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Analysis of two-phase ceramic composites using micromechanical models

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ABSTRACT

Micromechanical models of two-phase ceramic composites are created using a modified Voronoi tessellation approach. These representative Finite Volume (FV) microstructures are used to investigate the role of microstructure on fracture of advanced ceramics. An arbitrary crack propagation model using a cell-centred finite volume based method is implemented. In particular the effect of matrix content is examined. It is shown that the underlying microstructure significantly affects the local stress and strain distributions for a two-phase ceramic containing hard particles in a softer matrix. Simulation results indicate that an increase in the volume fraction of these hard grains leads to an increase in strength of the composite material. Furthermore, it is found that the homogeneity of the microstructure affects the overall strength.

1. Introduction

Advanced ceramics are a class of materials which exhibit superior properties when compared to traditional ceramics, such as abrasion resistance and high hardness. Due to these superior properties, the materials often find use in extreme conditions involving high temperature and impact loading, for example as tool materials for high speed machining and rock drilling [1]. These extreme conditions may lead to premature failure due to fracture or chipping.

According to Groeber et al. [2] and Ayyar and Chawla [3] early methods for modelling of microstructures did not consider the actual particle shapes and instead used cubes, spheres and ellipsoids as an approximation of the particle shape. However, in reality microstructures are complex and it is well established that mechanical and fracture properties of ceramic materials are affected by the underlying microstructure [4–6]. It has been shown by Carolan et al. [7,8] that the strength and toughness of certain advanced ceramics are affected by both the size of the primary phase and the percentage matrix content. Therefore it is desirable to be able to accurately model these microstructures in order to understand the mechanisms which contribute to failure and guide the development of improved materials. Furthermore, it is important to be able to correctly predict the stresses, crack initiation and propagation characteristics of complex microstructures [9].

Numerical models have been used extensively to model crack growth and in most cases this has been carried out using the Finite Element (FE) method [3]. However in the current work the Finite Volume (FV) method was implemented. Over the last number of years the FV method has become established as an alternative to the FE method for the solution of problems involving stress analysis. The method was first developed for the solution of solid mechanics problems by Demirdžić and co-workers [10–14]. Ivanković and co-workers have applied the FV method successfully to the solution of both fracture problems [15–19] and fluid structure interaction problems [20,21].

Numerous studies have been carried out to produce numerical microstructures using Voronoi tessellatio [22,23,24]. It is well established that polycrystalline microstructures can be modelled using Voronoi tessellations. Nygårds and Gudmundson [25] use Voronoi tessellations to create 3D geometrical models of 2-phase ferrite/pearlite steel with periodic boundary conditions. Kühn and Steinhauser [26] model polycrystalline materials using power diagrams which are a generalisation of Voronoi diagrams for arbitrary dimensions. Voronoi tessellations have also been used to investigate fracture. Espinosa and Zavattieri [27] investigate failure initiation in brittle materials, while Warner and Molinari [28] model compressive fracture of alumina ceramics. Similar to the current study, Zhou et al. [29] and Wang et al. [30] have used

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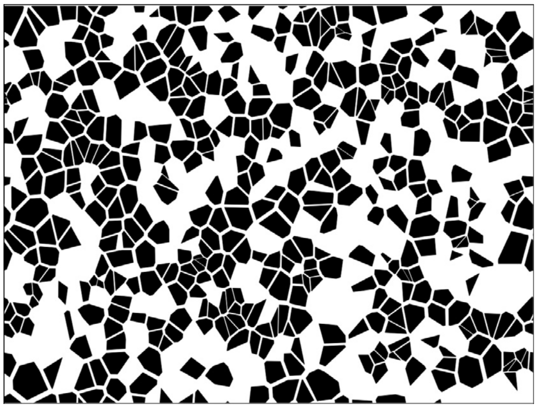

Fig. 1. Numerical ceramic microstructure with 50% particulates and matrix agglomeration.

Voronoi tessellations to investigate crack propagation in ceramic tool materials. Voronoi tessellations have also been used to investigate plasticity by modelling elasto-viscoplastic deformation of rubber-toughened glassy polymers [31].

Zhang et al. [32,33] used a controlled Poisson Voronoi tessellation model to generate polycrystalline microstructures. They introduced control parameters to control the regularity of the microstructure and ensure that the grain size distribution is statistically equivalent to real microstructures. As mentioned previously this is important in the case of fracture problems where the microstructure morphology will affect fracture initiation.

Nygårds and Gudmundson [25], Li et al. [34] and Wang et al. [35] have all created 2-phase microstructures using Voronoi tessellations. In this study we examine a two-phase ceramic structure consisting of randomly dispersed hard particles held together with a softer matrix material. The matrix materials can be either ceramic or metallic.

2. Microstructure generation

2.1. Voronoi tessellation approach

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 and metallic materials in both two- and three-dimensions. The Voronoi tessellation algorithm produces a random structure which is representative of a polycrystalline material as outlined in [36]. To create the two-phase ceramic structure each Voronoi tile is contracted around the circumcentre of the tile until the desired area fraction of the second phase is reached. When viewing micrographs of some advanced ceramics it may be observed that the grains cluster together resulting in regions filled predominantly with the second phase material. These regions will be referred to as matrix agglomerations (MA). In order to create these numerically a specified number of particles are removed from the synthetic microstructure while keeping the overall particle phase content constant, see Fig. 1.

The generated microstructures were all $100 \times 100\ \mu m$ in size with an average particle area of $30\ \mu m^2$. The particle size distributions follow a lognormal distribution as outlined in [36]. The percentage particles was varied from 30% to 70% in increments of 10% as shown in Fig. 2. Three different microstructures were generated for each volume fraction as it is expected that the geometrical variability on the microstructural level will affect the overall material. A further three 50% microstructures with matrix agglomerations were generated to investigate their effect on strength and fracture, see Fig. 2f.

3. Analysis

3.1. Finite volume analysis

Finite Volume (FV) analysis was carried out on the numerical microstructures using OpenFOAM 1.6-ext [38–40]. The simulations

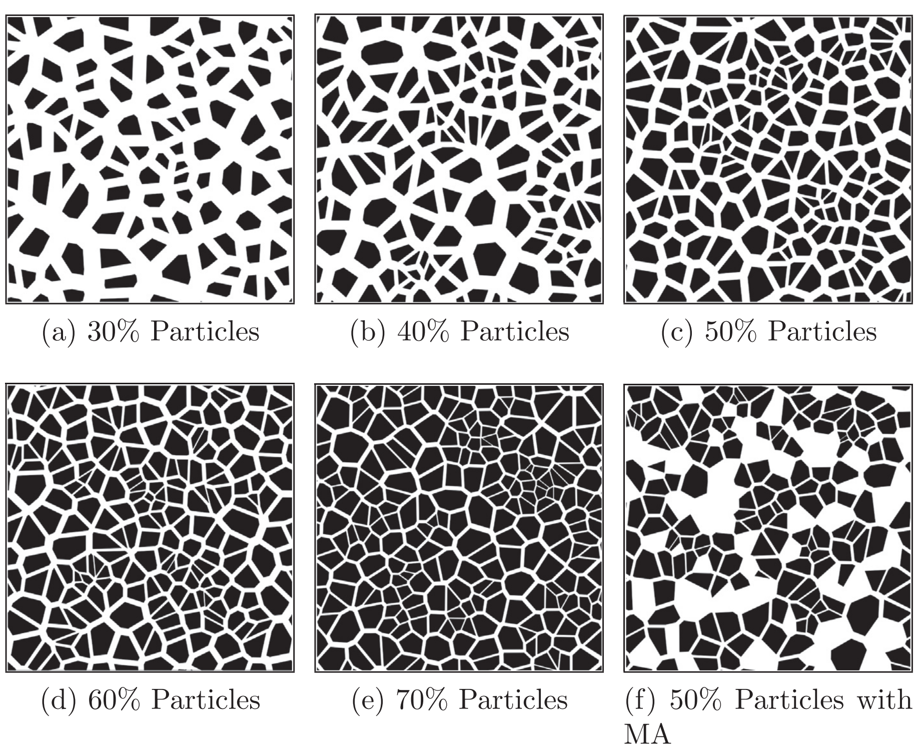

Fig. 2. Two-phase microstructures with varying percentage particulates.