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# Microstructure-level modeling and simulation of the flexural behavior of ceramic tool materials

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## ABSTRACT

The flexural behavior of ceramic tool materials is investigated by both experiments and numerical simulation. The Voronoi Tessellation hybrid random algorithms are utilized to construct a microstructure model to simulate the flexural behavior of ceramic. The secondary phase volume fraction, the nano-scale particle volume fraction, the grain centroid distribution, and the grain diameter distribution of the materials are considered in the model. The flexural strength of ceramic materials is calculated via the simulation of three-point bending tests. The effects of average grain diameter, nano-scale particle and secondary phase volume fraction on the flexural strength of ceramic materials are systematically studied. The numerical simulation results show good agreement with the experimental results.

## 1. Introduction

Ceramic materials possess a series of excellent properties which are indispensible for tool materials, such as high hardness, great wear resistance, good chemical stability and heat resistance [1,2]. Whereas, one of the intrinsic drawbacks of ceramic cutting tools is relatively low flexural strength and fracture toughness, which usually makes them more susceptible to excessive chipping or fracture when machining hardened materials [3]. During the past two decades, much effort has been made to improve the strength and toughness of ceramic materials. Several useful methods have been proposed, such as dispersion of different particles in a matrix, fiber or whisker reinforced composites and micro-nano reinforced composites [4–8].

Recently, grain size effects on mechanical properties of composite ceramics were widely studied [9–11]. The effects of $Al_2O_3$ particle size on the mechanical properties of alumina-based ceramics were investigated by Teng et al. [9]. The effect of starting powder size on $Al_2O_3$/TiC composites were studied by Liu et al. [11]. Conventionally, $Al_2O_3$-based ceramic tool materials were strengthened by the addition of micro-sized particles like TiC, TiN, $ZrO_2$, (W, Ti)C, $TiB_2$, etc. or SiC whisker to improve the mechanical properties [12–15]. Formerly, many studies have been carried out to evaluate the effect of addition of secondary phase on the microstructure and mechanical properties of ceramic. The effect of addition of TiC on the mechanical properties of $Al_2O_3$ based composites were examined by Cai et al. [12]. The effect of (W, Ti)C content on the microstructure and mechanical properties of $B_4C$/(W, Ti)C ceramic composites were studied by Deng et al. [14]. Since, Niilhara firstly reported that the addition of nano-particles to the $Al_2O_3$ matrix could improve mechanical properties notablely, especially the researches on nano $Al_2O_3$-based composites were conspicuously developed [16]. The investigation on preparation ceramic composites for cutting tools by adding nano-scale particle, such as TiC, $Al_2O_3$ and TiN, to the Al2O3 matrix have drawn more attention [17–19]. Davidge et al. [17] showed a clear evidence for significant strengthening and toughening due to the addition of approximately 100 nm SiC particles to $Al_2O_3$.

Microstructure plays an important role in determining the mechanical properties of ceramic tool materials [20]. The mechanical properties would be affected by grain diameter, grain distribution, grain shape and constituent phases [21,22]. It is difficult to quantify the correlation between microstructure and materials properties due to the complexity of ceramic microstructure. Recently many numerical and theoretical models have been developed to reveal this correlation [23–25]. Sukumar and Srolovitz [23] simulated the crack propagation of polycrystalline materials by the means of X-FEM. A simulation of crack propagation in microstructure of ceramic was presented by Wang et al. [24]. The effects of randomness in the distribution of microstructure parameters have been generally neglected or scarcely considered in these simulation models. To this end, the objective of this paper is to develop a microstructure-level model to simulate the flexural behavior of ceramic material. The model was based on the Voronoi Tessellation in which random algorithm was employed by taking into account

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the secondary phase volume fraction, nano-scale particle volume fraction, the grain centroid distribution and the grain diameter distribution of the materials.

In this paper, a type of $Al_2O_3$-based composite ceramic tool material simultaneously reinforced with micro-scale (W, Ti)C and nano-scale $Al_2O_3$ particles is fabricated by using hot-pressing technology, the experimental procedures and results are described in Section 2. Then, a microstructure model is developed by using Voronoi Tessellation and random algorithm. The detailed construction of microstructure model and the simulation procedures are presented in Section 3. The simulated results and discussion are given in Section 4. Eventually, some concluding remarks obtained from this study are given in Section 5.

## 2. Experimental procedures

### 2.1. Materials preparation

The starting materials are $\alpha$-$Al_2O_3$ powders with average grain size of approximately 0.5 μm (purity: 99.99%, Shanghai, China), nano-scale $Al_2O_3$ with an average particle size of approximately 140 nm (purity: 99.9%, Zibo, China) and (W, Ti)C with an average particle size of 1 μm (purity: 99.99%, Hefei, China). Nine different composition rations are tested as shown in Table 1. The nano-scale $Al_2O_3$ powders are prepared into suspensions using alcohol as the dispersing medium, and the dispersant PEG (polyethylene glycol, Shanghai, China) is added after ultrasonic dispersion (with SB5200 ultrasonic instrument and D-7401-III motor stirrer, China) for 10 min. The suspensions are dispersed ultrasonically for 20 min after a pH of 9.0 (with PHS-25 digimatic pH-meter, China) is attained by the addition of $NH_3{\cdot}H_2O$. After the nano-scale $Al_2O_3$ particle suspension is dispersed well, they are then mixed with micro $Al_2O_3$, micro (W, Ti)C. MgO and NiO (Shanghai, China) are used as sintering additives to promote the densification of the compacts and retard the grain growth of $Al_2O_3$ matrix during the sintering process. The mixed slurries are ball-milled for 48 h, and then dried in a vacuum dry-type evaporator (Moder ZK-82 A, China). After that, the dried powders are sieved through a 200-mech sieve for further use. The dried powders are placed into a graphite die and hot-pressed with an applied pressure of 32 MPa at 1650 °C with the holding time of 20 min in vacuum in a sintering furnace.

### 2.2. Characterization

Each sintered compact (with 42 mm diameter) is cut and machined into five bend bars with the dimension of 3 mm × 4 mm × 20 mm and then ground flat to a 10 μm finish. Flexural strength is measured using a three-point bending tester (Model WD-10, China) with a span of 20 mm and a loading velocity of 0.5 mm/min. The flexural strength for the nine composites is given in Table 1. The fracture surfaces are observed by scanning electron microscopy (SEM, SUPRA-55, ZEISS, Germany).

**Table 1**
Composition (vol.%) and flexural strength of different composites.

| Composites | Micro-scale $Al_2O_3$ (0.5 μm) | (W, Ti)C (1 μm) | Nano-scale $Al_2O_3$ (0.14 μm) | Flexural strength, $\sigma_f$ (MPa) |
|---|---|---|---|---|
| AW15 | 85 | 15 | 0 | 531.27 |
| AW25 | 75 | 25 | 0 | 723.40 |
| AW35 | 65 | 35 | 0 | 781.12 |
| AW45 | 55 | 45 | 0 | 796.95 |
| AW55 | 45 | 55 | 0 | 580.65 |
| W45N5 | 50 | 45 | 5 | 817.33 |
| W45N10 | 45 | 45 | 10 | 832.52 |
| W45N15 | 40 | 45 | 15 | 819.51 |
| W45N20 | 35 | 45 | 20 | 810.83 |

## 3. Numerical simulation procedures

### 3.1. Microstructure modeling of ceramic materials

Voronoi diagram (VD) is a kind of important geometric structure in Laguerre geometry. The space is divided into many regions in accordance with the shortest property of element in the set of objects (points or lines). The ceramic grain matrix is similar to the Voronoi cells in the shape. The matrix microstructure model is constructed by using of the VD in this paper. Some basic microstructure parameters of ceramic, including average diameter and centroid, are considered in the model. The incremental method is used to construct the VD based on hybrid programming of MATLAB and VC++. In the algorithm of incremental method, the new seed points are added gradually into the VD which has been constructed with seed points. There are two main steps to establish the model [24]. Firstly, the location of newly added seed point $p_{k+1}$ is checked in the VD ($p_k$). $VR_p$ ($p_i$) indicates the cell of seed point $p_i$ in the VD. In Fig. 1(a), the location of $p_{k+1}$ could be determined by comparing the distance between $p_{k+1}$ and the point in the set $P_k = \{p_1, p_2, \ldots, p_k\}$. Once the point $p_i$ with the minimum distance away from the $p_{k+1}$ is determined, the fact that the $p_{k+1}$ located in the $VR_p$ ($p_i$) could be found. Then, the Voronoi cell $VR_p$ ($p_{k+1}$) is produced by the point with minimum distance away from the $p_{k+1}$. The dotted line indicates the $VR_p$ ($p_{k+1}$) in Fig. 1(a). $VR_p$ ($p_i$) is separated into two parts by the straight bisector between $p_{k+1}$ and $p_i$. There are two intersection points ($q$ and $t$) in the boundary of $VR_p$ ($p_i$). The intersection points ($t$ and $n$) are found in the adjacent cell $VR_p$ ($p_j$) by using the same method. The process would be accomplished until a polygon appeared. Finally, the new cell $VR_p$ ($p_{k+1}$) is generated by deleting the boundary and vertex in that polygon. The new Voronoi cell in Fig. 1(b) is developed.

The simulation of ceramic microstructure starts with the generation of cell points. A set of cell points are generated by using the uniform distribution function based on the MATLAB. Then the cell points are inserted into the matrix one by one. With the addition of the cell points, the new VD is constructed correspondingly. The process is terminated until the grain diameter reaches a designated value. Then, the convex quadrilaterals are put into the matrix randomly to simulate the secondary phase (see Fig. 1(c)). The location of quadrilateral is determined by the uniform distribution function. In this process, it is inevitable that there are overlapping cells, which can be removed by a series of Boolean operations (see Fig. 1(d)). The total areas of added quadrilaterals are calculated with the adding process. The program would ceases to run when the area reach a designated value. After this step, the ceramic microstructure with secondary phase is constructed. In Fig. 2(a), the light-colored cells and the deep-colored cells indicate the $Al_2O_3$ matrix and the secondary phase of (W, Ti) C, respectively. In order to simulate the nano-scale particle $Al_2O_3$, dots with certain diameter are randomly added into the above generated model. The number of circles is determined by the volume fraction of nano-scale $Al_2O_3$. The microstructure model with nano-scale particle is shown in Fig. 2(b) in which the dots are the nano-scale particle $Al_2O_3$.

**Table 2**
Material parameters of microstructure.

| Material | $\rho$ (kg/m$^3$) | $E$ (GPa) | $\nu$ |
|---|---|---|---|
| $Al_2O_3$ | 3990 | 374 | 0.22 |
| (Ti, W)C | 9490 | 570 | 0.2 |