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Crack propagation simulation of polycrystalline cubic boron nitride abrasive materials based on cohesive element method

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ABSTRACT

A two-dimensional finite element model is established to simulate the crack propagation behavior of polycrystalline cubic boron nitride (PCBN) under tensile loading. The grain level microstructure of PCBN is created using Voronoi diagram. Cohesive elements are embedded in the potential crack paths to simulate both intergranular and transgranular fracture. The influence of grain size, bonding strength of grain boundaries and grain boundary stiffness on the crack patterns and fracture toughness are studied. The simulation result is compared with the previously reported experimental counterpart, and the identical changing trends are obtained. Finally, it is found that the influence of various microstructural factors on fracture toughness is mainly achieved by varying the crack patterns.

1. Introduction

Polycrystalline cubic boron nitride (PCBN for short) is a typical superhard material, which has been commonly used as the abrasive grains for grinding difficult-to-machine materials, such as titanium alloy and nickel-based superalloy [1]. Compared with the monocrystalline CBN grains, the unique microstructure of PCBN grains overcomes the drawback of anisotropic, which tends to a cleavage in grinding due to the limited slipping planes [2]. The PCBN abrasive tools mainly works in the extreme conditions such as high temperature, friction and impact load environment, which could lead to brittle fracture of the abrasive grains, resulting in a reduction in the number of effective abrasive grains to shorten the tool life [3]. Therefore, it is necessary to investigate the crack propagation and fracture toughness of PCBN abrasive materials as well as the influencing factors.

The mechanical properties of PCBN abrasive grains mainly depend on the internal microstructure, which consist of grain boundaries, grains with different sizes, shapes and constituents, inclusions and porosity [4]. Concerning the influence of the internal microstructures of PCBN on its mechanical properties, several experimental studies have been conducted. For example, Liu et al. [5] studied the effect of grain size on the mechanical properties of CBN-Si composite, in which it was found that the hardness and thermal stability increased with the increase of grain size, and the fracture toughness decreased with the increase of grain size. McKie et al. [6] investigated the influence of grain size and Al content on the hardness, fracture toughness and flexural strength of CBN-Al composite, based on which they pointed out that the hardness of CBN-Al composite decreased with the increase of CBN grain size and Al content, fracture toughness depended on combined relationship between the grain size and Al content and there was no significant relationship between flexural strength, grain size and Al content. Yue et al. [7] studied the influence of mass ratio of Ti_3SiC_2 on the flexural strength, compressive strength and Vickers hardness of CBN-Ti_3SiC_2 composite. It was found that the flexural strength decreased with the increase of Ti_3SiC_2 mass ratio and the compressive strength and hardness increased with the increase of Ti_3SiC_2 mass ratio.

The experimental studies mentioned above reveal the influence of the various microstructural characteristics of PCBN on its mechanical properties. However, it is usually time-consuming and cost-expensive to sinter PCBN and measure the various mechanical parameters of PCBN. Meanwhile, the control of the input parameters is limited in an experimental operation, because it is difficult to change one single parameter while keeping other parameters unaffected. However, resorting to finite element method, these problems would not exist. By means of the finite element method, various material parameters and load conditions can be set to simulate the mechanical behavior of the material under various working conditions, and the simulation results could be obtained conveniently in the post-processor. The cohesive model, put forward by Dugdale and Barenblatt, is a very effective method in simulation researches concerning crack propagation and fracture toughness of polycrystalline materials [8,9].

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Hillerborg [10] applied the cohesive model to study brittle fracture using finite element method for the first time. Needleman [11] was the first one to use the model for analyzing crack propagation of ductile materials. After the successful implementation of the cohesive model into finite element method, it has been widely used in the crack propagation simulation of brittle polycrystalline materials. Sfantos et al. [12] developed a cohesive grain boundary element formulation to model intergranular micro-cracking evolution in polycrystalline brittle materials. The stochastic effects of each grain morphology-orientation, internal friction and randomly distributed preexisting flaws on the overall behavior and micro-cracking evolution of a polycrystalline brittle material were studied respectively. Yin et al. [13] inserted cohesive elements with the bilinear softening law into both the mastic and the interfaces between the mastic and aggregates to simulate crack initiation and propagation of asphalt mixture under uniaxial tensile loading. The influence of aggregates distribution and parameters of the cohesive model on the performance of asphalt mixture were evaluated. Zhou et al. [14] utilized a cohesive element method to simulate the phenomenon of crack propagation in the microstructures of ceramic tool materials. The influence of grain size, grain boundary strength and microcracks on cracking patterns and fracture toughness were analyzed respectively. Kraft and Molinari [15] developed a two-dimensional finite-element model using cohesive interface approach to investigate transgranular fracture in polycrystalline alumina under tensile loading. The effects of grain boundary distributions on mesoscopic failure strength and fracture energy and the resulting percentages of transgranular fracture were examined. These studies revealed that the cohesive model can be used for a variety of materials to simulate a variety of fracture mechanisms.

The present investigation work mainly deals with the effects of grain size, bonding strength of grain boundary and grain boundary stiffness on the fracture toughness of PCBN abrasive materials under tensile loading. The potential crack paths of PCBN are represented through embedding cohesive elements based on traction-separation-law both in grains and along grain boundaries. Simulation calculations are performed through the general finite element analysis software Abaqus. In this research work, the energy dissipations due to fractures of various microstructures as well as the length of cracks and the percentage of transgranular fracture are calculated. The relationship between fracture toughness and crack characteristics is analyzed in detail.

2. Characterization and modeling for PCBN grains

2.1. Microstructural model based on Voronoi diagram

A Voronoi diagram is a partition of a spatial plane into regions based on distance to points, often called seeds, in a specific subset of the plane. For each seed, there is a corresponding region consisting of all points closer to that seed than to any other. All these regions together form the whole Voronoi diagram [16]. Many researches show that the grain level microstructures of polycrystalline materials can be represented by Voronoi diagram very well [17–19].

In this study, all the crack propagation simulations are based on the microstructures represented by Voronoi diagram. The Voronoi diagram is established by invoking the function mpt_voronoi of the multi-parametric toolbox (MPT) in Matlab. Comparing the real microstructure of PCBN (Fig. 1(a)) with the generated Voronoi diagram (Fig. 1(b)), it can be found that they are similar. The basic flow for building a Voronoi diagram is summarized in Fig. 2. The detailed procedure for building a Voronoi diagram is provided in Appendix A.

2.2. Cohesive element model

2.2.1. Cohesive element theory

The crack initiation and propagation process can be simplified as the cohesive element model. The constitutive behavior of the cohesive element used in the present work is based on the traction-separation-law. The traction-separation-law consists of three basic ingredients: the initial linear elasticity stage, the fracture initiation criterion and the fracture evolution criterion [21]. Fig. 3 shows a typical traction-separation-law with a failure mechanism. The initial elastic behavior is described by an elastic constitutive matrix that relates the nominal stresses to the nominal strains across the interface. So the relationship between the nominal stresses and the nominal strains can be defined as:

$$t = \begin{Bmatrix} t_n \\ t_s \\ t_t \end{Bmatrix} = \begin{bmatrix} E_{nn} & E_{ns} & E_{nt} \\ E_{ns} & E_{ss} & E_{st} \\ E_{nt} & E_{st} & E_{tt} \end{bmatrix} \begin{Bmatrix} \varepsilon_n \\ \varepsilon_s \\ \varepsilon_t \end{Bmatrix} = E\varepsilon \tag{1}$$

where t is the nominal traction stress vector, ε is the nominal strain vector and E is the elastic constitutive matrix. When the stress and/or strains satisfy certain damage initiation criteria, the process of degradation of the response of a material point begins. In this work, damage is assumed to initiate when a quadratic interaction function involving the nominal stress ratios reaches a value of one. This criterion is called quadratic nominal stress criterion, which is represented as:

$$\left\{\frac{\langle t_n \rangle}{t_n^o}\right\}^2 + \left\{\frac{t_s}{t_s^o}\right\}^2 + \left\{\frac{t_t}{t_t^o}\right\}^2 = 1 \tag{2}$$

where t_n^o, t_s^o and t_t^o represent the peak values of the nominal stress when the deformation is either purely normal to the interface or purely in the first or the second shear direction, respectively. Once the damage initiation criterion is reached, the rate at which the material stiffness is degraded is described by the damage evolution law. A scalar damage variable D is used in the damage evolution law to represent the overall damage in the material. Upon further loading after the initiation of damage, D monotonically evolves from 0 to 1. The effects of the damage on the stress components are described as:

$$\begin{cases} t_n = \begin{cases} (1-D)\bar{t}_n, & \bar{t}_n \geqslant 0 \\ \bar{t}_n, & \text{otherwise (no damage to compressive stiffness)} \end{cases} \\ t_s = (1-D)\bar{t}_s, \\ t_t = (1-D)\bar{t}_t. \end{cases} \tag{3}$$

where $\bar{t}_n$, $\bar{t}_s$ and $\bar{t}_t$ are the stress components predicted by the elastic traction-separation behavior for the current strains without damage. When the damage variable D reaches 1 at all of its material points, the cohesive element will fail and be removed. The energy dissipated due to the element failure is equal to the area enclosed by the traction-separation curve and the horizontal axis.

2.2.2. Embedding cohesive elements

During the fracture procedure of PCBN materials, cracks may propagation both along grain boundaries and into grains. Therefore, in order to simulate the intergranular fracture and transgranular fracture of PCBN materials, cohesive elements will be embedded as potential paths for crack propagation both in the grains and along the grain boundaries.

The entire model is first meshed with linear triangular elements, and then cohesive elements are embedded along each triangular element as the potential crack paths. The nodes and elements data of the triangular mesh require special treatment to