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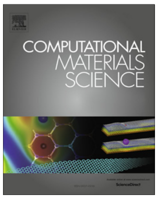

Simulation of crack propagation in single phase ceramic tool materials

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ABSTRACT

The crack growth simulation contributes to the investigation of the relationship between fracture toughness and microstructure of ceramic tool materials. In this paper, the Voronoi tessellation is used to represent microstructures of single phase ceramic tool materials. Cohesive element model has been built up to conduct the modeling of cracking propagation by embedding cohesive elements with fracture criteria in grains and along grain boundaries. Both single phase ceramic tool materials with pores and without pores are studied. The influences of grain size and porosity on fracture mode and fracture resistance are analyzed respectively. And the simulation results have a good agreement with the experimental phenomena.

1. Introduction

Study on how to improve the fracture toughness is one of the most important research subjects in ceramic tool material area all the time [1]. The mechanical properties of ceramic tool materials are primarily affected by microstructure. The microstructure of ceramic tool materials is comprised of grain boundaries and grains with different shapes, sizes and components, as well as impurities and porosities [2]. The complexity of microstructure increases the difficulty in investigating the relationship between microstructural morphologies and mechanical properties. The development of computer technology and related computational theory make computer simulation an important research approach in the ceramic tool materials.

The microstructure heterogeneities and the mechanical property anisotropies of composition phases need to be considered when studying the crack growth phenomena in microstructure of ceramic tool materials. Quantitative results cannot be obtained by analytical approach based on fracture mechanics theory. In recent years, numerical methods are commonly utilized to solve questions in this area. Continuum mechanics cannot be used to reflect the physical essence of microscopic fracture behavior for ceramic tool materials. During numerical simulation, discrete characteristics should be introduced into the crack tip to describe the effect of microstructure on crack growth path. And cohesive element method is frequently used in cracking behavior modeling of polycrystalline materials.

The basic theory of cohesive element method is proposed by Barenblatt as a traction–separation law when studying the atomic lattice decohesion [3]. The stress field singularity at crack tip which does not actually exist in continuum mechanics can be avoided by means of this method. In fracture simulation, cohesive elements are often embedded into material models as the potential crack path. Because of the computational efficiency and the simplicity of mathematical description, the approach of cohesive element has been widely used. Hillerborg et al. [4] performed the crack growth simulation in concrete with the help of cohesive element method. Xu and Needleman [5] utilized cohesive element approach to investigate the dynamic fracture behavior of brittle solids. Lin et al. [6,7] carried out a series of cracking simulation job for metallic materials. Rahul-Kumar et al. [8,9] published the detailed work for fracture in polymers and ductile cracking. These investigations reveal that cohesive element method is capable of processing various material systems and fracture mechanisms.

As for ceramic materials, in which fracture is a main failure type, many studies are conducted to explore the relationship between microstructure characteristics and mechanical behavior. Zhou and Zhai [10] studied the dynamic fracture behavior of Al_2O_3/TiB_2 microstructures by means of cohesive element method. Zavattieri and Espinosa [11,12] applied cohesive element approach to systematic research about intergranular fracture of Al_2O_3 microstructures under impact load. Tomar [13] conducted cracking simulation of $SiC–Si_3N_4$ nanocomposites with cohesive element

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theory and analyzed the effect of SiC dispersion on material strength.

This paper mainly deals with the crack growth simulation in the microstructure of single phase ceramic tool materials. The Voronoi tessellation is used to represent microstructures of ceramic tool materials. The cohesive element model is built up by introducing cohesive elements both in grains and along grain boundaries in the microstructure models as potential cracking path. Then the finite element calculation is conducted on the ABAQUS computing platform for the cracking modeling. Both intergranular and transgranular fracture mode are considered in our research. And the influences of microstructural morphologies on fracture patterns and mechanical response are also discussed.

2. Simulation models for single phase ceramic tool materials

2.1. Microstructure model – Voronoi tessellation

Voronoi tessellation is a kind of space subdivision form, which splits the space into several Voronoi areas based on a set of nuclei. Many studies have shown that the grain level structure of polycrystalline material can be modeled very well by Voronoi tessellation [11]. Due to the high calculation efficiency of Voronoi tessellation programming, many researchers have applied it to polycrystalline material. Ghosh et al. [14] employed Voronoi tessellation to describe the microstructure of composite and porous materials and conducted the stress–strain analysis. Bolander and Saito [15] discretized homogeneous, isotropic materials by means of Voronoi tessellation and modeled brittle fracture behavior of cement and concrete with a rigid-body-spring network. Liu et al. [16] utilized Voronoi tessellation to characterize the microstructure of multi-phase material and study the damage process under uniaxial tension and cyclic shear loading.

In this paper, all the crack propagation simulation jobs are carried out based on microstructures characterized by Voronoi tessellation. In order to obtain the Voronoi tessellation to represent the polycrystalline microstructure of ceramic tool materials, a number of random points should be generated as the nuclei of Voronoi polygons in the plane region. Voronoi tessellation can be obtained by calling the Voronoi generation function in Matlab. But it is impossible of getting closed Voronoi tessellation because there are not enough nuclei at the tessellation boundaries by using of this method. Therefore, certain algorithm should be designed to change the open Voronoi tessellation (Fig. 1(a)) into closed Voronoi tessellation (Fig. 1(b)). And the tessellation boundaries are single-line type.

2.2. Numerical simulation method – cohesive element method

2.2.1. Cohesive element theory

After the Voronoi tessellation which represents microstructure of ceramic tool materials is obtained, elements with fracture criteria (that is cohesive elements) should be inserted into the Voronoi tessellation to establish cohesive element model for cracking calculation.

According to [17], the crack initiation and propagation process can be simplified as the cohesive element model. Cohesive element model assumes that crack surfaces carry tractions that resist normal separation (Tn) and tangential sliding (Tt) before chemical bonds break, as illustrated in Fig. 2 [17]. The value of these tractions is a function of the respective normal and tangential displacements. The material deformation and fracture behavior can be simulated, if the traction–separation law of cohesive element model is utilized to describe the evolution procedure of the region at the front of crack tip.

Two kinds of traction–separation law (depicted in Fig. 3) can be used to describe the properties of cohesive elements. Fig. 3(a) shows ductile fracture, while Fig. 3(b) denotes brittle fracture. The traction–separation law is determined by two parameters: the maximum interface traction $T_{\max}$ and the interface fracture energy Γ. The area enclosed by the traction–separation curve equals to the interface fracture energy Γ. The fracture process begins as the interface traction reaches $T_{\max}$. And the interface will fail eventually when the mechanical energy release rate exceeds Γ. Since plastic deformation hardly exists before the fracture of brittle materials, interface traction will decay at once after arriving $T_{\max}$, as shown in Fig. 3(b). The detailed description of cohesive law can be found from [18]. In this work, the traction–separation curve in Fig. 3(b) is utilized to describe the properties of cohesive elements for ceramic tool materials.

Cohesive element model is directly based on tectonic displacement control equation. Therefore strain does not need to be solved by using the displacement field gradients in elements calculation. This greatly improves the stability of numerical simulation and makes cohesive element model suitable for processing strong nonlinear problems like multiple fracture, crack branching and solid crushing [19]. At the same time, cohesive element model has a high calculation efficiency since it integrates very well with traditional finite element method. In addition, it requires only two parameters ($T_{\max}$ and Γ) to describe the fracture process. Therefore, cohesive element model is particularly attractive for practical application. However, some numerical stability issues should be paid attention when solving fracture problems with cohesive element model [20].

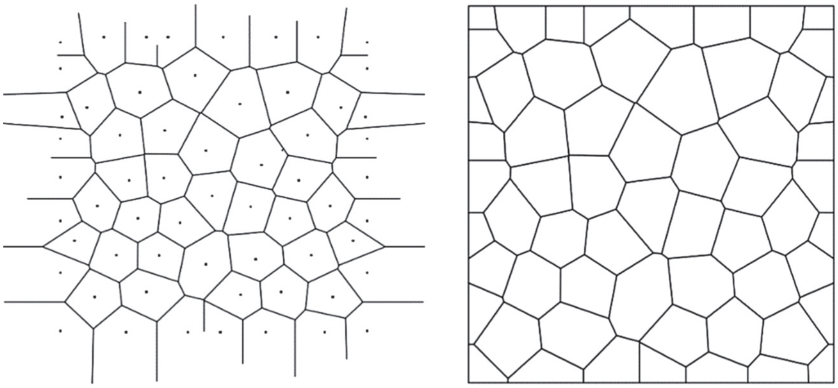
(a) Open Voronoi tessellation (b) Closed Voronoi tessellation

Fig. 1. Voronoi tessellation [11].