, Figure 4.21 and Figure 4.22. In case that \( \zeta \) is equal to zero and the GFEM and MDM’s crack paths are identical, we have a cluster of points at the origin of the graph (\( \zeta = \delta l = 0 \)). This zone, so called zone 1, is representative of those simulations that MDM and GFEM’s crack paths are identical and this is predicted by our model (\( \zeta = 0 \)). Graphs clearly show numbers of points on the vertical axes (\( \zeta = 0, \delta l \neq 0 \)). This zone, zone 2, is representative of cases that obtained crack paths are not identical, but the model can not find any suspicious junction and thus predicts the MDM’s crack path to be identical.
Figure 4.20: Correlation between $\delta l$ and $\zeta$ for analysis of samples with 80 centroidal Voronoi tessellations inside the process window. Different colors show different material properties.

with GFEM’s one. Investigations for this problem have shown that this problem happens due to the presence of equal angles. With avoiding the equal angles, this error in this model will be solved.

Zone 3, where $\zeta \geq 1$ and $\delta l \neq 0$, shows the cases that a suspicious junction presents and thus due to microstructural complexity of the junction, MDM cannot describe the crack path. In zone 4, where $\zeta \geq 1$ and $\delta l = 0$, there are points that can be seen on the horizontal axes. In these cases GFEM and MDM’s crack paths are identical while the model finds a suspicious junction. These are, indeed, the failures of our model to predict the crack path. This problem can be improved by developments in definition of $\zeta$.

In the following we will compare some statistics which have been obtained from analysis of 3 different geometry:

**80 grains sample (170×120 µm)**

<table>
<thead>
<tr>
<th>Statistics</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total number of analysis</td>
<td>200</td>
</tr>
<tr>
<td>Number of GFEM and MDM’s crack paths that are:</td>
<td></td>
</tr>
<tr>
<td>- Identical ($\delta l = 0$)</td>
<td>133 (67 %)</td>
</tr>
<tr>
<td>- Predicted by the model (zone 1, $\zeta = 0$)</td>
<td>120 (60 %)</td>
</tr>
<tr>
<td>- Not predicted by the model (zone 4, $\zeta \neq 0$)</td>
<td>13 (6.5 %)</td>
</tr>
<tr>
<td>- Non-identical ($\delta l \neq 0$)</td>
<td>67 (33.5 %)</td>
</tr>
<tr>
<td>- Predicted by the model (zone 3, $\zeta &gt; 1$)</td>
<td>59 (26 %)</td>
</tr>
</tbody>
</table>
4.5 GEOMETRICAL MODEL

Figure 4.21: Correlation between $\delta l$ and $\zeta$ for analysis of samples with 160 centroidal Voronoi tessellations inside the process window. Different colors show different material properties.

- not predicted by the model (zone 2, $\zeta = 0$): 17 (7.5%)

180 grains sample (170×240 $\mu$m)

- total number of analysis: 200
- Number of GFEM and MDM’s crack paths that are:
  - Identical ($\delta l = 0$): 124 (62%)
    - predicted by the model (zone 1, $\zeta = 0$): 92 (46%)
    - not predicted by the model (zone 4, $\zeta \neq 0$): 32 (16%)

- Non-identical ($\delta l \neq 0$): 76 (38%)
  - predicted by the model (zone 3, $\zeta > 1$): 59 (29.5%)
  - not predicted by the model (zone 2, $\zeta = 0$): 17 (8.5%)

340 grains sample (170×480 $\mu$m)

- total number of analysis: 200
- Number of GFEM and MDM’s crack paths that are:
  - Identical ($\delta l = 0$): 60 (30%)
    - predicted by the model (zone 1, $\zeta = 0$): 42 (21%)
Figure 4.22: Correlation between $\delta l$ and $\zeta$ for analysis of samples with 300 centroidal Voronoi tessellations inside the process window. Different colors shows different material properties.

- not predicted by the model (zone 4, $\zeta \neq 0$) : 18 (9%)
- Non-identical ($\delta l \neq 0$) : 140 (70%)
  - predicted by the model (zone 3, $\zeta > 1$) : 117 (58.5%)
  - not predicted by the model (zone 2, $\zeta = 0$) : 23 (11.5%)

As we mentioned before, for hexagonal grains MDM always predicts the true crack path. It is important to note that in all cases of hexagonal realizations, our model always gives $\zeta = 0$, which means that our model is perfectly reliable for crack path determination in hexagonal realizations.

The result of this section can be summarized as following: A topological procedure has been described. This model take the topology as an input and defines the crack path based on minimum deviation method, then, based on the defined crack path, the indicator $\zeta$ can be computed. It has been shown that for more than 60% of various cases that the MDM and GFEM analyses obtain the identical crack paths. Interestingly, The obtained crack paths can be clustered where $\zeta = 0$. For those cases that $\zeta \geq 1$, only a method which allows the detailed description of the stress field at the crack tip (e.g. Finite Element Method) can determine the crack path.
Chapter 5

Conclusion

5.1 General Summary

Intergranular fracture of brittle polycrystalline aggregates have been studied considering different type of topologies, test setups and varies material properties. Generalized Finite Element Method for polycrystalline [39] is used to simulate the failure of such materials. Brittle polycrystalline aggregates have been modeled using centroidal voronoi tessellations and also various random realizations of regular hexagonal grains. Crack propagation starts under quasi-static loading and the mode-I crack paths obtained from different test setups have been compared.

It has been observed in this study that for every mode-I test setup, for a specific material properties which is defined by means of cohesive law, intergranular crack path is insensitive to all boundary conditions and specimen size. Shabir et al. [36] have discovered that with special refinement rules, the intergranular crack path is insensitive to cohesive law parameters such as maximum cohesive strength or fracture toughness. Merging the result of their work with our investigations could be resulted in the following: mode-I intergranular cracking of brittle polycrystalline aggregates solely depends on its microstructure.

To investigate the localization of crack formation, the following question has been addressed: How many grains around the crack path could play a role in the fracture of brittle polycrystalline aggregates? To this end, an area in close vicinity of the crack tip has been explicitly investigated. It showed that as the crack tip meets an heterogeneity (grain junction), the only decisive factor for determining the crack path is the geometry of grain junction itself.

Based on all above findings, one can conclude that a geometrical approach to find the crack path (based on arrangement of grain boundaries) can lead to the identical crack path obtained via GFEM. Thus, heavy numerical simulation can be avoided. Two different techniques have been used in which both of them using topological procedure to obtain the crack path.

The first method is Dijkstra method which defines the shortest available path as the crack path. It has been observed that Dijkstra’s algorithm failed to predict crack propagation in brittle polycrystalline materials. Indeed, Dijkstra’s algorithm minimize the energy consumption globally (at specimen-size level) while this crack propagation is highly localized and there is a need to consider local minimization of mode-I energy consumption, as well.

The second method is Minimum Deviation Method (MDM). We predict the crack path based on minimum deviation of grain segments with respect to normal direction of loading. By comparing GFEM and MDM’s crack paths, obtained from analysis of different simulations, it has been
concluded that for special grain arrangements, it is possible to avoid the heavy finite element analysis and find the crack path based on MDM at relatively low cost.

Based on these findings, a topological model has been described. In this model, we have proposed an algorithm to study the obtained MDM’s crack path. Accordingly, a parameter $\zeta$ has been defined and it has been shown that for $\zeta = 0$, the crack path obtained from MDM is identical with GFEM one. In summary, the prescribed model is able to predict the crack path for specific topologies based on topological considerations.

### 5.2 Future Work and recommendations

In this study, a mode-I loading (at specimen-size level) has been assumed. Crack paths obtained base on mode-I loading condition has been explored and a topological model has been defined. However, it could be recommended to consider mode-II loading and mixed modes loading. Nevertheless, we assumed a quasi-static loading condition, which would be interesting to consider dynamic load condition and its effect on the failure of polycrystals and its crack path.

In our constructed model, we can predict the reliable crack path at a low cost but only in absence of suspicious junctions. Further development of the model, may able us to predict the crack paths even in presence of the suspicious junctions.
Bibliography


