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Micromechanical Modelling of Advanced Ceramics with Statistically Representative Synthetic Microstructures

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Abstract. Advanced ceramics are a class of material used in extreme conditions, such as high speed turning of aerospace alloys and rock drilling. Their high hardness makes them suitable for these uses, however their lower toughness means that failure due to fracture and chipping is a problem. They are composed of micron-sized particles of a primary hard phase together with either a ceramic or metallic matrix material.

A combined experimental-numerical method was used to investigate the role of microstructure on the fracture of advanced ceramics. Two dimensional, statistically representative microstructures of the advanced ceramics are created using Voronoi tessellation. The synthetic microstructures are compared to real microstructures in terms of particle size distribution and particle aspect ratio. Simulation results indicate that the computed elastic parameters are within the Hashin-Shtrikman bounds and agree closely with analytical predictions made with the Eshelby-Mori-Tanaka method.

It is found that the local stress and strain distribution within the model is significantly affected by the underlying microstructure, which in turn affects fracture properties. Hence, tailoring the microstructure can optimise the bulk strength parameters of the material.

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 produce stronger or tougher materials for specific applications.

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 [5-7]. However there is little in the literature to show that these 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 as outlined in [8]. The Voronoi tessellation algorithm produces a random structure, which is representative of a two-phase material, Fig. 1a. 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, Fig. 1b.

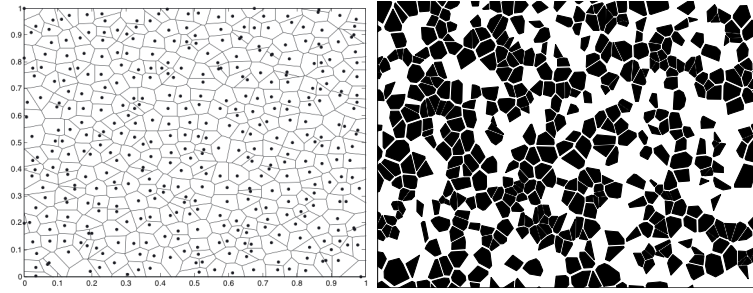


Figure 1: (a) Voronoi tessellation of a microstructure and (b) numerical microstructures with 50% primary phase

Image Analysis

Ideally, the microstructure would be characterised in 3D using serial sectioning. However, sectioning of these extremely hard materials is extremely difficult. As a compromise, a 2D micrograph is used to obtain an approximation of the underlying microstructure. Certain microstructural properties such as grain size distribution and volume fraction can be determined at high magnification from images obtained using scanning electron microscopy (SEM). It is often necessary to work with a binary image when carrying out such image analysis. The process in which the grey-scale image is converted to a binary image is called thresholding.

Watershed segmentation. A difficulty that arises is the problem of touching or overlapping grains. If two or more grains are touching, they will be seen as a single feature by the image analysis software. A common method used for segmenting touching features is the watershed segmentation method [9-11]. The binary image (2b) is converted into a Euclidean distance map, (2c), where the pixel intensity represents the distance of that pixel from an edge. The distance map is then eroded until only the brightest points remain (2d). Finally, the image is dilated from these points at a constant velocity, known as flooding, and when two or more flooded basins meet a dam is built which is the watershed line, (2e), [12]

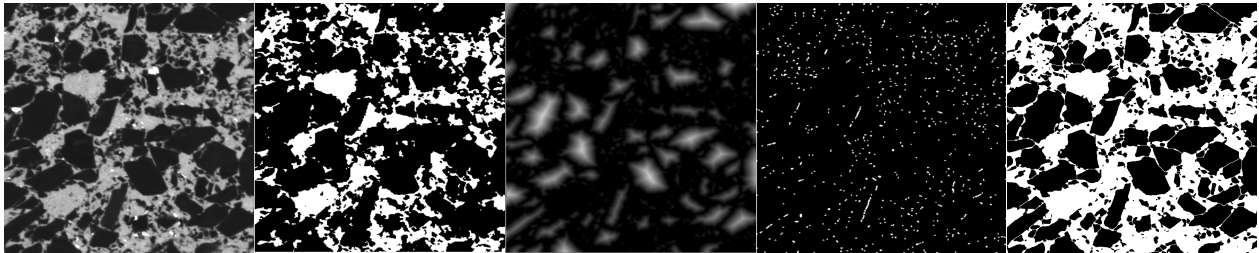


Figure 2: Watershed segmentation sequence with (a) original image, (b) binary image, (c) Euclidian distance map, (d) ultimate eroded point and (e) the segmented image

Comparison of real and numerical microstructure. Grain size distribution, percentage particle phase and aspect ratio were obtained for both the numerical and a corresponding real microstructures. A comparison between the two confirms that the numerical model is a good representation of the real microstructure. Using image analysis it was found that the average primary phase content of the real microstructures was 50.5%, while the generated microstructure, shown in Fig. 1b, had particle content of 50%. The grain size distribution of both the real and the numerical microstructure follow a lognormal distribution with a greater number of small grains (see Figure 3b and 3e). The real microstructure has a higher percentage of these small grains than its numerical counterpart due to small fragmented grains. These small fragments are likely to affect bulk properties, however they have been excluded due to increased computational cost. It is intended to include these in future work. The aspect ratio of the real and the numerical microstructures show excellent agreement, as shown in Figure 3c and 3f. Visually it was also observed that the numerical microstructure resembled the real microstructure, see Figures 3a and 3d.

Finite volume analysis.

Finite volume based stress analysis was carried out on the six generated microstructures using OpenFOAM 1.6-ext [13]. Each generated microstructure was $100 \times 100 \mu\text{m}$ 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.

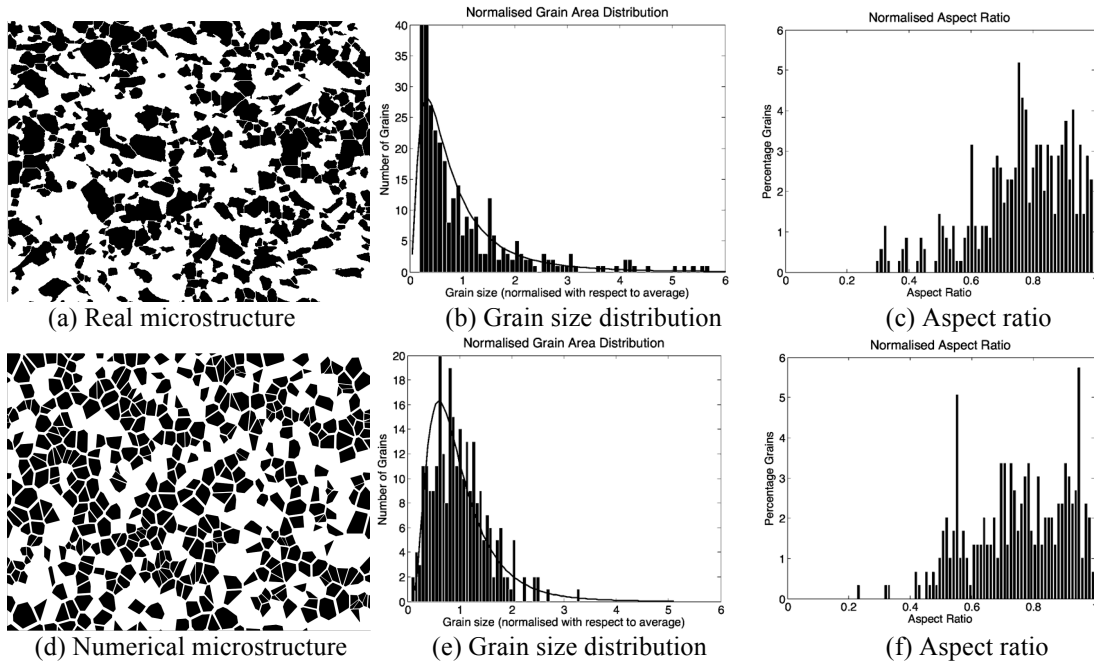


Figure 3: Comparison of real (a,b,c) and numerical (d,e,f) microstructures

Effective elastic properties. The Young's modulus of a multiphase material depends on the properties of the individual phases. The Young's modulus of the numerical microstructure were calculated using four methods: (i) the effective Young's modulus was found by averaging the local stress and strain in the volume [14], (ii) using Hooke's law, 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 [18-20]. The results are shown in Fig. 4.

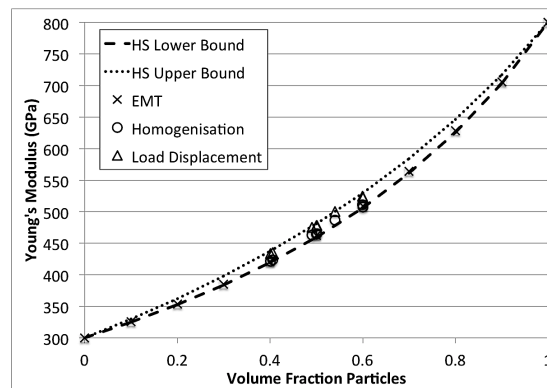


Figure 4: Graph of volume fraction versus elastic properties found using the Hashin-Shtrikman (HS), Eshelby-Mori-Tanaka (EMT), homogenization and load-displacement methods.

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. Homogenisation 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

Conclusion

A method of developing statistically representative numerical models of advanced ceramic microstructures was presented. The microstructures were generated using an adapted Voronoi tessellation procedure. It has been shown that the Voronoi Tessellation technique is a reliable method for the generation of synthetic microstructures for numerical analysis.

The current work 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. Future work will concentrate on extending the predictive capabilities of the micro mechanical models to capture both strength and fracture behaviour.

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