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Micromechanical study of strength and toughness of advanced ceramics

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Abstract

Numerical investigations using the finite volume (FV) method were conducted to examine the effect of microstructure and microstructural properties on the fracture strength of advanced ceramics with industrial applications. Statistically representative microstructural volumes were created using a diffuse-interface model using OpenFOAM-1.6-ext. Crack initiation and growth was modeled using a recently developed arbitrary crack propagation model. It was found that by varying the Young's modulus of the second phase material, a significant change in the maximum failure load was observed. It was also shown that there exists an optimum Young's modulus for which a maximum failure load will be reached. A number of microstructures with a varying percentage second phase material were investigated in this study. Results indicate that for a given set of material and cohesive parameters the maximum failure load was insensitive to the percentage second phase material. This study highlights the role that microstructure and constituent

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properties of brittle ceramics have on influencing the fracture strength of such material. With this in mind, a parametric study was undertaken to examine the competition between crack deflection and crack penetration at the interface between two materials. It was found that appropriate choice of interface strength and toughness as well as second phase material compliance was required in order to promote an overall strength and toughness increase through crack deflection and bridging. Such numerical modeling is essential in order to gain a greater understanding into the structure-property relationship that exists for such advanced ceramics.

Keywords: Fracture strength; Microstructural modeling; Finite volume method.

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1. Introduction

Advanced ceramics are a class of material typically used in demanding material removal operations such as rock drilling. The material under examination is composed of an interlocking matrix of hard grained material, with a small percentage second phase matrix in between the primary phase. During operational conditions these materials are subjected to high temperatures and repeated high rate impacts. The suitability of these materials to such operations is characterized by high hardness, excellent thermal conductivity and high abrasive resistance ([4]). However such materials have a relatively low fracture toughness and strength, and subsequently are prone to premature failure. It is therefore of interest to gain an understanding into the influence of the microstructure on the failure mechanism with a view to

developing a roadmap for the development of improved grades of advanced ceramics.

Recently, it has been shown by [17] that the bulk mechanical and fracture properties of the material under investigation are affected by the underlying microstructure. Much of this work has been conducted experimentally and only provides material properties at the macro-scale. There are many microstructural features, such as phase morphology, phase distribution and microstructural constituents that can significantly influence the properties of such materials. Consequently, it is often difficult to develop an accurate structure-property relationship without considering the stochastic nature of microstructures and how this affects the properties of the material at the micro-scale level. The trial and error experimental approach for development of materials is often costly and time consuming. It is of interest to develop computational models which offer an alternative approach to material design and testing.

Design of improved microstructures involves a detailed understanding of how cracks initiate and propagate within a complex microstructure. There have been multiple approaches to investigating fracture with the Cohesive Finite Element method (CFEM) being among the most widely implemented ([22], [8], and [14]). However, this study will use the Finite Volume (FV) method for all numerical simulations. The use of the Finite Volume (FV) method has become an increasingly popular alternative to solving problems involving stress analysis ([5]). The FV method has been successfully implemented in a wide range of fracture problems. [16], successfully predicted dynamic crack propagation in PMMA, [9] solved fracture problems involving

adhesively bonded joints and more recently, [2] applied the FV method in the area of advanced ceramics.

Prediction of stresses, and fracture paths that are representative of the material failure are facilitated through accurate modeling of the microstructure. Generation of representative volume elements (RVE) for polycrystalline microstructures has traditionally focused on triangulations, through the use of Voronoi tessellation, ([12], [19], and [6]). While it is well established that polycrystalline materials are accurately simulated by Voronoi tessellations, it is often difficult to explicitly represent certain microstructural features accurately, such as discrete pools of second phase materials dispersed within a polycrystalline structure and between grain boundaries.

Another approach taken is the phase-field method ([7], [3], [10], and [15]), where ordered parameters are defined for each individual grain orientation and the microstructure evolves over a specified time. This modeling method is known as a diffuse-interface model, where a finite width describes the boundaries between grains. The advantage of using a diffuse-interface approach over other methods is that the main topological and morphological features of the microstructure are described during the evolution. In three-dimensional systems, such topological changes are described by the disappearance of edges, triangular and two-sided faces, tetrahedral grain and three-faced grains ([13]).

2. Microstructural Model

2.1. Diffuse-Interface Model

The Finite Volume (FV) numerical method is used to generate representative volume elements, (RVE) for the material under investigation. All simulations in this work have been conducted using OpenFOAM-1.6-ext ([20]).

A diffuse-interface model approach, not unlike the phase-field method used for modeling diffusional phase transformations, has been adapted for microstructural generation. In this particular application, grain boundaries are considered as diffuse interfaces, that is across the grain boundary of a finite width, the orientation, or value of a grain changes continuously into the orientation of an adjacent grain. The orientation state of a point in the microstructural system consisting of p grains is described by a set of independent field variables which are continuous functions of both position r , and time t , $\eta_1(r, t), \eta_2(r, t), \dots, \eta_p(r, t)$. For the purpose of modeling grain growth all orientation field variables are solved using equation (1):

$$\frac{\partial \eta_i}{\partial t} - \nabla^2 \eta_i = 0, \quad (1)$$

The origin of the grain boundaries comes from the gradient energy terms, $\nabla^2 \eta_i$, which are non-zero at grain boundaries. For example, for a polycrystalline microstructure comprising of N grains, the grain belonging to an orientation denoted η_i has the properties $\eta_i = 1$ and $\eta_j = 0$ within the grain itself. At the boundary between grains, the orientation of η_i changes continuously from 1 to 0 and everywhere outside the grain its value is 0.

2.2. Microstructure Generation

In order to generate statistically representative 2D microstructures, it was first necessary to generate 3D microstructures where the total percentage second phase material could be controlled. Once a 3D microstructure was generated 2D cuts are taken from this and used for the subsequent 2D simulations, Fig. 1.

The initial microstructure is created by assigning a number of field variables to random points within the computational domain described by $\eta_1(r, t), \eta_2(r, t), \dots, \eta_p(r, t) = 1$. Everywhere else the initial value is $= 0$. As nucleation initializes, the field variables fill the surrounding domain and interact with each other. This results in the annihilation of some grains and the proliferation of others. Topological changes consistent with polycrystalline grain growth are preserved, such as the removal of three-sided grains resulting in triple points where three grains meet ([11]). Between the grains exists the second phase material and once this reaches a desired percentage the simulation is ended.

For the initial 3D simulations, a computational domain of 10 mm x 10 mm x 10 mm was used. This was discretized to have a uniform cell size $\Delta x = 50\mu m$ in all directions with the total number of cells being 8 million. The time-step chosen for the simulation was $\Delta t = 0.005$, and once the second phase material reaches the desired percentage the simulation finishes.

3. Results and Discussion

The microstructures are two-dimensional and plane strain is assumed. A strain rate of $1 \times 10^{-4} \text{ s}^{-1}$ was applied to both the top and bottom boundaries, while the left and right boundaries were treated as periodic. Table 1, shows

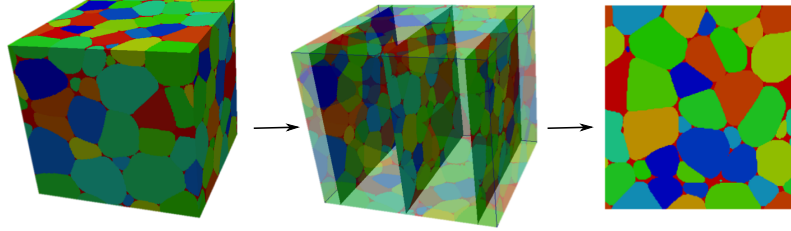


Figure 1: Initial 3-D microstructure with 2-D cuts and resulting microstructure

the initial material properties used in the study.

Table 1: Material properties for advanced ceramic used in this study

	Young's modulus (<i>GPa</i>)	Density (<i>kg/m³</i>)	ν
Grain	800-950	4000	0.1
Second Phase	200	8500	0.33

To examine the role of the second phase material on the overall strength, a number of microstructures with a second phase ranging from 3% - 8% area fraction were tested. A recently developed arbitrary crack solver by [1] was implemented, and a linear traction separation law was specified for the cohesive zone. A cohesive strength, $\sigma_{max} = 1000$ MPa was chosen based on previous experimental work on the material under investigation ([18]). The fracture energy used in this study was $G = 100$ J/m².

It was found that the failure loads for all the microstructures were comparable, failing between 60 - 70% of the maximum σ_{max} value. The data was subsequently fitted to a Weibull distribution for further analysis. The fitted strength distribution was found to have a Weibull modulus of 13.73 (Fig. 2).

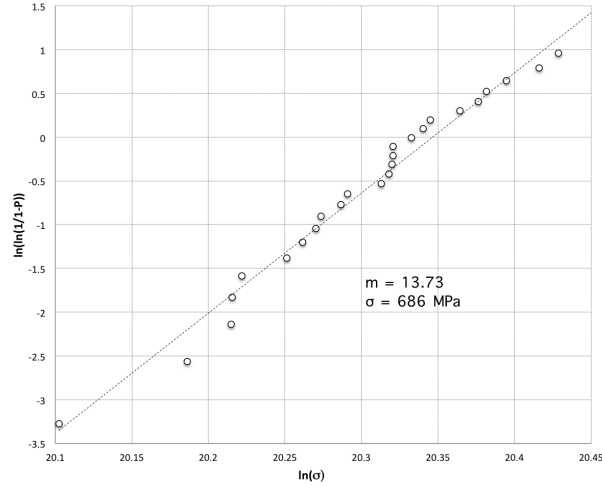


Figure 2: Weibull distribution of strength data using material properties in Table 1

For brittle ceramics, a high Weibull modulus such as this, indicates a low scatter in the measured strength data ([21]). For the range tested in this study, the overall strength of the microstructure was found to be insensitive to the percentage second phase material.

To explore the effect of Young’s modulus mismatch on strength, simulations were conducted with the second phase modulus varying from between 5 - 900 GPa, while keeping the Young’s modulus of the grains constant. A Young’s modulus of $E = 5 \text{ GPa}$ effectively represents a porous sample in this case because the stiffness of the grains is so high, as indicated in Table 1, while the final case is a situation where the second phase is stiffer than the grains themselves. Figure. 3, illustrates the effect of stiffness variation on the overall fracture strength of the material. Taking $E = 200 \text{ GPa}$ as a reference value, it is shown that reducing the Young’s modulus significantly affects the overall strength of the microstructure. This is a result of an increase in the

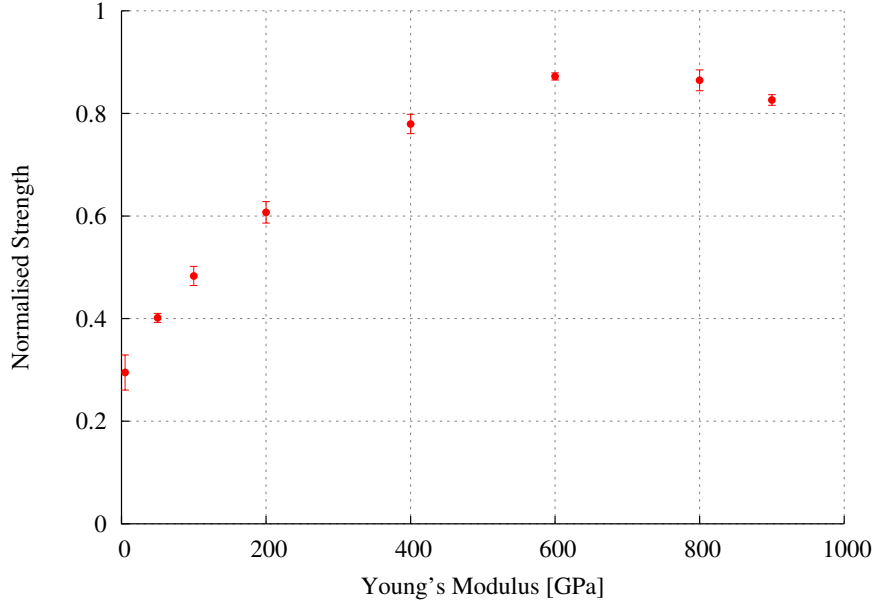


Figure 3: Change in failure strength with second phase Young's modulus

stress concentration factor between the stiff grains and the more compliant second phase. Consequently the grains and grain boundaries adjacent to the compliant second phase will be exposed to a higher level of stress which can lead to premature failure. On the other hand, once the Young's modulus is increased the overall microstructure stiffness increases and the stress concentrations at the interface between the second phase and the grains reduce, resulting in a higher overall failure strength. It can be seen that there exists a maximum Young's modulus for which the greatest strength is achieved. This value corresponds to the stiffness of the grains and once the second phase becomes stiffer than the grain their roles are reversed and the stress concentration factor once again increases and causes a reduction in strength.

Results indicate the microstructure and its constituent properties play

a major role in determining the strength and failure characteristics of advanced ceramics. With this in mind, it is of interest to investigate the role these properties have on the fracture of the material under investigation. A simple case of a circular inclusion surrounded by a stiff matrix under tension was used for this study. The matrix, inclusion and interface strength and toughness remained constant throughout all tests. To explore the effect of modulus mismatch on the crack propagation only the modulus of the inclusion was varied.

Figure 4, illustrates the effect of modulus mismatch on the fracture energy. For a compliant inclusion, where there exists a moderate modulus mismatch, crack penetration through the inclusion was observed, resulting in little if any increase in toughness over a homogenous matrix. For cases with a large modulus mismatch, it was found that crack deflection became increasingly unlikely. However, as the modulus mismatch increased the dominant failure mechanism changed from crack penetration to the inclusion exhibiting ductile ligament bridging across the crack (Fig. ??) which acts to increase the overall fracture energy. As the second phase inclusion increased in stiffness, so too did the tendency for crack deflection which also led to increases in the toughness compared to the case with no inclusion (Fig. ??). Due to the inherent brittle nature of many advanced ceramics an understanding of the microstructural conditions necessary to promote toughness increase is of great importance. It is interesting to note that when the matrix and inclusion have comparable values of stiffness, crack penetration is particularly pronounced and results in a similar fracture energy to that of the homogenous matrix.

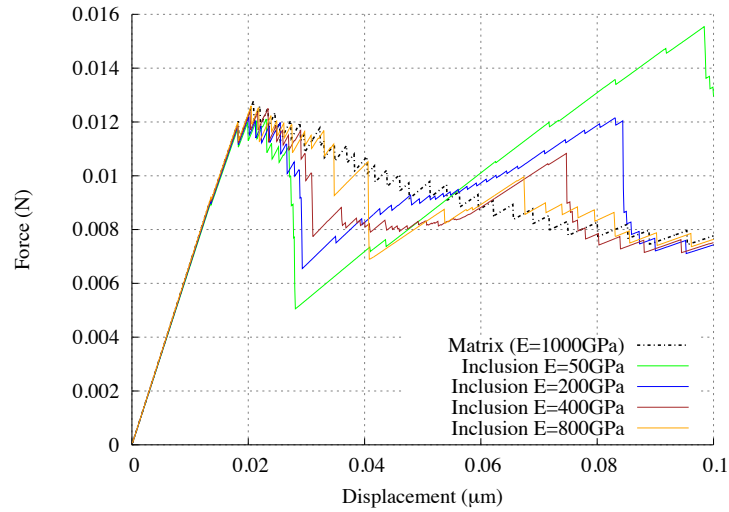


Figure 4: Effect of modulus mismatch on the fracture energy

4. Conclusion

A micro-mechanical FV approach for investigating the effect of microstructure on the strength and toughness of advanced ceramics was presented. A diffuse-interface model was developed to generate representative volume elements for the polycrystalline material under investigation. It was found that the strength of the microstructure was insensitive to the area percentage sec-

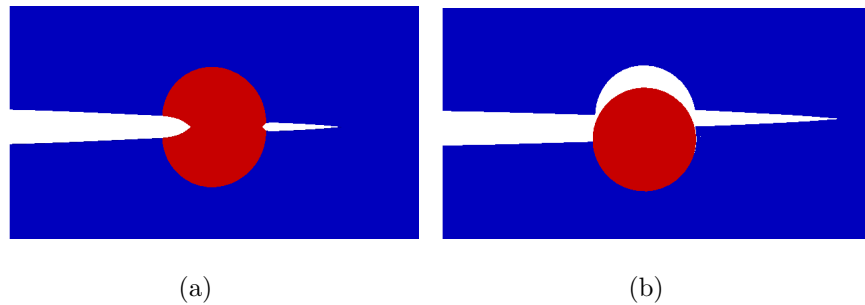


Figure 5: Change in fracture mechanism associated with modulus mismatch

ond phase material for the limited range considered. Simulations show that varying the mismatch between the grains and second phase material had a significant effect on the overall strength and there exists an optimum modulus for which a maximum strength can be achieved. A simple model was simulated to test the effect modulus mismatch has on the feature energy. By varying the modulus of the second phase a transition in fracture mechanism was observed. Crack bridging was observed for the compliant cases and crack deflection became the dominant mechanism as the second phase inclusion modulus increased. From this study the influence of phase morphology and constituent behaviour on the overall mechanical and fracture properties of advanced ceramics has been demonstrated. Continued investigation will lead to future insights into the dominant failure mechanisms and allow the development of an accurate roadmap for future material design.

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