# Micromechanical modelling of advanced ceramics using statistically representative microstructures

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**Abstract**. Advanced ceramics are a class of materials used as cutting tools in some of the most demanding material removal operations. Their high hardness makes them extremely suited for use at these extreme conditions. However they have a relatively low fracture toughness when compared to other conventional tool materials.

A combined experimental-numerical method was used to investigate the role of microstructure on the fracture of advanced ceramics. In particular, the effect of grain size and matrix content were examined. Representative finite volume (FV) microstructures were created using Voronoi tessellation. It is shown, by comparing with real micrographs, that the method captures the features of real microstructures in terms of grain size distribution and grain aspect ratio. It was found that the underlying microstructure significantly affects the failure of this class of materials. Furthermore, it was found that by altering the microstructural parameters in the numerical model, such as grain size and matrix content, it is possible to specify material improvements.

## Introduction

In this study, we examine a two-phase ceramic structure composed of stiff hard particles together with a softer ceramic matrix material. Carolan et al [1, 2] have shown that the strength and toughness of two-phase materials are affected by both the grain size and matrix content. Therefore it is desirable to be able to virtually optimise these parameters to be able to produce stronger or tougher materials for specific applications. By specifying materials virtually, the influence of individual material parameters on the microstructural scale can easily be investigated and altered to change bulk material properties.

A number of authors [3, 4] have generated finite element meshes directly based on actual microstructural images. In this work, however, a representative synthetically generated geometry is produced. Numerous studies have been carried out to produce numerical microstructures using Voronoi tessellation [5, 6]. However there is little in the literature to show that numerical microstructures are actually representative of the real microstructures they were created to replace. This is important, especially in the case of fracture problems, where the morphology of a grain boundary interface is of added importance in initiating fracture.

## Synthetic microstructure generation

Voronoi tessellation was used to generate the geometrical model of the microstructure. It is a commonly used method for the generation of numerical microstructures of ceramic [8, 9] and metallic [7, 10] materials in both two- and three-dimensions. The Voronoi tessellation algorithm produces a random structure, which is representative of a two-phase material. Each Voronoi tile is then reduced in area around the circumcentre of the tile until the desired area fraction of the second interpenetrating phase is reached, see Fig.1.

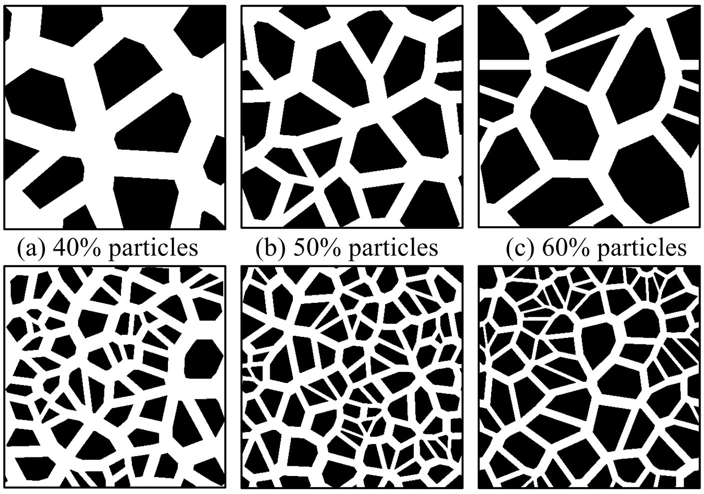
(a) 40% particles (b) 50% particles (c) 60% particles
(d) 40% particles (e) 50% particles (f) 60% particles

Figure 1: Numerical microstructures with (a-c) 5×5 grains and (d-f) 10×10 grains

**Comparison of real and numerical microstructure.** Six synthetic microstructures were generated for investigation, as shown in Fig. 1. Grain size distribution, aspect ratio and percentage primary phase were obtained through image analysis. The generated microstructures had a particle content of 40%, 50% and 60%. This was found to be in good agreement with micrographs of the real advanced ceramics being investigated. The real microstructures have a higher percentage of small grains than its numerical counterpart due to small fragmented grains. However, it is not thought that these small fragments affect the mechanical properties of the bulk material.

## Results

**Finite volume stress analysis.** Finite volume based stress analysis was carried out on the six generated microstructures using OpenFOAM 1.6-ext [11]. Each generated microstructure was 100×100 μm in size with approximate particulate content of 40%, 50% and 60%, but with varying grain sizes. The simulations were 2-dimensional and plane strain was specified in the third direction. The Young's modulus and Poisson's ratio for the grains are 800 GPa and 0.1 respectively, while for the matrix material $E$ = 300 GPa and $\nu$ = 0.1 were chosen for illustration. Both the particulates and matrix were treated as linear elastic over the course of the simulation.

The microstructures were subjected to a normal traction rate of 10 MPa/s in the positive y-direction for a total loading time of 10 seconds, while periodic boundary conditions were applied in the x-direction, see Fig. 2. The periodic boundary conditions ensure that both material and displacement distribution are continuous from right to left.

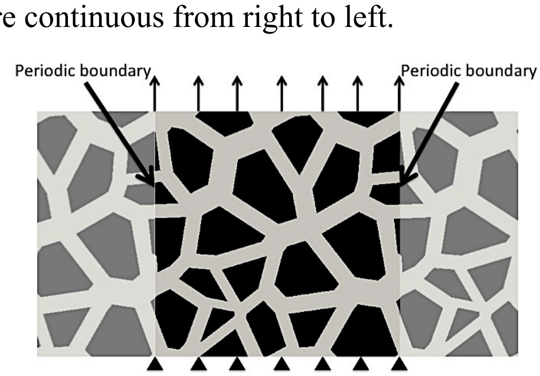


Figure 2: Generated microstructure with periodic boundary conditions subjected to a fixed traction on top surface

**Effective elastic properties.** The Young's Modulus value of a multiphase material depends on the properties of the individual phases. The Young's modulus of the numerical microstructures were calculated using four methods; (i) the effective Young's Modulus was found by averaging the local stress and strain in each cell [18], (ii) a numerical value was found by calculating the average tractions and displacements on the loading boundaries, (iii) a theoretical value was found using the

Eshelby-Mori-Tanaka approach [15–17], and (iv) theoretical upper and lower bounds were found using the Hashin-Shtrikman method [12-14]. The results can be seen in Table 1.

| **Microstructure** | $V_f$ | $E_{HOM}$ **[GPa]** | $E_{LD}$ **[GPa]** | $E_{EMT}$ **[GPa]** | $E_{HS}$ **[GPa]** |
|---|---|---|---|---|---|
| 5×5 | 0.406 | 423.8 | 435.2 | 423.5 | 421.4 – 439.6 |
| 5×5 | 0.501 | 465.1 | 477.8 | 462.5 | 460.0 – 481.1 |
| 5×5 | 0.599 | 510.8 | 524.8 | 508.6 | 505.8 – 528.8 |
| 10×10 | 0.401 | 421.7 | 433.4 | 421.6 | 419.5 – 437.5 |
| 10×10 | 0.500 | 464.8 | 477.8 | 462.1 | 459.6 – 480.6 |
| 10×10 | 0.600 | 507.6 | 522.3 | 509.1 | 506.3 – 529.3 |

Table 1: Elastic properties of numerical microstructures where $E_{HOM}$ is calculated using the homogenisation method (i), $E_{LD}$ is calculated using the load-displacement method (ii), $E_{EMT}$ is calculated using the Eshelby-Mori-Tanaka method (iii), and $E_{HS}$ is calculated using the Hashin-Shtrikman method (iv). $V_f$ is the volume fraction of particulates.

The Young's modulus of the 5×5 and 10×10 microstructures with the same volume fraction of the second phase material was found to be very similar using all the methods for calculating the Young's modulus. This suggests that the Young's modulus is not affected by the grain size.

It was found that the load-displacement method consistently gave higher results than both the Eshelby-Mori-Tanaka and the homogenisation methods. The load-displacement values were found to lie close to the upper bounds of the Hashin-Shtrikman limits. The homogenising was found to give realistic values for Young's modulus, and these values were found to be in good agreement with the Eshelby-Mori-Tanaka method. Both these values tend to lie close to the lower bound of the Hashin-Shtrikman limits.

Fig. 3 plots the distribution of Von-Mises equivalent strain for both the 5×5 and 10×10 microstructures. The highest strains are seen in the more compliant matrix phase. Furthermore, it was noted that the strains were observed in the microstructure with 40% particles and decreased as the particle content increased. This would suggest that as the particle content increases more of the strain is absorbed by the harder phase. Hence, as particle content increases, the material strength also increases.

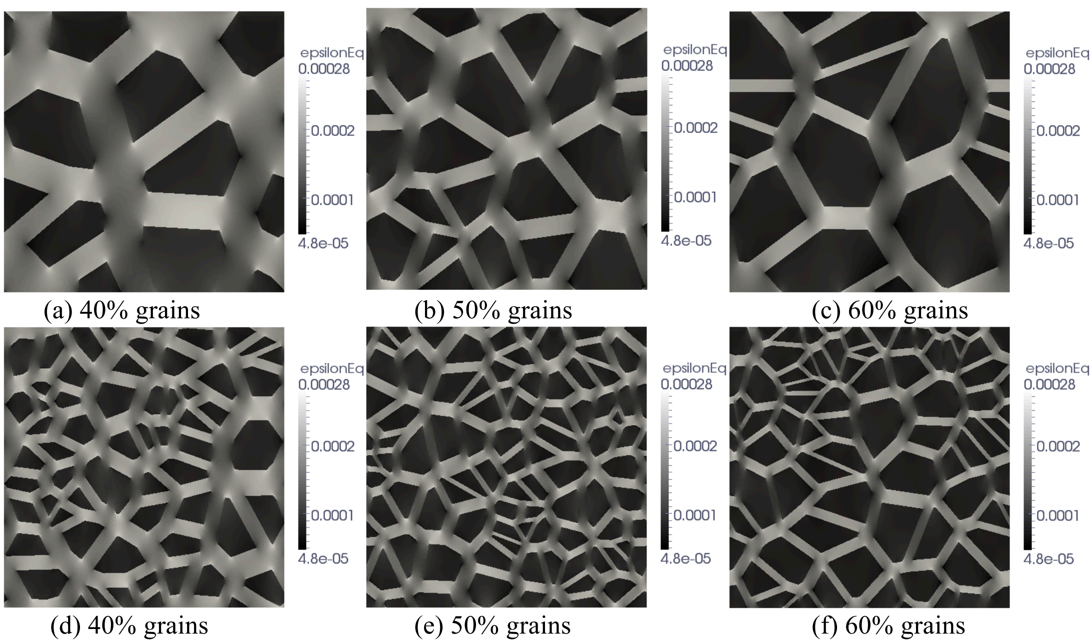


Figure 3: The Von-Mises equivalent strain distribution in the numerical microstructures with (a-c) 5×5 grains and (d-f) 10×10 grains subjected to a normal traction of 100 MPa.

## Conclusion

The purpose of this paper was to develop statistically representative numerical models of advanced ceramic microstructures. The microstructures were generated using the Voronoi tessellation algorithm and subsequently altered to add a specified percentage primary inclusion phase. In the current paper it has been shown that the Voronoi Tessellation technique is a good method for the production of synthetic microstructures. Using the numerically generated microstructures, Finite Volume analysis was carried out to investigate the stress and strain distributions in the microstructures and hence calculate the effective Young's modulus. It was observed that the higher strains occur in the more compliant second phase material. Furthermore, it was observed that as percentage particulates increased, the stress and strain decreased.

The current paper presents a useful and implementable tool for investigating the effect of microstructural parameters on the microscopic stress and strain distribution in a two-phase material. It is intended to extend the predictive capabilities of the models to capture strength and fracture behaviour.

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