Simulation of microcrack initiation in nanocomposite ceramic tool materials

T Zhou 1, * and C Huang 2

1 School of Mechanical and Automotive Engineering, Qilu University of Technology, Jinan 250353, P. R. China
2 Center for Advanced Jet Engineering Technologies (CaJET), School of Mechanical Engineering, Key Laboratory of High-efficiency and Clean Mechanical Manufacture (Ministry of Education), Shandong University, Jinan 250061, P. R. China
*Corresponding author. E-mail address: zhoutingting506@163.com

Abstract. In this work, the microcrack initiation behavior of nanocomposite ceramic tool materials caused by the residual stress initiated during the cooling stage is simulated by means of a micromechanical model based on the Voronoi tessellation and the cohesive element theory. Influences of microstructure morphologies such as nanoparticle size, nanoparticle volume content and microstructure types on the microcrack distribution and material properties are analyzed respectively. The conclusions are useful for providing theoretical basis for the development of nanocomposite ceramic tool materials.

1. Introduction

The brittle fracture is known as the main fracture mode of ceramic tool materials. Cracks usually initiate from internal defects like pores and microcracks in ceramic tool materials. On one hand, a crack grows under external load and is affected by microstructural heterogeneities such as grain boundaries, porosities, impurities and second phase particles. On the other hand, residual stress forms during the cooling stage after sintering procedure due to the mismatch of thermal expansion coefficients and elastic modulus between matrix and second phases in composite ceramic tool materials, which also has an important effect on the crack path. If the superimposition of the residual stress on the external stress caused by applied load is above the fracture strength of materials, microcracks are liable to initiate in the vicinity of the main crack tip. Microcracking consumes extra fracture energy, releases the stress concentration around the crack tip and is useful for the material toughening. However, if the residual stress is too large, the strength of materials tends to be reduced.

Nanocomposite ceramic tool materials possess more excellent mechanical properties compared with microcomposite ceramic tool materials\(^1, 2\). Due to the size differences between nanoparticles and microsized matrix grains in nanocomposite ceramic tool materials, in which nanoparticles distribute both along GBs and in grains, the residual stress field and the microcrack initiation caused by the residual stress are different from that in the microstructure of microcomposite ceramic tool materials, as well as the toughening mechanism of the residual stress and the microcrack initiation. Therefore, studying the residual stress distribution and the microcrack initiation behavior of nanocomposite ceramic tool materials is able to provide useful theoretical basis for material development.

In this work, the microcrack initiation in nanocomposite ceramic tool materials caused by the residual stress initiated during the cooling stage will be simulated. And influences of nanoparticle size,
nanoparticle volume content and microstructure types on microcrack initiation and material properties will be discussed as well.

2. Simulation models
The simulation of microcrack initiation and cracking behavior will be carried out by means of a micromechanical model based on the Voronoi tessellation and the cohesive element theory. The microstructure models are developed by programming with MATLAB\(^3\). The Voronoi tessellation is utilized to characterize microstructures of nanocomposite ceramic tool materials. And nanoparticles generation are implemented until the size and the volume content of nanoparticles reaching the set value. Then cohesive elements with fracture criteria should be placed along all triangular volumetric element boundaries in order to form the arbitrary cracking paths. Finally, an inp file is compiled to introduce the cohesive model to ABAQUS for FEM calculation after the nodes and elements that lie in matrix grains, matrix GBs, nanoparticles and interfaces are determined.

Figure 1 (a) is a microstructure model represented by the Voronoi tessellation. And Figure 1(b) is the Voronoi tessellation diagram after generating cohesive elements and triangular elements. In Figure 1(b), each Voronoi polygon stands for a matrix grain, while white triangles indicate volumetric elements of matrix grains and blue triangles stand for volumetric elements of nanoparticles. Red and yellow quadrilaterals indicate cohesive elements along matrix GBs and those in matrix grains respectively. Black and green quadrilaterals characterize cohesive elements along interfaces and those in nanoparticles respectively. For easy display reason, the thickness of cohesive elements is magnified and coarser finite element mesh is adopted in Figure 1(b). It is obvious that cohesive elements with fracture criteria distribute among arbitrary adjacent volumetric elements, no matter in grains or along GBs of matrix phases and nano phases. Therefore both intergranular and transgranular cracking can be simulated with our model.

It should be noted that the addition of cohesive elements around volumetric finite elements easily induces the stiffness reduction of a numerical model. However, this issue can be ignored by carefully choosing the cohesive element strength and the finite element size\(^4\).

![Figure 1. Cohesive element model.](image)

3. FEM boundary conditions and parameters setting
Residual stress and microcracks tend to initiate in materials during the cooling stage. In this work, 1500\(^\circ\)C is taken as the temperature at which the residual stress initiates during the cooling stage and the room temperature is set as 20\(^\circ\)C. Therefore, the initiation of residual stress and microcracks can be modeled and the influence of microstructure morphologies on the microcrack distribution can be analyzed. Free boundary conditions are adopted in this step. Then external load is applied and the microscopic cracking behavior in the presence of residual stress and microcracks can be modeled. Explicit integration is employed to conduct the cracking simulation and constant velocity load is imposed symmetrically at the top and bottom edges of the model. The corresponding velocity load can be obtained by the expression \( \nu = \dot{\varepsilon} \cdot h \), while the constant strain rate \( \dot{\varepsilon} = 5 \times 10^3 \) is adopted in the simulation and \( h \) is the height of the model. Bilinear traction-separation law for brittle fracture is used
to describe the properties of cohesive elements.

Al$_2$O$_3$/SiC$_n$ nanocomposite ceramic tool materials are taken for the research subject. The thermal expansion coefficient for Al$_2$O$_3$ matrix is $8 \times 10^{-6}$ and that for SiC is $4.35 \times 10^{-6}$. The other material parameters are shown in Table 1.

Table 1. Material properties for the microstructure of Al$_2$O$_3$/SiC$_n$.

| Element type                      | $E$ (GPa) | $\nu$ | $T_{\text{max}}$ (MPa) | $\Gamma$ ($\text{j/m}^2$) |
|-----------------------------------|-----------|-------|-------------------------|---------------------------|
| 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                       |

4. Simulation results and discussions

4.1 Influences of nanoparticle size

Due to the size differences between nanoparticles and matrix grains, nanoparticles can distribute in matrix grains as well as along matrix GBs in nanocomposite ceramic tool materials. Figure 2 and Figure 3 respectively show intergranular (all the nanoparticles are located along matrix GBs) and intragranular (all the nanoparticles are located in matrix grains) microstructure models for Al$_2$O$_3$/SiC$_n$ with different sizes of nano SiC particles. The microstructure models have the same morphology with the average Al$_2$O$_3$ matrix size $d_{\text{matrix}} = 1 \mu m$ and volume content of nano SiC $V_{\text{nano}} = 10%$. The nanoparticle sizes in Figure 2 and Figure 3 are 70nm and 150nm respectively.

![Figure 2. Microstructure models with $d_{\text{nano}} = 70nm$.](image_url)
The numerical results of residual stress field in the microstructures with $d_{nano} = 70nm$ after FEM calculations are represented in Figure 4. Because of the fact that the thermal expansion coefficient of SiC is smaller than that of Al$_2$O$_3$ matrix, the shrinkage of nano SiC particles is smaller than that of Al$_2$O$_3$ matrix grains during the cooling stage. Thus compressive stress acts in nano SiC particles, whereas tensile stress prevails in Al$_2$O$_3$ matrix grains. More complicated stress condition exists between nanoparticles and matrix grains, which is affected by the location of nanoparticles. It can be observed from Figure 4 that the residual stress distributing around nanoparticles acts as compressive stress in the radial direction and acts as tensile stress in the tangential direction, no matter what kind of the microstructure types is.

The numerical results of microcrack initiation in the microstructures are shown in Figure 5 ($d_{nano} = 70nm$) and Figure 6 ($d_{nano} = 150nm$). It can be observed that the microcrack length is equivalent with the nanoparticle size and shorter microcracks initiate in the microstructure models with smaller nanoparticles, which indicates that the fracture strength of materials increases as the nanoparticle size decreases.

The radial residual stress and the tangential residual stress around nanoparticles can be expressed as \[5\],

$$
\sigma_r = P \left( \frac{R}{r} \right)^3
\]
$$

Where, $r$ is the distance between adjacent nanoparticles. $R$ is the radius of nanoparticles.

It can be deduced from equation (1) that lower tangential tensile stress initiates in microstructures with smaller nanoparticles, which produces smaller microcracks in size. Besides, the pinning effect of smaller nanoparticles on the GBs is stronger\[6\], which leads to smaller matrix size after the sintering procedure. Therefore, conclusions can be drawn that nanocomposite ceramic tool materials with smaller nanoparticles possess higher fracture strength. This is one of the reason why the microcrack size is
smaller in the microstructure of ceramic tool materials with smaller nanoparticles.

Levin et al.\cite{7} regarded that the fracture strength of matrix is liable to be reduced after the addition of nano SiC to ceramic tool materials, which contributes to transgranular cracking. However, the fracture toughness of materials tends to decrease if the fracture strength of matrix is reduced too much. The effect of tensile stress area in the matrix on the fracture toughness of materials can be expressed as\cite{8},

$$K_{IC} = K_{I0} - 2q\sqrt{\frac{2D_l}{\pi}}$$

Where, $K_{I0}$ is the critical fracture strength factor of matrix. $q$ is the local residual tensile stress. $D_l$ is the length of tensile stress area. In terms of nanocomposite ceramic tool materials with the same volume content of nanoparticles, reducing the nanoparticle size is liable to increase the number of nanoparticles and decrease the distance between nanoparticles. The length of the tensile stress area $D_l$ is relevant with the distance between nanoparticles, therefore $D_l$ is liable to be reduced, as well as the weakening effect on the matrix strength. Accordingly, it is beneficial for improving the fracture toughness of ceramic tool materials by reducing nanoparticle size based on equation (2).

![Microcracks in microstructures](image)

(a) Intergranular  
(b) Intragnanular

**Figure 5.** Microcracks initiated in microstructures with $d_{nano} = 70nm$. 
4.2 Influence of nanoparticle volume content

The microstructure models for nanocomposite ceramic tool materials with the volume content of nano SiC as 5%, 10%, 15% and 30% respectively are established. The microstructures are all the intragranular/intergranular structures with the average matrix grain size $d_{\text{matrix}} = 1 \mu m$ and the average nanoparticle size $d_{\text{nano}} = 70nm$.

Figure 7 represents the simulation results of microcrack initiation. With the increase of nanoparticle volume content, the distances between partial nanoparticles decrease and microcracks connect with each other, which is disadvantageous for the improvement of material strength. When the volume content of nanoparticles is too high (30%), some nanoparticles agglomerate and the residual tensile stress increases. Accordingly, microcracks are more liable to initiate around agglomerated nanoparticles. Therefore, it should take measures to control the nanoparticle dispersion during the actual sintering procedure in order to avoid the nanoparticle agglomeration.
4.3 Influence of microstructure types

In order to explore the influence of nanoparticles distribution on mechanical properties, intragranular and intergranular models for Al₂O₃/SiCₙ are established, as shown in Figure 3. The average size of Al₂O₃ matrix grains equals to 1μm, while the average size and the volume content of nano SiC are 150nm and 10% respectively.

4.3.1 Simulation of microcrack initiation. The simulation results of microcrack initiation in intergranular and intragranular microstructures are shown in Figure 6. It can be found that microcracks tend to initiate at matrix GBs around nanoparticles in the intergranular microstructure, since the tangential tensile stress forms around nanoparticles located along matrix GBs and the fracture strength of GBs is weaker than that of grains. As to the intragranular microstructure, in which nanoparticles are all located in the matrix, microcracks produce in the radial direction of some in-matrix nanoparticles under the tangential tensile stress.

4.3.2 Simulation of microscopic cracking behavior under the external load. External load is applied to the microstructure models with microcracks in order to study the effects of intragranular and intergranular microcracks on the fracture mode and the critical fracture energy release rate of materials. Figure 8 is the cracking paths in the intergranular microstructure. It can be observed that transgranular cracking is more evident in the microstructure without microcracks in comparison with the microstructure with microcracks. It indicates that intergranular cracking tends to happen due to the radial microcracks around nanoparticles that are located at GBs, which is disadvantageous for improving the fracture toughness of materials.

Figure 9 represents the cracking paths in the intragranular microstructure. It can be observed that transgranular cracking happens in the intragranular microstructure with microcracks under the applied load (Figure 9(a)), while cracks tend to propagate along GBs in the intragranular microstructure without microcracks (Figure 9(b)). It implies that microcracks around in-matrix nanoparticles in the intragranular microstructure play an important role in the fracture mode transition.

The results of critical fracture energy release rate during the cracking process for the intergranular and intragranular microstructures are shown in Figure 10. For the intergranular microstructures, the critical fracture energy release rate for the model with microcracks is less than that for the model without microcracks. As to the intragranular microstructures, the critical fracture energy release rate for the model with microcracks is close to that for the model without microcracks. Microcracks induced by residual stress tend to cause stress concentration and have a negative effect on the fracture strength of materials. Besides, the fracture surface energy is liable to be reduced since the existence of microcracks tends to decrease the actual fracture surfaces during the propagation process of main crack. Although
microcracks around nanoparticles located along GBs is liable to induce the transgranular cracking in materials to some extent, it is still disadvantageous for the fracture toughness improvement of materials.

![Image](a) With microcracks  
(b) Without microcracks

**Figure 8.** Cracking paths of intergranular microstructures under external load.

![Image](a) With microcracks  
(b) Without microcracks

**Figure 9.** Cracking paths of intragranular microstructures under external load.

![Diagram](Critical fracture energy release rate of microstructures with and without microcracks)

**Figure 10.** Critical fracture energy release rate of microstructures with and without microcracks.
5. Conclusions
In this paper, the numerical simulation of microcrack initiation behavior in nanocomposite ceramic tool materials caused by the residual stress is carried out by means of a micromechanical model based on the Voronoi tessellation and the cohesive element theory. Influences of microstructure morphologies such as nanoparticle size, nanoparticle volume content and microstructure types on the microcrack initiation and material properties are analyzed respectively. The following conclusions can be obtained.

Shorter microcracks initiate in microstructures with smaller nanoparticles, which is good for the material strength. The microcrack density increases as the nanoparticle volume content rises. When the nanoparticle volume content increases to some extent, microcracks located among adjacent nanoparticles are liable to connect with each other, which results in the decrease of fracture toughness. For the intergranular microstructure, microcracks mainly form at GBs around nanoparticles. As to the intragranular microstructure, microcracks primarily produce in the vicinity of nanoparticles that are located in matrix grains. And it can be concluded from the numerical simulation under the applied load that the presence of microcracks in materials is liable to reduce fracture surface areas in the process of crack propagation and decrease the fracture surface energy of materials, which has a negative effect on the fracture toughness of materials.

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