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.

Keywords: finite element analysis; finite-discrete element method; fracture mechanics; modelling; ceramics; grains and interfaces

# Introduction

Cemented tungsten carbide (WC-Co) is a well-established material that displays excellent hardness and fracture toughness, around 1400 Hv and 15 MPa.m0.5 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% - 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 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 multiligament 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.

# 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.m0.5; whereas high binder volume compositions will approach the pure Co fracture toughness of ~130 MPa.m0.5 [27]. In practice, manufactured composites will contain between 5 and 30% Co, with fracture toughness’s ranging between 7 MPa.m0.5 and 25 MPa.m0.5 respectively [27]. In addition, the microstructural parameter binder mean free path, λ, which is a measure of the average length of binder between carbide grains and represented by the diameter of the circles, show larger binder mean free paths tend to fall above the average, whereas small values are below. It is therefore important that numerical models which are used to study the fundamental behaviour of WC-Co need to be able to simulate the interaction between the two phases. In order to do this, modelling at the mesoscale is chosen, with domain size in the order of 10 μm to 20 μm. At this scale distinct WC grains, which are typically in the order of 0.5 μm to 5 μm in size, which form the carbide skeleton can be modelled. Furthermore, one of the benefits in modelling is the ability to control these variables fully. Due to the difficulty in isolating individual parameters in the manufacturing process, experimental studies rely on empirical relationships which often vary from one study to another.



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].

A similar FDEM method was employed by Kraft et al [29, 30] to study the compressive and tensile loading of ceramic material aluminium oxide (Al2O3). Discretisation of grains allowed simulation of both intergranular and transgranular fracture. Results showed an interesting effect whereby when attempting to promote one fracture mode (intergranular) another was initiated instead (transgranular). Although the desired increase in mechanical performance of the bulk material was achieved, the crack path was very different to that anticipated. Instead of the fracture toughness being increased through increasing fracture path tortuosity, the fracture had to penetrate through the Al2O3 grains which have a higher fracture toughness compared with grain boundaries. This highlights the importance of trying to gain a full understanding of microstructural effects and although not the same material, the study shows that FDEM simulations could be useful to studying technical ceramics.

The focus of this paper is to investigate if FDEM is a suitable technique to analyse tensile fracture behaviour of the two-phase composite material WC-Co. This will also include studying the full fracture process from microcracks in the WC to coalescing of Co voids as described by Sigl and Exner. To assess the suitability of this approach a real microstructure is used to validate the model against phenomenological observations and current understanding of the fracture process. The limitations of the current model and some proposed solutions will also be discussed. Effort will be made throughout the paper to highlight material assumption and minimise empirical formulations. It is hoped that such an approach will help our understanding of differing experimental results and subsequent theories.

# Numerical Simulation Theory and Implementation

## Pre-processing and meshing

A brief introduction to Y-Geo is provided for the reader’s benefit with algorithms pertinent to the work described. A thorough explanation of the FDEM engine is given by Munjiza [21] which collects published articles into a single body of work. Further details of the additional functionality that Y-Geo provides are given by Mahabadi et al. [22].

The mesh consists of linear triangular elements that are created in a standard way using a coordinate matrix which defines nodes and element matrix defined by nodes. Prior to initialisation of the simulation, the software adds in a joint or cohesive element between all elements, see Fig. 2.

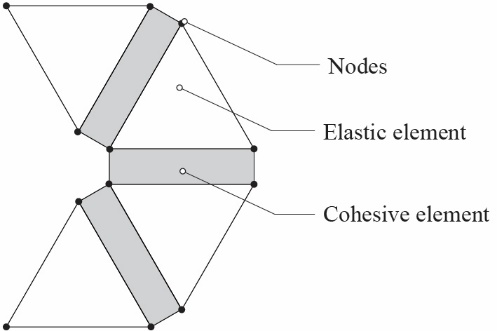


Fig. 2. A simple model showing mesh structure and element types.

Elastic behaviour is simulated using the FEM approach of constituent laws. All material properties are assumed isotropic and linear elastic. The plane strain assumption is used in all simulations in this paper. This presumes that plastic flow perpendicular to the plate is constrained causing a triaxial stress state. This appears reasonable given that a rigid carbide skeleton structure would be surrounding any domain of interest.

The addition of cohesive elements enables explicit simulation of fracture. This is performed through the removal of cohesive elements once a failure criterion has been met. Once cohesive elements are removed this will alter how stresses are distributed within a domain. This process is of interest as fracture propagation of WC-Co has been described as a series of discrete steps. However, as there is no adaptive mesh refinement algorithm, meshing of the domain needs to be sufficiently fine at the outset in order to obtain an accurate stress solution around geometric stress raisers and thereby predict fracture behaviour.

## Fracture simulation

The fracture model handles the transition between continua and discontinua. This process is implemented through a cohesive zone model (CZM), a concept first introduced by Barenblatt and Dugdale [31]. To maintain numerical stability as well as computational optimisation, the stress-strain curve is split into two sections, see Fig. 3. The first section being relatively simple to implement in the standard way through the constitutive law (i.e. stress-strain relation) until element stresses reach a critical stress value, *σ*c; the second section is formulated using a stress-displacement relation. This approach is similar to the traction-separation failure criterion that was implemented in XFEM simulations by Debski and Sadowski and the McHugh and Connolly approaches discussed earlier. The latter, however, used a gradual reduction in stress and stiffness based on time steps rather than displacement. Furthermore, the finite elements were only ‘numerical removed’ meaning that residual values are attached to these elements. In the FDEM approach elements are physically removed from the domain.



Fig. 3. Stress-strain relationship until element stress equals tensile stress b) Stress-displacement relationship until element hits critical displacement.

The cohesive element is broken and removed when displacement of the element reaches the critical displacement, *δ*c, which is defined as:



Where *h*e is the element size and *G*IC is the fracture toughness. A fracture penalty function, *p*f, determines the stiffness of the cohesive elements. If an appropriate value of *p*f is chosen, the value of *δ*c will default to the second condition. To apply a critical strain value to the cohesive elements, the equation needs to be rearranged to incorporate this term. From the definition of strain, displacement of a single element at fracture can be described as:



Where *ε*c is critical strain. Substitution from second conditions of Equation yields:



In order apply the material’s *ε*c Equation is used to calculate *G*IC.

## Additional DEM parameters

Although other important DEM mechanics, including friction, contact detection and element interaction, are coded, these terms are not of interest to the simulations performed in this study as only tensile loading is considered.

## Modelling strategy

Mesh generation with the Y-GUI environment is not well developed, therefore the Abaqus pre-processor is used to create an unstructured triangular mesh and the input file (.inp) exported. This text file has coordinate and element matrices which can be imported into Y-GUI. Simulation parameters, element properties, element relationships and boundary conditions are all setup in Y-GUI, after which a Y-Geo readable text file (.y) can be exported. A separate Matlab script was run to import the material property matrices from the .inp file and added to the Y-GUI created .y file. A flow diagram of the modelling process is provided in Fig. 4.

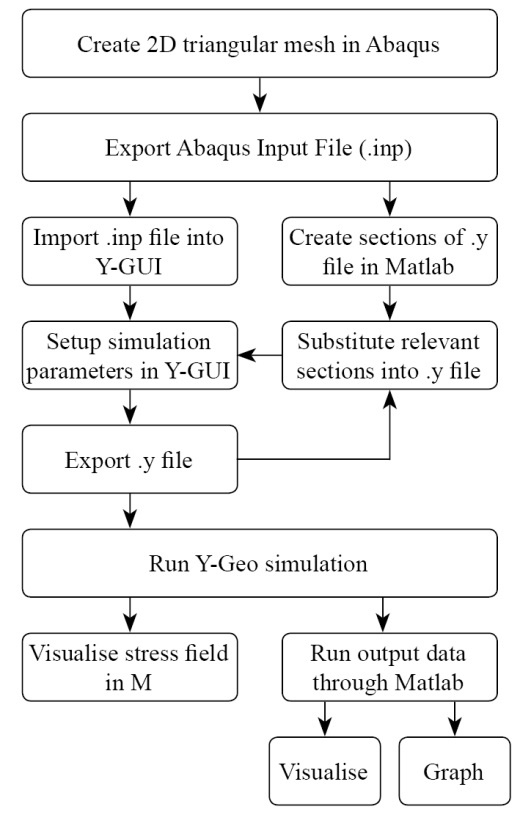


Fig. 4. Modelling and simulation process.

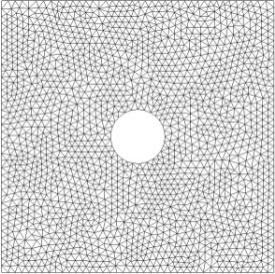
# Validation

## Simulation set-up

In order to validate the ability of the software to accurately predict stress concentration around geometry as well as fracture propagation, simulations were run for stress around a circular hole. The stress distribution could then be compared to the analytical LEFM solution by Kirsch [32]:



A plate with a hole (modelled as a void) at the centre with a radius of *a* is modelled, as shown in Fig. 5. A mesh was generated with element size *h*e = 20 which was found to provide good accuracy and created a mesh with 21668 elements. As critical fracture displacement is defined by element size the mesh size is kept equal over the whole domain.



a) b)

Fig. 5. a) Plate with hole simulation parameters and b) Mesh generated.

In order to create uniaxial tensile loading velocity, boundary conditions are applied to all nodes along the horizontal edges of the domain creating a displacement controlled simulation.

## Elastic properties

There have been many studies on the mechanical properties of WC-Co, along with the many literature reviews which summarise these findings [25, 33-35]. The majority of studies which focus on WC-Co material properties however only consider the bulk material response. In order to model at the mesoscale material properties for the constituent phases is required. Nanoindentation has been shown to be a suitable technique for determining the properties of individual phases in-situ [36].

The Young’s modulus for the binder phase, *E*Co, has been found to be similar to its bulk material properties 200-250 GPa [37, 38]. WC grains, which have an irregular hexagonal structure, one basal {0001} and two prismatic {10–10}, have been found to be anisotropic. Studies using nanoindentation have found basal facets exhibit approximately ×1.5 higher elastic modulus compared to prismatic facets, 400 – 700 GPa and 500 – 900 GPa respectively [38, 39].

However, indention results are restricted to Young’s modulus measurements and hardness measurements. Furthermore, the latter is not an intrinsic material property, but rather a material behaviour that is a result of a complex interaction between multiple material properties. Hardness can be described through other mixture of parameters such as toughness and ductility making modelling using this value next to impossible and therefore cannot be used directly as a modelling parameter.

The elastic material property values used in similar numerical studies have tended to fall within the same order of magnitude. Co properties have ranged from 176 GPa to 227 GPa for Young’s modulus and Poisson’s ratio typically ranging from 0.3 to 0.32.

Although anisotropy of WC has been shown experimentally, with such a large scatter in results in the literature and no clear consensus on the magnitude of difference between the planes, implementing this aspect would be challenging and create even more unknown variables. To date, numerical studies have modelled WC as an isotropic material with Young’s modulus ranging from 600 GPa to 714 GPa and Poisson’s ratio between 0.18 and 0.25. Simulations were performed using the elastic material properties of WC and Co as shown in Table 1, which represents average values found in experimental and numerical studies.

Table 1

Elastic material properties used in simulation [27, 40]

|  |  |  |
| --- | --- | --- |
| Elastic Property | WC | Co |
| Young’s modulus / GPa | 700 | 210 |
| Poisson’s ratio | 0.24 | 0.31 |
| Density / g cm-3 | 15.6 | 8.9 |

## Fracture properties

Although elastic properties are fairly well established, there is much less consensus for the material fracture properties. Values used in simulations appear to vary significantly in the literature especially for the Co phase, with yield strength ranging from between 279 MPa and 2950 MPa. The lower values are approximately equal to the expected values for pure Co (295 MPa – 485 MPa [27]), while upper estimates are based on a one-third hardness value assumption, a factor which has been found approximately true for most metals [41]. This difference has not fully been explained in the various studies although hypothesis put forward for this difference include: alloying of the binder during the sintering process with modifies the composition; size effects; FCC crystal structure as a result of the sintering process which holds Co in its high-temperature structure compared to HCP in its pure form; and the physical effect of the surrounding WC skeleton. These factors have yet to be reconciled.

A numerical investigation by Sadowski and Nowicki [40] into the mechanical properties of each phase a Co yield value of 279 MPa was used. A similar value of 297 MPa was also used by Dębski and Sadowski [18].

There have been some studies on fracture properties of WC-Co. During the sintering process the cobalt binder mixes with tungsten and carbon from the WC powder creating a Co-W-C alloy [42]. Tensile tests were performed by Roebuck et al. [43] on specimens with this composition. Unfortunately no yield properties were reported, however tensile strength values of alloy compositions of interest were in the range of 700 MPa to 950 MPa and fracture strain of between 4% – 12% which are similar in value to those of pure Co.

Although there has been significantly less modelling of WC fracture, likely due to numerical issues discussed earlier, a similar discrepancy of critical stress values has occurred for the WC phase. In fatigue studies of WC-Co by Özden et al. [19, 20] a value of 4000 MPa was used. This is significantly higher than that of WC which is generally quoted by manufacturers of between 350 and 550 MPa [27]. A value within this range, 356 MPa, was used by Dębski and Sadowski as the failure stress of the WC/Co interface.

As the premise of this modelling approach is that the interaction between the individual phases creates the bulk material behaviour, critical stress values are assumed to be within the range of the original material properties. This assumption also agrees with the elastic properties which appear to be similar to their bulk material properties. Simulations were performed using the fracture material properties for WC and Co, as shown in Table 2.

Critical strain values are used to define the critical displacement, as discussed in Section 3.2. Shear strength is calculated using the von Mises yield criterion which takes shear yield stress to be 3-0.5 of the tensile strength. The critical shear strain is assumed to be equal to the critical tensile strain.

Table 2

Fracture material properties used in simulation [27, 40]

|  |  |  |
| --- | --- | --- |
| Fracture Property | WC | Co |
| Critical Tensile Stress / MPa | 450 | 280 |
| Critical Shear Stress / MPa | 260 | 160 |
| Critical strain / % | 0.1 | 8 |
| Mode I Fracture Energy\* | 3×106 | 187×106 |

\* Value calculated from Eq .

## Validation results

The numerical results show how both FEM and DEM parts of the software work. Using the mesh shown in Fig. 5, simulation results showing stress distribution can be obtained, see Fig. 6.



a)



b)

Fig. 6. The transition between continuum and discontinuum behaviour a) stress builds as a tensile force is applied to top and bottom edges and b) fractures propagate outward from the point of maximum stress.

It can be seen from Fig. 6a that as a tensile force is applied tensile stresses slowly build around the hole. A similar stress distribution would be expected from FEM simulations. Once stresses exceed the tensile strength, fracture initiates from the edge of the hole at the point of maximum stress. Stresses in the plate redistribute around this fracture as the fracture itself becomes a point of maximum stress, causing the fracture to propagate outwards along the edges of elastic elements.

Results from the simulation stress distribution along A-A is compared with the analytical solution, see Fig. 7. The simulation shows good agreement with Kirsch’s analytical solution of *σ*yy and *σ*xx. Stresses at the edge of the hole at the point of maximum stress approach the predefined tensile strength of the material just before fracture initiation occurs.



Fig. 7. Stress concentration comparison along A-A between analytical solution and simulation results for WC material simulation just before fracture.

## Validation discussion

This simulation demonstrates the advantage of this type of modelling. While FEM is able to simulate elastic behaviour, failure of the component is assumed when a stress value in the domain exceeds that of the yield strength of the material. This would give a result similar to that seen in Fig. 6a. FDEM, on the other hand, is able to continue to simulate the next phase in this process by simulating fracture initiation and propagation.

From Kirsch’s analytical solution the stress value at the point of highest concentration is three times that of the remote stress (when *r* = *a* and *θ* =π/2). Fracture in the WC and Co simulated materials should occur at 153 MPa and 93 MPa respectively. Simulation results for stress distribution along A-A show good agreement with these values with stress at the edge, where *r*/*a* = 0.2, equal to 160 MPa and 99 MPa for WC and Co simulations respectively. The slightly higher stress values perhaps suggest a slight underestimation of stress concentration, which leads to an overestimation of the stress distribution across the plate.

One of the limitations of the method employed is the lack of dynamic mesh refinement. This becomes very apparent in fracture propagation where bifurcation occurs much more frequently in simulations than would be expected. It typically happens when the corner of an element is in line with the fracture path with each edge angled symmetrically along the fracture path, see Fig. 8a. This makes mesh biasing a crucial consideration in this type of simulation. Typically mesh bias is avoided in numerical studies as it can result in erroneous stress distribution, however in fracture modelling it can be used to provide a more accurate solution when they mimic naturally occurring weaker interfaces such as grain boundaries and slip planes within a crystal lattice. For example, when a bias mesh is used on the plate and hole example with elements aligned along the centre line a horizontal fracture path with no branching can be achieved, see Fig. 8b.

a) b)

Fig. 8. Mesh bias a) showing how it can result in fracture branching and b) simulated fracture path using a bias mesh and Co material properties.

Although not investigated any further, the interaction between the two halves could be studied to understand friction between the two faces through the interaction laws defined in FDEM. This could be important once fracture has occurred and when a shear load across this face is applied.

# Microstructure Simulation Methodology and Set-up

The next stage is to validate against experimental results. An approach similar to that used by Özden et al. [19, 20] is used (discussed earlier), whereby phenomenological observations from an experimental fracture path through the microstructure is compared and contrasted again numerical results.

Fracture experiments conducted by Sigl and Exner [9] provide a good reference as SEM images provide a clear picture of how fracture interacts with microstructural features. A Chevron notched WC-10Co sample (35 mm × 6 mm × 2 mm) was subjected to a loading in three-point bend test, rollers 28 mm apart, and the resulting fracture analysed. The sample microstructural properties are given in Table 3.

Table 3

Sample microstructural properties [9]

|  |  |
| --- | --- |
| Microstructural property | Value |
| Volume fraction / % | 16.5 ± 2.1 |
| Average grain size / μm | 2.18 ± 0.02 |
| Mean free binder path / μm | 0.84 ± 0.02 |

Stable crack propagation was obtained using very slow loading-rate control, 20 N.s-1, allowing the fracture to be arrested before propagating through the whole sample and provide a snapshot in time. A SEM image of the fracture path obtained from the experiment is shown in Fig. 9.



Fig. 9. a) SEM image of fracture path (propagating left to right) in WC-Co [13] and b) skeleton structure used for mesh and annotated with key WC grains and fracture locations: WC (blue) and Co (green).

A triangular mesh based on the microstructure shown in Fig. 9a was created in Abaqus and imported into the Y-Geo environment which represents a domain of approximately 8 μm × 12 μm. This mesh is slightly different to the mesh used in a follow-on FEM study by Sigl and Schmauder [13] in two respects. Firstly, for unknown reasons the microstructure differed slightly to the experimental images. Secondly, in the FEM model it was assumed that fracture had already formed ahead of the main fracture in the carbide phase and therefore fractures at A, B-C, D-E and F-G were introduced, see Fig. 9b. This was performed by introducing voids in the domain to create pre-existing stress raisers. As FDEM can explicitly model fracture, only a single void is introduced into the domain at A by preventing cohesive elements from being introduced between grain *i* and *ii*. This is similar to the experimental study where a Chevron notch introduces a stress raiser.

WC-Co is modelled as a heterogeneous material using intrinsic material properties as per Table 1 and Table 2. WC and Co material was discretised further effectively allowing simulation of the four types of fracture in WC-Co classified by Sigl and Exner, namely:

* fracture along WC and Co interfaces (WC/Co)
* intergranular fracture along WC grain interfaces (WC/WC)
* transgranular fracture within WC grains (WC)
* transgranular fracture through the Co phase (Co)

There is assumed to be WC/WC interaction between WC grains, this aligns with the established theory that there is a continuous carbide skeleton as proposed by Dawihl [44]. Furthermore, continuity of WC grains is assumed i.e. the interface properties between WC/WC are the same as between WC elements within a single grain, although mesh bias is introduced as cohesive elements align along the WC/WC interfaces. The mesh and associated boundary condition described is shown in Fig. 10.



Fig. 10. Mesh created for Y-Geo simulation based on micrograph, using heterogeneous microstructure: WC (blue) and Co (green).

Similar to the plate and hole model, loading is introduced to the domain along the top and bottom edges (*E*2 and *E*4) in order to create a tensile stress through the application of a velocity boundary condition. The magnitude needs to be low enough for stresses to stabilise while considering computational time to induce a large enough force to initiate fracture. Vertical edges (*E*1 and *E*3) are constrained in the *x*-axis to mimic conditions in the experimental setup whereby surrounding elements will constrict the domain. Element size is *h*e = 200 nm, creating a domain of 8343 elements.

As WC and Co elements are now interacting with each other additional definition is required for cohesive elements along the WC/Co interface. Experimental studies by Sigl and Exner [9] found fracture to occur alongside carbide/binder interfaces in the binder phase rather than exactly on it. This would suggest that the cobalt binder properties would dictate fracture at this interface, therefore Co fracture properties are applied to WC/Co interface elements.

# Results

The previous numerical simulation by Sigl and Schmauder only studied the stress distribution in the binder phase for reasons discussed earlier. This, combined with the assumption of linearly elastic elements means that the stress distribution is therefore only valid for small-scale yielding. On the other hand, FDEM is a dynamic simulation and the progression of the fracture through the domain can be visualised. Fig. 11 shows a sequence of images from simulation results plotting stress (*σ*yy) distribution across the domain. Together they illustrate key stages of the crack propagation process.



Fig. 11. Simulation visualisation results of fracture propagation process, showing change in stress yy distribution as the discontinuity advances. Circles and arrows highlighting a) stress concentration in WC grain interfaces b) fracture propagating along WC/Co interface and jumping across binder region creating microfracture ahead of the main crack tip c) microfracture propagating ahead of crack tip and d) microfracture joining up with main fracture and repeat of microfracture process ahead of main crack tip.

As force is applied stress throughout the microstructure increases, with stresses mainly being transferred through WC grains. Local stress concentrations are naturally formed at the interface between grains which are angular due to the shape of the WC crystal, see Fig. 11a.

The initiation notch creates a local stress concentration which starts to propagate along the WC/Co boundary, see Fig. 11b. This propagation halts when it reaches the Co phase which is much more ductile than the ceramic phase. Stress continues to build at the crack tip, but fracture in the Co phase is prevented as the surrounding WC structure constricts displacement. Forces are therefore required to disperse through the adjacent WC grain structure until stresses are sufficiently high enough to cause fracture along a nearby WC/WC interface between grains *iii* and *iv*, see Fig. 11b. Fracture initiates between two grains where a natural stress raiser is created at the interface between two angular grains. Redistributed stresses from the crack tip can initiate fracture at this point and causes the crack to jump across the Co region.

This second microfracture propagates along the WC/WC and WC/Co interfaces in both directions, see Fig. 11c. Stresses in grains *iii* and *iv* fall to zero as the primary load bearing structure is removed. This causes stresses to once again redistributed in the microstructure, resulting in a further increase in stress between grains *v* and *vi*. Failure of the surrounding skeleton structure then allows for further deformation of the binder between point A and B. This imposed strain then leads to sufficient build-up of stress in the binder that failure is initiated. This causes fracture to propagate through the Co phase toward the initial fracture until it finally connects, creating a continuous fracture.

This whole process is repeated as once again the fracture appears to jump across the binder phase between C and D once critical stress is exceeded between grains *v* and *vi*, see Fig. 11d. This initiates another microfracture ahead of the crack front at a WC/WC interface.

A visualisation of the final fracture path, as well as comparison with experimental results, is provided in Fig. 12. Key fracture locations along WC grains at B-C and D-E, as well as connecting fractures through the Co phase between A-B, C-D and E-F are replicated exactly by the simulation. The final fracture path along F-G is not so accurately simulated, reasons for which will be discussed later.



Fig. 12. Final simulated fracture path (red) with respect to microstructure phases WC (blue) and Co (green). Compared with results from experimental fracture of WC denoted by dashed lines.

# Discussion

## Elastic behaviour

In the simulation transfer of stress is initially through the carbide structure, with some stress concentrations occurring in the binder phase at WC grain corners. This indicates that WC-Co behaviour is dominated by WC initially. This result is counter to the behaviour described by Sundstrom whereby the stress-strain relation was first controlled by plastic deformation of the binder phase, followed by yielding of the carbide network. This result would only be possible if the binder can detach from the WC. Furthermore, this behaviour was not observed in fracture experiments which found only slight deformation to the binder phase outside the fracture path and this was limited to within a few λ of the fracture path.

One of the major drawbacks of FEM models is that they are only able to simulate the stress-strain relationships up to the point of failure. Although good correlations between areas which would enter the plastic regime and the location of voids in the binder phase from experimental studies can be obtained, as highlighted by Fischmeister et al. [45], only statistical estimates of where fracture is likely to initiate can be established. Without a method of incorporating the discontinuous nature of fracture the stress redistribution within the domain that follows cannot be captured. Stresses will therefore change as the domain changes and is a significant advantage of the FDEM approach.

## Fracture behaviour

The dynamic simulation results correspond well to experimental observations of the fracture process as described by Sigl and Exner, principally that smaller carbide fractures advance ahead of the crack tip followed by failure of the Co phase which links these fractures, therefore supporting this hypothesis. Furthermore, the final simulated fracture path through the microstructure closely resembles that obtained from the experiment.

The effect of localised stress concentration was observed by Lee and Gurland [46] as a result of compressive loading by hardness tests. FEM simulations by Sigl and Schmauder also highlighted the effect that angular grains had on the stress distribution within the binder phase when subjected to tensile loading. However, relatively little credit has been given to the importance of the geometry in determining the initiation point of fracture in the advancing WC phase microcracks. With stresses concentrated in the WC phase, areas of reduced cross section in the continuous carbide skeleton result in stress raisers being formed. These sections of the microstructure are first to fracture. This initial point then plays a major role in determining the final fracture path as it will dictate the stress field in the surrounding microstructure. Once fracture occurs in the carbide its load carrying capacity reduces to zero, forcing load to be taking up by either surrounding WC grains or in the binder phase. As previously highlighted in previous FEM studies the combination of an existing fracture and increased stress caused by the geometry of the microstructure leads to fracture in the binder phase.

Despite the assumption that fracture properties at the interface between WC grains are assumed equal to the grain itself, the simulation still predicts fracture at these interface points as a result of localised stress concentrations. Once again this lends weight to the importance of microstructure over material properties in determining fracture path. One fracture toughening mechanism that can be created in the microstructure is through increasing fracture tortuosity; that is to say, that the microstructure prevents the fracture from propagating linearly by diverting it around features in the microstructure thereby increase effective fracture length.

However, the simulation deviates from experimental observations in grain *vii* along path F-G, which could be due to a few of reasons. Firstly, because it is a 2D model certain physical characteristics are not captured accurately enough such as where grains are located in the *z*-axis which then affects how they interact with one another. More likely however is that the domain is not large enough to correctly model the fracture. As demonstrated by fractures across B-C and D-E, the surrounding carbide skeleton affects how stresses are distributed around a fracture. Because this is the primary mode in which stresses are transferred through the structure the absence of a modelled microstructure adjacent to the fracture along F-G is likely to impact how stresses are distributed in this area of the domain. Although a fixed boundary condition is applied along both vertical edges, this is not sufficient to overcome this restriction.

Bifurcation is also seen much more in the simulation than in experimental studies which have found little evidence of this. As discussed earlier, this is a result of mesh bias and lack of dynamic mesh refinement. Although mesh bias was introduced along WC/WC grain interfaces, mesh bias was not used to mimic the naturally formed slip planes in the WC crystals. This results in a much more irregular fracture path fracture which propagates where stresses are highest in the WC grain rather than propagating along the weaker crystal planes.

## Future work

There are many opportunities to develop and improve the accuracy of this model. Although not studied in this simulation due to lack of information, the introduction of different fracture properties along WC/WC would be trivial to introduce into the model. This would be particularly important where there is very low binder fraction leading to more WC/WC than WC/Co interfaces. Fracture is therefore likely to progress primarily through the WC and fracture path will be more influenced by properties of WC grain and WC/WC interface, rather than the contrast in properties between the ceramic and binder phase.

WC areas rather than alternating through WC and Co phases as with the domain studied which had 10 wt.% binder content. There is also evidence that grain orientation affects the fracture process [47]. Provided that accurate material properties can be measured for the individual facets, it is possible to implement the structure through specifying different material properties and bias meshing to mimic preferential slip directions.

Numerically, this approach could be developed through the introduction of non-linear stress-strain behaviour and refinement of the damage laws, in particular for the ductile binder phase. Adaptive mesh refinement for fracture models is also of particular interest as unlike standard FEM, the dynamic simulation leads to redistribution of stress as the fracture propagates. This means that the region of interest, usually requiring greater mesh density, moves around the domain. Other more complex phenomena such as thermally induced in-situ stresses and phase transformation in the cobalt which affects the material properties could also be introduced. Although there have been numerical studies into three-dimensional models, the authors believe that the resources required for the additional computational complexity could be better spent on solving the aforementioned phenomena.

One of the primary challenges for modelling is that intrinsic fracture properties are still not well understood, especially for individual in-situ phases of the composite. Shear strength is of particular interest, and although the von Mises yield criterion is likely suitable for the Co phase as it applies to ductile materials, its applicability to the WC phase is questionable. Use of the Mohr-Coulomb criterion would probably be more appropriate for the WC. This is used to define the yield strength of brittle materials and is often employed in geomechanical applications and has therefore already been implemented in Y-Geo. Measurement of these intrinsic properties would need to be carried out experimentally. Previously, experimental studies tend to either measure bulk material properties or restrict material property measurements to only a few variables, making modelling even more challenging to validate. In this study material properties obtained from macro tests of the commercially pure materials were used. However, modern techniques are now able to measure at the microscale. Nanoindentation studies have shown that some material properties are altered as a result of the manufacturing process such as hardness and Young’s modulus. Extension of such work to study other affected material properties, such as interface properties, would be invaluable to modelling a more accurate microstructure. New material data can be incorporated easily into the model through updating element properties. Finally, consideration should be made of the applied strain rates for experimental tests, which can dramatically affect the measured material properties. In the majority of studies, including the simulation presented in this paper, quasi-static loading is used but the applicability of this assumption in a wear system where high strain rates are experienced is questionable. Dynamic loading effects have been demonstrated in Y-Geo previously [48], although the correlation between simulation and experimental values has not been investigated.

# Conclusion

The study successfully demonstrates the suitability of FDEM to analyse the fracture behaviour of the two-phase composite material WC‑Co at the mesoscale. Validation against fracture paths obtained using experimental techniques on WC-10Co and 2 μm grain size show good agreement. This is the first time that the discrete fracture steps in WC‑Co, which has been described using experimental images, has been replicated through simulation. The model uses fundamental material properties, which is important in two respects. Firstly, it supports this fracture process description without having coded it directly. Secondly, it allows this method to be used across any microstructure of interest without multiple variables.

This project opens up a new avenue in research for WC-Co and further our understanding of the wear mechanisms. Development of a comprehensive model would allow us to systematically study the effects of individual material and microstructural influences which are difficult to isolate in experimental studies. Fundamental understanding of this nature could lead to manufacture of optimised WC-Co structures. The model could also be extended to incorporate a full abrasive wear system including 2nd and 3rd bodies, similar to the approach used by Mpagazehe and Higgs [49] who developed a chemical mechanical polishing wear model which integrates multiple physical interactions.

The study also highlights some areas of weakness in our current understanding of the material and which requires further study. Computational work is heavily reliant on intrinsic properties of the materials studied and a larger range of material data would aid validation of numerical models.

Finally, the FDEM approach would also be appropriate to study compressive failure as well as other composite material design in which there well-defined heterogeneous structure. It is particularly useful to understand microstructure influences on the material strength.

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# Data Access

All data supporting this study are openly available from the University of Southampton repository at http://dx.doi.org/10.5258/SOTON/xxxxxx

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