17th International Research/Expert Conference
”Trends in the Development of Machinery and Associated Technology”
TMT 2013, Istanbul, Turkey, 10-11 September 2013

NUMERICAL SIMULATION OF FRACTURE BEHAVIOUR OF CEMENTED CARBIDES

Marin Petrovic, Avdo Voloder, Dzenan Ismic
University of Sarajevo, Mechanical Engineering Faculty
Vilsonovo setaliste 9, 71000 Sarajevo
Bosnia and Herzegovina

ABSTRACT
Cemented carbides are one of the most successful composite engineering materials ever produced. Their unique combination of strength, hardness and toughness satisfies the most demanding applications. These materials have a unique combination of high hardness and good toughness within a wide range and thus constitute the most versatile hard materials group for engineering and tooling applications.
After the fracture tests on notched cemented carbide specimens have been conducted and the relevant properties at initiation determined according to linear elastic fracture mechanics, an appropriate numerical model needs to be developed for the calibration of cohesive laws in order to reproduce the obtained experimental results.
Finite volume modelling of three-point bend tests was performed and numerical results obtained. The impact speed and measured material properties were provided as input parameters, and the cohesive strength for each grade of material was determined across the range of loading rates used in the experiments at room temperature. The numerical simulations were compared to the experimental data and very good agreement was obtained, where the computed force-time curves lie very close to the experimental signals.
Keywords: Cemented carbides, Fracture, Three-point bend, Finite volume analysis

1. INTRODUCTION
The cemented carbides are a range of composite materials, which consist of hard carbide particles bonded together by a metallic binder. They are one of the most successful composite engineering materials ever produced. Their unique combination of strength, hardness and toughness satisfies the most demanding applications. A key feature of this material is a potential to vary its composition so that the resulting physical and chemical properties ensure maximum resistance to wear, deformation, fracture, corrosion and oxidation.
The super hard materials all suffer from lower toughness and poor resistance to sudden fracture. The cemented carbides have a unique combination of high hardness and good toughness within a wide range, along with a good thermal conductivity, and thus constitute the most versatile hard materials group for engineering and tooling applications. They have a wide range of application, from cutting tools and wear parts to drilling in oil and gas industry and mining applications.
The grades used in this analysis contain tungsten-carbide (WC) and cobalt (Co) as the main elements, although small additions or trace levels of other elements can also be found as added to optimize their properties. Two different grades were used in this analysis and are classified according to their WC grain size:
- 4μm average WC grain size, which is referred to as a fine grade (FG)
- 20μm average WC grain size, which is referred to as a coarse grade (CG)

The series of tests on laser-cut notched cemented carbide specimens were previously performed in laboratory conditions at room temperature. Loading rate was varied from quasistatic of 1mm/min up to dynamic of 5m/s using the same procedure as outlined earlier in [1,2]. Using standard equations, the fracture toughness, fracture energy, flexural strength and Young's modulus were determined according to linear elastic fracture mechanics.

2. NUMERICAL METHOD

After the experiment was performed and the relevant properties at initiation determined, an appropriate numerical model needed to be developed for the calibration of cohesive laws in order to reproduce the obtained experimental results. Calibrated cohesive zone models could subsequently be used in analysing more complex components such as WC-Co bits under given in-service conditions.
The behaviour of the continuum is governed by a conservation of linear momentum. An implicit Finite Volume (FV) method was employed in this work, as described by Jasak and Weller [3,4]. An open source software package called OpenFOAM [5] was used in this work. In OpenFOAM the physical entities are described by tensors that vary across time and spatial domains. The Dugdale cohesive zone model was used to describe the damage/failure process of the cemented carbide in terms of the local material traction-separation relationship in the vicinity of the crack tip.

3. MODEL DESCRIPTION

The model of the PCD specimen was created and meshed manually by setting up the code directly in blockMesh, the OpenFOAM mesh generation utility. The spatial domain was discretized using an unstructured computational mesh consisting of hexahedral cells. In order to obtain a converged, mesh independent solution, the mesh was locally refined close to the notch root, as well as close to the symmetry plane. The solution domain and the boundary conditions used in the simulation, as well as the mesh generated, are shown in Figure 1, with close up view of the notch root. The length, width and thickness of the modelled specimen are 14.25mm, 6.25mm and 1.0mm, respectively. A blunt notch was modelled, with average root radius of 155μm, which corresponds to the notch root of the examined specimens. Only half of the specimen is considered due to symmetry, where the left surface is represented initially by a symmetry plane. When the normal traction on the plane reaches a cohesive strength σ_{max}, Dugdale cohesive boundary condition is activated to describe the damage region ahead of a crack. In this case, the traction is assumed to be constant everywhere in the cohesive region ahead of the crack tip. The striker loading was represented by specifying a constant striker velocity boundary condition, while the support cells were fixed. All other surfaces were modelled as stress free boundaries. Plane strain conditions were assumed.

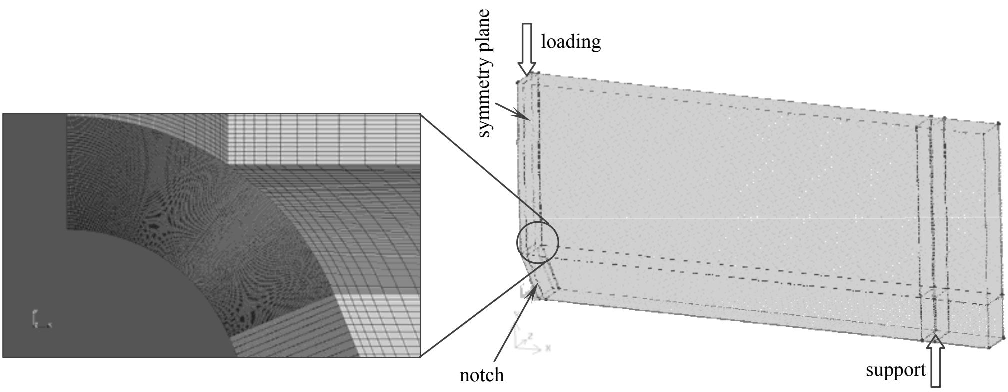

Figure 1. Spatial discretisation of the specimen.

4. RESULTS AND DISCUSSION

Two main parameters must be specified in a cohesive description of material failure: the cohesive strength σ_{max} and the separation energy (fracture resistance) G, which is equal to the area under the traction-separation curve.

At first, the cohesive strength σ_{max} was assumed to be equal to the experimentally obtained value of the flexural strength σ_f. This returned too low ranges of initiation forces, which is understandable as the flexural strength obtained in the experiments was underestimated due to surface flaws and layering effects. For this reason, the cohesive strength values were varied until the numerical initiation load matched the experimental value for a given notch root radius. A linear function between the cohesive strength and the initiation load was obtained across the entire range of simulated loading rates.

For striker loading rate of 1 mm/min, the load-time trace obtained numerically for FG specimen was compared to the experimental ones as shown in Figure 2. The time step of 1 ms was used. Stresses in all faces of the loading patch are calculated and multiplied with corresponding face areas. The sum of all stress-area products represents the loading force.

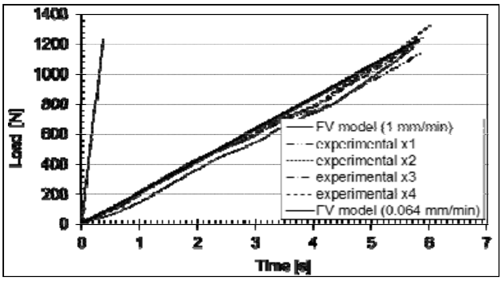

Figure 2. Force vs. time obtained in OpenFOAM for FG specimen loaded at 1 mm/min.

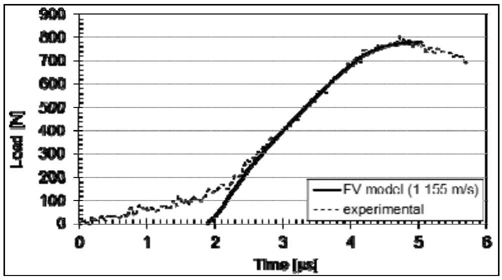

Figure 3. Force vs. time trace obtained in OpenFOAM for FG specimen loaded at 5 m/s.

It can be seen from the graph that the model predicts perfectly linear elastic behaviour as expected and after 0.37 s the crack initiation is predicted (when the opening stress at the crack tip equals the cohesive stress). Once the crack initiation occurs, propagation takes place extremely quickly. The rate of experimental loading and fracture initiation happened more slowly due to the differences in stiffness of the cemented carbide which is an order of magnitude higher than the stainless steel loading rig. The more compliant striker will elastically deform so that the actual impact velocity is lower than the prescribed striker velocity. By applying the lower effective loading rate of 0.064m/s, determined according to the 2D FV simulation matching the strains experimentally and numerically, experiment can be fully matched, as presented in the same graph. Compared to these results, an analysis was also performed for the dynamic case of the FG specimen experimentally loaded at 5 m/s with the time step of 5 ns, for which the load-time trace is presented in Figure 3. Comparison of experimental and numerical load-time traces for CG specimens for two different sampling rates is given in Figures 4 and 5. As can be seen, a good agreement was obtained between the finite volume predictions and the experimental data.

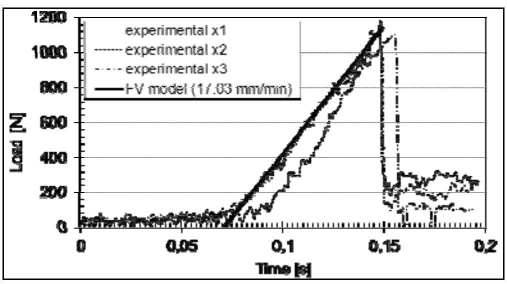

Figure 4. Force vs. time trace obtained for CG specimen loaded at 100 mm/min.

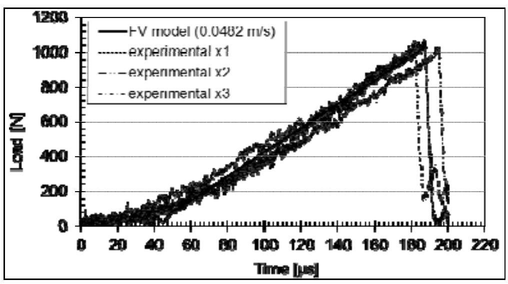

Figure 5. Force vs. time trace obtained for CG specimen loaded at 0.3 m/s.

The cohesive strength values which resulted in good agreement between the numerical initiation forces and the experimental values are given in Table 1.

Table 1. Cohesive zone model parameters used in simulations.

Applied loading rate	FG		CG	
	G_{Ic} [J/m^2]	σ_{max} [MPa]	G_{Ic} [J/m^2]	σ_{max} [MPa]
1 mm/min	387,09	5080	730,11	3000
100 mm/min	329,71	4450	707,79	2590
0.3 m/s	268,91	3770	550,45	2240
1 m/s	205,72	3560	441,21	2080
5 m/s	112,28	2560	250,34	1460

In order to check a universal validity of the determined cohesive strength and its general applicability as a material constant, a sharpened notch of FG specimen was also modelled with the root radius of 27.4 µm, which was a mean radius of the notches of 5 experimentally tested specimens that were previously sharpened. The cohesive strength σ_{max} was varied until the breaking load returned by OpenFOAM matched the experimental breaking load of F = 770N, as shown in Figure 6. The value of σ_{max} = 5050MPa was determined, which is very close to previously obtained 5080MPa for the blunt notch. This means that the cohesive strength numerically determined in these simulations is the material constant and can be used in simulations of realistic geometries.

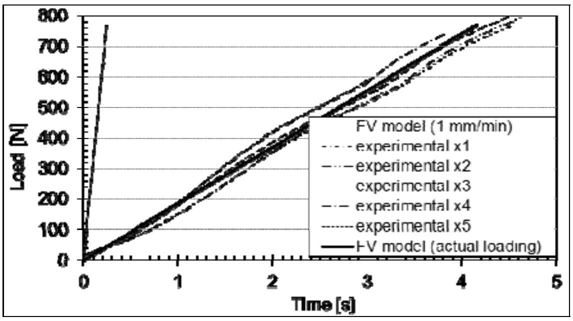

Figure 6. Force vs. time obtained in OpenFOAM for sharpened FG specimen loaded at 1mm/min.

6. CONCLUSIONS

The 2D models used in this research show the suitability of the finite volume method for modelling the fracture of superhard materials. The impact speed and measured material properties were provided as input parameters. The numerical model calibration of force and strain in three-point bend simulations strongly agree with the experimental signals obtained in the fracture tests. Fracture initiation forces from the experiment were matched numerically and the magnitudes of the cohesive strength noted across the range of loading rates. The cohesive zone model parameters obtained in these simulations were confirmed to be accurate and valid for simulation of realistic parts.

7. REFERENCES

[1] Petrovic M., Ivankovic A., Murphy N.: The mechanical properties of polycrystalline diamond as a function of strain rates and temperatures, Journal of the European Ceramic Society, 32:3021-3027, 2012.

[2] Petrovic M., Ivankovic A., Murphy N.: High rate and high temperature fracture behaviour of polycrystalline diamond, Key Engineering Materials, 488-489:670-673; 2012.

[3] Jasak H., Weller H.G.: Application of the finite volume method and unstructured meshes to linear elasticity, International Journal for Numerical Methods in Engineering, 48:267-287, 2000.

[4] Jasak H., Weller H.G.: Finite volume methodology for contact problems of linear elastic solids, Proceedings of 3rd ICCSM, Croatia, pp. 253-260, 2000.

[5] Jasak H., Tukovic Z., Jemcov A.: OpenFOAM: A C++ library for complex physics simulations, International Workshop on Coupled Methods in Numerical Dynamics IUC, Dubrovnik, Croatia, 2007.