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Explicit fracture modelling of cemented tungsten carbide (WC-Co) at the mesoscale

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ABSTRACT

Using Y-Geo software, the combined finite-discrete element method (FDEM) has been used for the first time to simulate fracture explicitly of cemented tungsten carbide (WC-Co). Although originally designed for geomechanical applications, this study has investigated the use of this numerical approach to model WC-Co material at the mesoscale. The composite material is modelled as a heterogeneous structure using fundamental mechanical properties of the respective phases. A series of simulations are validated against both analytical solutions and experimental observations; these cover both elastic and fracture behaviour of the model. Results show good agreement with both analytical stress distribution solutions and experimental fracture path results. For the first time the discrete fracture process, which has previously been described from experimental images, has been replicated by simulation. The study shows the potential of using the finite-discrete element method as a tool for studying fracture of WC-Co, although the paper also highlights areas of understanding that needs to be improved to achieve a robust model. Ultimately by being able to model fracture behaviour accurately, this would enable a systematic study of microstructural variables in isolation to optimise composition to improve fracture toughness, something which is difficult to do experimentally.

1. Introduction

Cemented tungsten carbide (WC-Co) is a well-established material that displays excellent hardness and fracture toughness, around 1400 Hv and 15 MPa $m^{0.5}$ respectively for the grades of interest; thus it is ideally suited for high abrasion environments. The composite is primarily comprised of a ceramic reinforcement with a metal matrix, not typically making up more than 30% of the total weight. The hard tungsten monocarbide (WC) grains have an interpenetrating network of a softer, ductile binder metal from the iron group of metals, most often cobalt (Co). This combination results in the desirable properties required by many engineering applications such as machining, fluid control valve trim, mining and oil and gas drilling.

Under severe abrasive wear conditions brittle materials, such as WC, are particularly susceptible to highly concentrated stresses from 2nd or 3rd bodies which result in microcracking. Analysis by Larsen-Basse et al. [1] of rotary drill bits after rock cutting operations found microfracturing of WC-Co which led to the removal of large wear debris being detached from the surface. Surface cracks have also been seen to form shortly after percussive drilling starts by Beste et al. [2]. Analysis of the surface of worn rock drilling buttons often reveals a very angular surface with exposed and fractured WC grains, suggesting brittle mode fracture is dominant [3]. Extensive fracture of WC grains has also been observed in tribological laboratory experiments including scratch and microabrasion tests [4–8]. With fracture playing such a critical role in the degradation mechanisms of WC-Co, a fundamental understanding of fracture modes and behaviour would assist in prediction of material behaviour under various conditions and aid development to improve material performance.

A comprehensive experimental study by Sigl and Exner [9] of fracture paths in various WC-Co grades (ranging from 6% to 15% Co) confirmed and expanded on earlier findings from Chermant and Osterstock [10]. Using SEM images, it could be inferred that fracture progressed in discrete steps as follows:

1. Initially, there is the formation of fractures (both intergranular and transgranular) in the WC phase ahead of the crack tip;
2. This is followed by deformation of the Co binder which forms voids and ligaments;
3. Finally, these voids coalesce to form the final fracture path.

Furthermore, although the binder deforms plastically, WC-Co

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behaviour is dictated by the dominant WC phase and can be classed as a brittle material.

Despite the extensive research that has been performed on the wear of WC-Co, surprisingly little progress has been made in the modelling of the material. This is likely due to the challenges of modelling brittle materials in general. While the typical numerical modelling approach uses the finite element method (FEM), a technique based on equations for linear and non-linear stress-strain relationships, this does not adequately describe the brittle nature of ceramics.

Accordingly, early modelling studies [11,12] used available FEM techniques to obtain bulk elastic material properties from real microstructures, where 2D meshes representing real microstructures were modelled with individual WC and Co phases. These generally gave good predictions of bulk material response when compared to experimental results and analytical solutions based on the rule of mixtures approach. Some of the early limitations of these models were the uncertainties associated with the material properties used, an issue which has continued into more recent studies and will be discussed later in further detail.

One of the first attempts at modelling fracture of WC-Co was performed by Sigl and Schmauder [13] also using a 2D FEM. This compared results directly with experimental observations. This study was limited to small-scale yielding of the binder phase as no plastic or fracture behaviour was included. Simulations were initialised with voids in the WC phase to represent the fracture initiation points described in step 1 of the fracture process. Simulations were able to show stress distribution in the binder phase and how this was affected by stress concentrations around existing WC fractures and also neighbouring WC grains. A prediction of fracture path within the binder phase could be made using results from the plane stress condition, which appeared to correspond well with the observed final fracture path. The simulation also supported evidence from experimental observations that the plastic zone does not exceed the binder mean intercept length. The limitations of FEM have led to similar parametric studies focused on binder failure (step 2 of the fracture process) using idealised structures to understand the effect of the binder phase around existing WC fractures [14,15].

McHugh and Connolly [16] extended this approach to idealised structures by using Abaqus finite element software with the addition a modified Rice and Tracey [17] damage model which was implemented through the use of a user defined function. This introduced the effect of ductile failure in the Co phase through the use of a damage parameter in order to predict void growth based on the stress and strain of an element. During the simulation finite elements were effectively removed from the domain once a critical value of the damage parameter had been reached, thereby allowing the model to explicitly simulate crack propagation in the binder phase. A model of an idealised multi-ligament zone (MLZ), which forms in the binder phase in the wake of crack propagation through the ceramic phase, was used to perform a number of parametric studies. The study used an interesting mix of homogeneous and heterogeneous modelling of the WC-Co structure, nevertheless it was able to demonstrate the toughening effect of the binder in WC-Co through a series of crack resistance curves (R-curves). These showed binder ligaments increased fracture toughness by arresting crack propagation.

Dębski and Sadowski [18] compared the Rice and Tracey modelling approach used by McHugh and Connolly with the extended finite element method (XFEM) in Abaqus which used a traction-separation law. The focus of this study was micropores which are created during the manufacturing process and how they lead to void growth. This meant that modelling was restricted to the analysis of the WC/Co interface. The mesh used was based on a very low binder content composition with WC grains surrounded by a thin layer of Co. The two methods approached a qualitative convergence for varying levels of porosity and both indicated a non-linear relationship between porosity and mechanical properties. Although this result was in agreement with other studies no quantifiable validation was presented and the structure modelled is very differently to that used in many engineering applications.

While there has been some research into the fracture of WC-Co, published literature has focused primarily on Co fracture. One of the few times that WC fracture has also been considered is in studying the similar but different field of fracture fatigue. Özden et al. [19,20] performed FEM simulations using Abaqus and applied similar formulations to the tensile fracture simulations. Similar to McHugh and Connolly, a subroutine removed elements once a fatigue failure criterion had been met. The model applied this to a real microstructure which was used in an experimental study. Results showed that it was able to simulate the evolution of fracture propagation under fatigue with good agreement with experimental results. This method of validation was able to both give a visual indication of the accuracy of the simulation and help to understand the nature of fracture propagation.

2. A new approach

More recently, the research software Y-Geo has emerged as a powerful two-dimensional solver that uses a hybrid finite-discrete element method (FDEM) allowing it to model both continuum and discrete element behaviour. This builds on the finite element method (FEM) by adding the ability to simulate particle dynamics through the discrete element method (DEM). The transition from continua to discontinua enables the software to simulate fractures explicitly without predefining fracture paths. Originally developed by Munjiza [21], Y code was further developed by Mahabadi et al. [22] to create Y-Geo. This enhanced the software capability as well as added a graphical user interface (Y-GUI) to simplify and speed up the set-up of simulations [23]. As with much of the research into the modelling of brittle failure, the focus of these studies was civil and geomechanical applications such as concrete and rock core strength modelling. The use of this software has yet to be applied to technical ceramics.

Experimental studies have found that in addition to the material properties of the respective phases, microstructural parameters such as grain size and binder mean free path also have a significant impact in determining the bulk material properties [10,24–26]. This is demonstrated in Fig. 1 where both binder volume fraction and binder mean free path affect the bulk material fracture toughness. Under the rule of mixtures based approach fracture toughness of low binder volume compositions will approach the pure WC fracture toughness of ~4 MPa $m^{0.5}$; whereas high binder volume compositions will approach the pure Co fracture toughness of ~130 MPa $m^{0.5}$ [27]. In practice, manufactured composites will contain between 5% and 30% Co, with

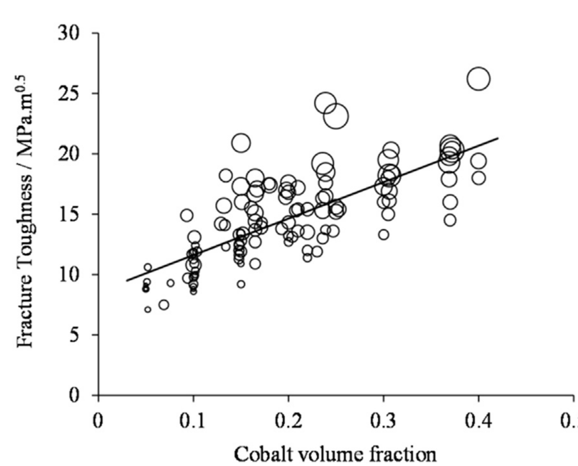

Fig. 1. The relationship between fracture toughness and binder volume. Diameter of circle represents binder mean free path. WC grain size varies between 0.6 μm and 8 μm. Adapted from Ravichandran [28].