



Article Simulation of Microscopic Fracture Behavior in Nanocomposite Ceramic Tool Materials

Tingting Zhou ^{1,2,*}, Lingpeng Meng ^{1,2}, Mingdong Yi ^{1,2} and Chonghai Xu ^{1,2}

- School of Mechanical Engineering, Qilu University of Technology (Shandong Academy of Sciences), Jinan 250353, China
- ² Shandong Institute of Mechanical Design and Research, Jinan 250031, China
- Correspondence: zhoutingting506@163.com

Abstract: In this paper, the microstructures of nanocomposite ceramic tool materials are represented through Voronoi tessellation. A cohesive element model is established to perform the crack propagation simulation by introducing cohesive elements with fracture criteria into microstructure models. Both intergranular and transgranular cracking are considered in this work. The influences of nanoparticle size, microstructure type, nanoparticle volume content and interface fracture energy are analyzed, respectively. The simulation results show that the nanoparticles have changed the fracture pattern from intergranular mode in single-phase materials to intergranular–transgranular–mixed mode. It is mainly the nanoparticles along grain boundaries that have an impact on the fracture pattern change in nanocomposite ceramic tool materials. Microstructures with smaller nanoparticles, in which there are more nanoparticles dispersed along matrix grain boundaries, have higher fracture toughness. Microstructures with a nanoparticle volume content of 15% have the most obvious transgranular fracture phenomenon and the highest critical fracture energy release rate. A strong interface is useful for enhancing the fracture toughness of nanocomposite ceramic tool materials.

Keywords: nanocomposite ceramic tool material; microstructure; fracture behavior; Voronoi tessellation; cohesive element

1. Introduction

Nanocomposite ceramic tool materials possess excellent mechanical properties, along with nanoparticles that have great specific surface area, high chemical activity and large dispersivity [1,2]. Fracture is a primary failure mechanism for nanocomposite ceramic tool materials, just like ordinary ceramic materials. Grain boundaries (GBs), nanoparticles and thermal expansion mismatch between matrix grains and nanoparticles may lead to crack deflection, pinning and bridging, which tend to improve the fracture energy of materials [3]. Therefore, investigating the fracture behavior of nanocomposite ceramic tool materials in microscale contributes to the exploration of the relationship between microstructures and macroscopic properties, like fracture strength and toughness.

Due to the heterogeneous microstructures and the mechanical property anisotropies of constituent phases, the microscopic fracture behavior of ceramic tool materials cannot be reflected by means of continuum mechanics, which are suitable for predicting the average response of heterogeneous materials. Therefore, a proper approach is needed to perform the cracking simulation of polycrystalline materials; which does not only characterize microstructural heterogeneities, but also tracks the microscopic damage process, such as crack initiation, propagation and coalescence [4]. The cohesive element model is an approach that could achieve both objectives.

Dugdale [5] conducted the earliest studies on the cohesive element theory and found that cohesive tractions along the fracture process zone were constant for metallic materials under the condition of ideal elastic–plasticity. Xu and Needleman [6] carried out the dynamic crack growth simulation of isotropic elastic solids based on the cohesive element



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Copyright: © 2023 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (https:// creativecommons.org/licenses/by/ 4.0/). model they proposed previously. Wang et al. [7] proposed a computational framework for the impact fracture of laminated glass based on the cohesive element model, which was applied to the impact fracture simulation of a laminated glass plate. The simulation results were found to be in agreement with the experimental ones. Geng et al. [8] conducted numerical simulations on two-dimensional standard concrete specimens under axial compression and tension based on the cohesive element theory. Their results indicated that the proposed method exhibited exceptional capabilities in predicting initial stiffness, uniaxial strength and corresponding strain. Xu et al. [9] studied the interface cracking mechanism of calcium-magnesium-alumino-silicates (CMAS)-corroded thermal barrier coatings based on the cohesive element model. Their theoretical model validated the spalling phenomena of thermal barrier coatings caused by CMAS corrosion at high temperatures. Zavattieri and Espinosa [10,11] developed a grain level micromechanical model of brittle materials in the context of cohesive elements to model crack initiation and propagation. Simulations of wave propagation experiments on alumina are used to illustrate the model capabilities in the framework of experimental measurements. Zhou, Tomar and Zhai [4,12] investigated the dynamic fracture process of Al₂O₃/TiB₂ microstructures and discussed the effects of heterogeneous phases on crack paths. Sun et al. [13] investigated the fracture behavior of graphene-toughened Al₂O₃ ceramic materials and characterized the Al₂O₃/graphene interface properties using the cohesive element method. The effects of phase interface bonding strength and graphene content on fracture behavior were analyzed and some toughening mechanisms induced by nano-graphene, such as crack bridging, crack branching, microcracks and pull-out of graphene, were discussed.

This paper mainly deals with microscopic cracking simulations based on nanocomposite ceramic tool materials. Although many studies have been carried out regarding the microscopic cracking behavior of both single phase ceramic tool materials and composite ceramic tool materials reinforced with microsized particles, little attention has been paid to the work on the microscopic fracture mechanisms of nanocomposite ceramic tool materials. It is meaningful for the optimization of mechanical properties to investigate the microscopic fracture behavior of nanocomposite ceramic tool materials, and to analyze the effects of microstructure heterogeneities such as nanoparticle distribution and the nanoparticle size on cracking paths.

In this paper, a micromechanical model of $Al_2O_3/SiCn$ nanocomposite is developed by embedding cohesive elements with fracture criteria into microstructures represented using the Voronoi tessellation. Then crack propagation modeling is conducted in order to explore the effects of microstructural morphologies, like nanoparticle size, microstructure type, nanoparticle volume content and interface fracture energy, on fracture patterns and mechanical responses.

2. The Cohesive Element Model for Microscopic Cracking Simulation

2.1. Traction–Separation Law

In the cohesive element model, it is assumed that crack surfaces carry cohesive tractions that resist normal separation (T_n) and tangential sliding (T_t) before cracking [14]. The relationship between cohesive traction (T) and cracking displacement (δ) can be described using the traction–separation law.

In this work, the linear traction–separation law for brittle materials (Figure 1) is utilized to characterize the properties of cohesive elements in ceramic tool materials. When the cohesive traction increases to a maximum value T_{max} , the damage process begins. As the traction gradually reduces to zero, the cohesive interface will fail completely and reach the maximum displacement (δ_{max}). The area under the traction–separation curve equals the interface fracture energy Γ . It is obvious that the traction–separation law can be determined by two parameters: the maximum interface traction T_{max} and the interface fracture energy Γ . This makes the cohesive element model very attractive for practical applications.



Figure 1. Traction-separation law for brittle fractures.

2.2. Development of the Cohesive Element Model

In this work, all the crack propagation simulation jobs are performed based on the microstructures of ceramic tool materials, which are represented by a Voronoi tessellation. Many studies have shown that the grain level structures of polycrystalline materials can be modeled very well by the Voronoi tessellation [15], and the influences of microstructure heterogeneities and neighboring elements on grain shapes can be reflected by the Voronoi tessellation. This feature gives the Voronoi tessellation the ability to quantitatively describe the characteristics of microstructures, such as the volume content, the size, the shape and the orientation of each composition phase. Due to the high computational efficiency and the simplicity of programming, the Voronoi tessellation has been widely used to characterize microstructures of polycrystalline materials [16–18].

In order to conduct the microscopic fracture simulation, a cohesive element model should be established by embedding cohesive elements with cracking law among adjacent volume elements using the Voronoi tessellation. Therefore, the Voronoi tessellation should be meshed with triangular volume elements first. In contrast with the simulation procedures for single phase ceramic tool materials described in [19], nanoparticles should be generated after the microstructure models are divided by triangular elements. In order to conduct the simulation of intergranular and transgranular cracking in nanocomposites, rectangular cohesive elements with cracking law should be embedded among all triangular volume elements to implement the arbitrary extension of the crack. The process of generating the Voronoi tessellation, the nanoparticles and the cohesive elements is carried out through programing with MATLAB 2020. The simulation procedures are illustrated in Figure 2.

Figure 3a shows the microstructure model represented with the Voronoi tessellation, in which each Voronoi polygon represents a matrix grain. And Figure 3b is the Voronoi diagram after embedding cohesive elements and triangular elements. It is observed from Figure 3b that white triangles indicate volume elements of the matrix and blue triangles denote volume elements of nanoparticles. Cohesive elements in matrix grains and those along matrix GBs are represented by yellow and red quadrilaterals, respectively. Cohesive elements in nanoparticles and along interfaces are characterized by green and black quadrilaterals, respectively. For presentation purposes, the thickness of cohesive elements is magnified in Figure 3b.

The addition of cohesive elements among volume elements has a negative effect on the stiffness of the FEM model. The density of cohesive elements increases as finite elements are refined, which will intensify the reduction of stiffness [12]. However, this issue can be avoided by carefully choosing a lower bound of finite element size and the constitutive parameters of elements. On the other hand, for the purpose of ensuring computational accuracy, there should be several cohesive elements distributed in the cohesive zone, which imposes an upper limit of finite element size. According to the reference [12], in order to

ensure simulation accuracy and calculation convergence, the finite element size h takes the form:

$$\left(\frac{\lambda_{cr}\delta_0}{T_{max}}\right)\frac{E'\left(\sqrt{2}+1\right)}{(1-\nu)} \le h \le \frac{9\pi E\Gamma}{32(1-\nu^2)T_{max}^2} \tag{1}$$

where E' = E for plane stress and $E' = E/(1-\nu^2)$ for plane strain. *E* and ν are the elasticity modulus and Poisson's ratio, respectively. $\lambda_{cr} = \delta_0 / \delta_{max}$ is the critical effective displacement jump.

Substituting the constitutive parameters of cohesive elements into Equation (1), the range of finite element size is specialized to 0.0016 μ m $\leq h \leq 2.54 \mu$ m. In our work, the finite element size of $h = 0.073 \mu$ m is adopted, which is reasonable for achieving accurate modeling.



Figure 2. Flowchart of simulation procedures.



Figure 3. Cohesive element model. (**a**) Before the addition of cohesive elements. (**b**) After the addition of cohesive elements.

3. Implementation of FEM Simulation

The microscopic fracture problems depicted in Figure 4 can be solved with the cohesive element model. An initial crack added in the simulation model aims to form the stress concentration, which can form regular crack paths under loading and is convenient for analyzing the influences of microstructures on cracking behaviors. In this work, the initial crack is set along grain boundaries and its length is equivalent to grain size. The effect of the initial crack on simulation results can be ignored, since the length of the initial crack is smaller than 1/10 of the microstructure model's length. The constant velocity load is imposed symmetrically at the top and bottom edges of the model. The corresponding velocity load can be obtained using the expression $v = \varepsilon \cdot h$, while the constant strain rate is $\varepsilon = 5 \times 10^3$ and *h* is the microstructure height. The total simulation time is 0.5 µs.



Figure 4. Boundary conditions.

The linear decaying cohesive law (Figure 1) is used to characterize the properties of cohesive elements. In this work, all modeling calculations are based on Al_2O_3/SiC_n nanocomposite ceramic tool materials. The material parameters for various elements are listed in Table 1.

Element Type	E (GPa)	ν	T_{max} (MPa)	Γ (J/m ²)
Triangular elements in Al ₂ O ₃	390	0.23	_	_
Cohesive elements in Al ₂ O ₃	390	0.23	644	2.3
Cohesive elements in GBs	78	0.25	186	1
Triangular elements in SiC	430	0.2	—	—
Cohesive elements in SiC	430	0.2	950	5.8
Cohesive elements in interfaces	250	0.25	712	2.5

Table 1. Material properties for the microstructure of Al_2O_3/SiC_n .

4. Simulation Results and Discussion

4.1. Influence of Microstructure Type

In nanocomposite ceramic tool materials, nanoparticle size is under nanoscale and matrix grain size is under microscale or sub-microscale. Therefore, nanoparticles distribute in matrix grains as well as along GBs. According to the distribution of nanoparticles in matrix phases, nanocomposite ceramic tool materials can be divided into three microstructure types, which are intragranular, intergranular and intragranular/intergranular structures. In order to explore the influences of nanoparticle distribution on mechanical properties, models of the intergranular, intragranular and intragranular/intergranular microstructures for Al_2O_3/SiC_n have been established, as shown in Figure 5. The average size of Al_2O_3 matrix grains is 1 µm, while the average size of nano SiC is $d_{nano} = 70$ nm and the volume content of nano SiC is $V_{nano} = 10\%$.

(a) Intergranular



(c) Intragranular/intergranular



(b) Intragranular

The cracking paths of microstructure models are shown in Figure 6. It can be observed that transgranular cracking is predominant in the intergranular structure (Figure 6a), and the crack is deflected continuously into Al₂O₃ grains by SiC nanoparticles located along matrix GBs. For the intragranular structure (Figure 6b), only intergranular cracking happens. The transgranular fracture in the intragranular/intergranular structure is less remarkable than that in the intergranular structure (Figure 6c). As for Al_2O_3/SiC_n nanocomposite ceramic tool materials, SiC nanoparticles and Al₂O₃ matrix grains usually bond tightly together and no glass phases exist. Many researchers have observed this phenomenon by means of high resolution TEM. Figure 7 displays the interface between the Al_2O_3 matrix and the SiC nanoparticle in Al_2O_3/SiC_n [20]. In addition, S. Jiao [21] concluded that the fracture surface energy of interfaces between Al_2O_3 and SiC in Al_2O_3/SiC_n is higher than that of Al_2O_3 grains at home temperature, according to experimental results and empirical formulae. The high-strength interfaces between nanoparticles and matrix grains have a pinning effect on the intergranular crack. At matrix GBs without nano SiC particles, the intergranular cracking is predominant. When the intergranular crack encounters nano SiC located along GBs, it is liable to be deflected into Al₂O₃ matrix grains, and transgranular cracking occurs. As the crack travels along GBs without nanoparticle distribution, the intergranular cracking continues until it is deflected into matrix grains again by another nanoparticle located at GBs. Figure 8 shows the SEM morphologies of Al₂O₃-based nanocomposite ceramic tool materials, in which typical cleavage steps caused by transgranular fractures are clearly observed, and nanoparticles located at GBs are indicated by red arrows [22]. In the case of the intragranular structure (Figure 6b), the intergranular cracking will not be hindered by nanoparticles located in matrix grains. Therefore, the transgranular fracture hardly arises.



Figure 6. Crack growth paths of different microstructure models.



Figure 7. Interface between Al₂O₃ matrix and SiC nanoparticle [20].



Figure 8. SEM morphologies of Al₂O₃-based nanocomposite ceramic tool materials [22].

Based on the energy equilibrium theory of cracking systems [23], as a crack propagates for the length of c, the critical fracture energy release rate G_C can be expressed as:

$$\frac{dU_S}{dc} = -\frac{d(U_E - W)}{dc} = G_c , \qquad (2)$$

where U_S is the fracture energy dissipated during facture, which can be obtained through simulation.

The critical fracture energy release rate G_C is usually regarded as a quantitative description of the fracture resistance of materials. The relationship between fracture toughness K_{IC} and the critical fracture energy release rate G_c is given by:

$$K_{IC} = \begin{cases} \sqrt{G_c E} & Plane \ Stress\\ \sqrt{\frac{G_c E}{1-v^2}} & Plane \ Strain \end{cases}$$
(3)

Figure 11 shows the calculation results of G_C during the fracture process. The G_C of the intergranular structure is higher than that of the intragranular/intergranular structure, and the intragranular structure exhibits the lowest level of G_C . Since the fracture surface energy of matrix grains is above that of matrix GBs (shown in Table 1), the transgranular fracture will consume more energy than the intergranular fracture during the cracking process. Therefore, if taking no consideration of residual stress and merely analyzing the effect of interface bonding strength, nanoparticles located along GBs dominate in the fracture mode transformation from intergranular to transgranular cracking, and in the improvement of fracture toughness for nanocomposite ceramic tool materials.

4.2. Influence of Nanoparticle Size

Figure 9 shows two intergranular microstructure models with different nanoparticle sizes ($d_{nano} = 150$ nm in Figure 9a and $d_{nano} = 70$ nm in Figure 9b). The two models have the same matrix morphologies, with the average matrix grain size $d_{matrix} = 1\mu$ m and the volume content of nanoparticles $V_{nano} = 10\%$.



Figure 9. Microstructures with different nanoparticle sizes.

The cracking paths of the two microstructure models after FEM calculation are shown in Figure 10. For the single phase ceramic tool materials, the main fracture mode is basically intergranular cracking due to weak grain boundaries, while transgranular cracking is more liable to occur in metals with strong grain boundaries [24–26]. Compared with the intergranular cracking in single phase ceramic tool materials, the fracture mode of nanocomposite ceramic tool materials has changed to the mixed mode of intergranular and transgranular cracking. And the transgranular cracking is more obvious in the microstructure with smaller nanoparticles ($d_{nano} = 70$ nm). Nanoparticles located along GBs represent strong obstacles to crack propagation due to their higher mechanical properties. The intergranular crack tends to be deflected into matrix phases when meeting nanoparticles at GBs.

The results of G_C for the intragranular, intergranular and intragranular/intergranular microstructures with two different sizes of nanoparticles (150 nm and 70 nm) are summarized in Figure 11. It can be found that microstructure models with smaller nanoparticles generally exhibit higher levels of G_C , and the characteristics of G_C resulting from different nanoparticle sizes are most remarkable in the intergranular microstructure. As for nanocomposite with the same content of nanoparticles, the toughening effect of microstructures with smaller nanoparticles is improved. That is because microstructures with smaller nanoparticles that are more widely dispersed along GBs, which results in more significant effects on crack pinning and deflection into matrix grains. Crack deflection will absorb extra fracture energy, and the transgranular cracking consumes more energy compared with the intergranular cracking during the fracture process.



Figure 10. Crack growth paths of microstructures with different nanoparticle sizes.





In addition, based on the grain growth theory, nanoparticles located along matrix GBs have a pinning influence on the migration of matrix GBs. The relationship between average matrix grain size and nanoparticle size is given as follows [27]:

$$D \propto R/V_f,$$
 (4)

where *D* is the average matrix grain size, *R* is the nanoparticle size and V_f is the volume content of nanoparticles.

Smaller nanoparticles have a stronger pinning effect on matrix GB migration during the sintering procedure, which will lead to a refinement of matrix grains in microstructures. Cheng [28] observed this phenomenon by fabricating nanocomposite ceramic tool materials with different sizes of nanoparticles at the same volume content. It is known that grain

refinement contributes to improving the fracture strength of materials, since the length of inherent cracks in ceramic materials is commonly the same as the maximum grain size, and materials containing shorter inherent cracks exhibit higher fracture strength based on the Griffith fracture theory [3,29]. From the above, conclusions can be drawn that smaller nanoparticles are useful for the enhancement of the fracture strength and toughness of nanocomposite ceramic tool materials.

4.3. Influence of Nanoparticle Volume Content

Figure 12 shows microstructure models for nanocomposite with $V_{\text{nano}} = 3\%$, 5%, 10%, 15%, 20% and 30%, respectively. The microstructures have the same matrix morphology, with $d_{matrix} = 1 \ \mu\text{m}$ and $d_{nano} = 70 \ \text{nm}$.



Figure 12. Microstructures with different nanoparticle content.

The cracking paths for the microstructures are shown in Figure 13. When the volume content of nanoparticles (V_{nano}) is lower (3%~10%), the intergranular cracking dominates. The microstructure with 15 vol% nanoparticles exhibits obvious transgranular cracking. As V_{nano} arrives at 20%, nanoparticle agglomeration does not arise and the transgranular cracking appears at some sites of the crack path, although V_{nano} is at a higher level and the distances among nanoparticles are relatively small. Some nanoparticles agglomerate together when V_{nano} reaches 30%. The main crack propagates from some region with weaker properties at the bottom of the microstructure model, rather than from the initial crack. The transgranular cracking still exists at some sites of the crack path, but is at a relatively lower level.



Figure 13. Crack growth paths of microstructures with different nanoparticle content.

The results of G_C are plotted in Figure 14. As depicted in Figure 14, G_C firstly shows an increase, and then a decrease trend as the nanoparticle content increases. G_C reaches the peak at $V_{nano} = 15\%$, which indicates that the fracture resistance is at its highest. Many researchers carried out theoretical and experimental investigations on the effect of the volume content of nano SiC on the fracture toughness. Niihara et al. [30] found that the fracture toughness of Al_2O_3/SiC_n reached the maximum with 5 vol% SiC through experiments, as depicted in Figure 15. Levin et al. [31] investigated the relationship between the fracture toughness of Al₂O₃/SiC_n and the SiC volume content, and obtained similar results to Niihara. Conclusions can be drawn from the modeling results in this paper that the microstructure with 15 vol% SiC has the maximum fracture toughness, which is obviously higher than the results published by other researchers. The primary reason for this difference is that the residual stress caused by the thermal expansion mismatch between nano SiC and matrix Al₂O₃ is not taken into account in our model. As the nanoparticle content is at a relatively higher level, there are more nanoparticles in the matrix grains, and the area of residual tensile stress (the thermal expansion coefficient of the Al₂O₃ matrix is higher than that of the SiC nanoparticle) increases as well. Cracking happens easily under the residual tensile stress. That is why the predicted nano SiC content with the maximum fracture toughness is higher in this work compared with other researchers' results.



Figure 14. G_C versus nanoparticle volume content (simulation results in this work).



Figure 15. Relationship between the fracture toughness of Al_2O_3/SiC_n and the volume content of SiC (published by Niihara et al.) [24].

The dispersion of nanoparticles in this work is well controlled by programming. For instance, nanoparticles' dispersion remains excellent in the microstructure as nano SiC content is 20 vol% (Figure 13e), while the agglomeration usually occurs as the nano SiC content arrives at 10% and higher in sintering experiments. Compared with the sintering experiments, more excellent nanoparticle dispersion in our work may be another reason why the predicted nanoparticle volume content with optimum toughening effect is relatively higher. Under the condition of excellent nanoparticle dispersion, fracture toughness increases as the nanoparticle content rises. All of the above analysis leads up to the conclusion that excellent dispersion procedures contribute to improving the fracture toughness of materials.

4.4. Influence of Interface Fracture Energy

In nanocomposite ceramic tool materials, there exist not only GBs among matrix grains, but also interfaces between nanoparticles and matrix grains. Interface bonding strength, matrix GB strength and matrix grain strength will affect the macroscopic strength and fracture toughness of materials through their effects on cracking paths. Interface bonding strength between matrix grains and nanoparticles can vary from different processing methods and conditions, and many investigations have shown that it has a significant effect on the fracture mode. Due to the small grain size and complicated microstructure morphologies, it is very difficult to measure the interface bonding strength by means of experiments. In this section, the influence of the interface bonding strength between nanoparticles and matrix grains on cracking paths and fracture toughness will be discussed.

In actual ceramic tool materials, the strength of nanoparticles is usually higher than that of matrix grains in order to obtain a good toughening effect. Therefore, only the influence of the fracture energy proportions among the interface, matrix grain and matrix GB on the fracture mode is taken into account in this work. Three levels of the proportions of the fracture energy of the interface Γ_{inf} , the matrix grain Γ_{grain} and the matrix GB Γ_{gb} ($\Gamma_{inf} : \Gamma_{grain} : \Gamma_{gb} = 3 : 2 : 1$, $\Gamma_{inf} : \Gamma_{grain} : \Gamma_{gb} = 2 : 3 : 1$ and $\Gamma_{inf} : \Gamma_{grain} : \Gamma_{gb} = 1 : 3 : 2$) are considered. These values indicate strong, intermediate and weak interfaces, respectively. Figure 16 represents three different microstructure models, which are the intergranular, intragranular/intergranular and intragranular structures. The average size of the matrix grain and the average nanoparticle size are 1 µm and 150 nm, respectively. The volume content of nanoparticles is equal to 10%.



Figure 16. Different types of microstructure models ($d_{nano} = 150$ nm).

Figure 17 shows the cracking paths of all microstructures with different fracture energy proportions. It can be seen from Figure 17(a1) that transgranular cracking occurs in the intergranular microstructures with strong interfaces ($\Gamma_{inf} : \Gamma_{grain} : \Gamma_{gb} = 3 : 2 : 1$). Since the interface fracture energy is higher than that of the matrix grain, the intergranular crack is liable to extend into the matrix when encountering nanoparticles located at GBs. Comparing Figure 17(a1) with Figure 18 ($\Gamma_{inf} : \Gamma_{grain} : \Gamma_{gb} = 4 : 2 : 1$), it can be concluded

that the higher the interface bonding strength, the stronger the pinning and deflecting effect of nanoparticles at GBs on the intergranular crack, and the more remarkable the transgranular fracture phenomenon. In Figure 17(b1), where the interfaces are stronger than GBs but weaker than matrix grains ($\Gamma_{inf} : \Gamma_{grain} : \Gamma_{gb} = 2 : 3 : 1$), the intergranular crack tends to surround nanoparticles as it encounters those located at GBs, and continue travelling along GBs when meeting matrix GBs. Similar fracture patterns appear in the intergranular microstructures with weaker interfaces (as shown in Figure 17(c1) with $\Gamma_{inf} : \Gamma_{grain} : \Gamma_{gb} = 1 : 3 : 2$).



Figure 17. Crack paths in different types of microstructures with different fracture energy proportions.



Figure 18. Crack path in the intergranular microstructure with Γ_{inf} : Γ_{grain} : $\Gamma_{gb} = 4:2:1$.

As for the intragranular/intergranular microstructures, transgranular cracking still exists in the model with strong interfaces (Figure 17(a2)). Due to relatively fewer nanoparticles located at GBs in the intragranular/intergranular microstructure, the transgranular fracture phenomenon is less pronounced compared with that in the intergranular microstructure with the same material parameters. In microstructures with intermediate Γ_{inf} : Γ_{grain} : $\Gamma_{gb} = 2 : 3 : 1$ and Γ_{inf} : Γ_{grain} : $\Gamma_{gb} = 1 : 3 : 2$ (Figure 17(b2,c2)), where the interfaces are weaker than matrix grains, cracks are liable to propagate around nanoparticles lying at GBs if they encounter them. And the intergranular fracture continues once the crack meets the matrix GB.

In the case of the intragranular microstructures, the intergranular cracking is predominant for the three fracture energy proportions (Figure 17(a3–c3)), which indicates that nanoparticles distributed in matrix grains have little pinning and deflecting effect on the intergranular crack.

Figure 19 shows the results of G_C for microstructures with different interface strengths. It can be found that for the same microstructure type, materials with strong interfaces $(\Gamma_{inf}:\Gamma_{grain}:\Gamma_{gb}=3:2:1)$ exhibit the highest level of G_C , as well as the highest fracture toughness. This is in good agreement with the simulation results, that the most remarkable transgranular fracture can be observed in microstructures with Γ_{inf} : Γ_{grain} : $\Gamma_{gb} = 3:2:1$. In models with weak interfaces (Γ_{inf} : Γ_{grain} : Γ_{gb} = 1 : 3 : 2), although a few transgranular cracks arise, G_C is the lowest due to the low interface fracture energy. From the above, strong interfaces (Γ_{inf} : Γ_{grain} : Γ_{gb} = 3 : 2 : 1) seem to have a positive effect on the fracture toughness of materials, while weak interfaces (Γ_{inf} : Γ_{grain} : Γ_{gb} = 1 : 3 : 2) may be disadvantageous for material toughening. The results of G_C are in accordance with the results of cracking paths presented in Figure 17. The results of G_C in the intergranular models are relatively higher than other microstructures with the same interface bonding strength. Compared with other microstructure types, G_C in intragranular microstructures is at the lowest level no matter how strong the interface bonding effect is, since nanoparticles in this matrix have negligible impact on the transition of the intergranular cracking to the mixed mode of intergranular and transgranular cracking. Actually, nanocomposite ceramic materials prepared using the sintering method primarily possess the intragranular/intergranular microstructure. Thus, in actual nanocomposite ceramic tool materials, strong interfaces have a significant effect on the fracture mode transition to the mixed mode of intergranular and transgranular cracking, which is advantageous for the enhancement of fracture toughness of materials.



Figure 19. G_C in different types of microstructures with different fracture energy proportions.

Yu [32] modeled the cracking extension in Al_2O_3/TiB_2 composite ceramic tool materials and investigated the relation between Al_2O_3/TiB_2 interface bonding strength and cracking behavior. He found that high interface bonding strength (higher than that of matrix grains) would result in the transition of the fracture mode from purely intergranular cracking to a mix of intergranular and transgranular cracking, as well as the enhancement of the fracture toughness of materials. Zhai [4] studied the influences of interface bonding strength on the cracking behavior of Al_2O_3/TiB_2 composite ceramic materials and reached the conclusion that strong interfaces contribute to enhancing the critical energy release rate of microstructures. These results agreed well with our conclusion.

It should be noted that the conclusion drawn from the numerical results—that weak interfaces are disadvantageous for enhancing the fracture toughness of materials—is based on the premise of the simulation model, in which the interfaces between second phases and matrix phases are all weakly bonded and an intergranular main crack is easily formed under an applied load. However, things may be different in materials with weak-interface-bonding particles independently distributed through the strong interface network. On one hand, weak interfaces are liable to fracture to form microcrack zones under an applied load, which can facilitate microcrack toughening. On the other hand, strong interfaces are able to prevent the coalescence of the main crack and microcracks, and the material strength will not be reduced [33,34]. This is the toughening mechanism for the weak-interface-toughening materials, which is not dealt with in this paper.

5. Conclusions

The macroscopic mechanical properties of ceramic tool materials are determined by microstructures. In order to reduce the brittleness and enhance the fracture toughness of materials, it is necessary to carry out a simulation in microscale and investigate the strengthening and toughening mechanisms in essence. In this work, the cohesive element model of nanocomposite ceramic tool materials is built up by embedding cohesive elements with fracture criteria into microstructures represented with the Voronoi tessellation. Then, the microscopic fracture behavior simulation is carried out to explore the relationship between microstructural morphologies and material responses. This research provides some mean-

ingful investigation results for the design and development of nanocomposite ceramic tool materials, which aims to optimize the tools' fracture toughness. The effect of microstructure type on the cracking patterns and critical energy release rate G_C is analyzed. It shows that the existence of nanoparticles changes the fracture mode from the intergranular cracking of single phase ceramic tool materials into mixed intergranular/transgranular cracking. Nanoparticles located at matrix GBs play a predominant role in the fracture mode transition of nanocomposite, while nanoparticles located in matrix grains have little effect on the intergranular cracking. The influence of nanoparticle size on microscopic fracture behavior is also discussed. Under the condition of the same nanoparticle content, the microstructure with smaller nanoparticles possesses more remarkable transgranular cracking and higher fracture resistance. The relationship between G_C and nanoparticle content is also examined. Finally, the influence of interface bonding strength between nanoparticles and matrix grains on cracking patterns and fracture toughness is investigated, resulting in the conclusion that strong interfaces contribute to improving the fracture toughness of nanocomposite ceramic tool materials.

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