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Numerical simulation of fatigue crack propagation in WC/Co based on a continuum damage mechanics approach

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Abstract

WC/Co referred also as hardmetal is one of the most widely used composite materials because of its high strength and wear resistance. The two interpenetrating phases of this advanced material have different mechanical properties: the brittle (elastic) WC phase contributes to the very high hardness whereas the ductile (elasto-plastic) Co phase contributes to the increased toughness of the material. There is a common agreement in literature that the hardmetals exhibit high fatigue sensitivity and the fatigue occurs predominantly in the ductile binder phase featuring ductile failure mechanisms.

In this study the main focus was given to the numerical study of the microscale fatigue crack development in WC/Co. In this respect a damage model based on a continuum damage mechanics approach was implemented in commercial solver Abaqus/Explicit for simulating the crack propagation in the material. Separate damage laws based on brittle failure and fatigue are implemented for the WC and the Co phases, respectively.

In order to evaluate the performance of the approach a numerical model based on a real damaged microstructure was generated. Based on the simulation results, the numerical model reflected strong agreement in comparison with the real crack pattern generated during the experiment. Results of this study indicate a strong dependence of the fatigue crack on accumulated plasticity within the binder phase; this suggests a novel understanding of the fatigue mechanism of this material and provides a basis for larger microstructural models.

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Keywords: WC/Co; Finite Element Method (FEM); Continuum Damage Mechanics (CDM); Fatigue; Crack propagation.

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1. Introduction

WC/Co referred also as hardmetal is one of the most widely used composite materials because of its high strength and wear resistance. The two interpenetrating phases of this advanced material have different mechanical properties in which the brittle (elastic) phase WC contributes to the very high hardness of the material whereas the ductile (elasto-plastic) phase Co contributes to the increased toughness of the material. There is a common agreement in literature that the hardmetals exhibit high fatigue sensitivity and the fatigue effects of hardmetals as well as the ductile failure mechanisms occur predominantly in the binder phase (Schleinkofer et al. (1997), Sailer et al. (2001), Nakajima et.al (2007)). Multiligament zone model suggested in the work of Sigl and Exner (1987) is well accepted as the main mechanism driving the micro crack initiation and evolution in WC/Co under monotonic loads. However, fatigue damage behavior in hardmetals has not been fully understood and contradictory observations on the damage effect of the binder content are present in literature. Some observations indicate an increase of fatigue strength with increasing binder content (Nakajima et al. (2007)) whereas others argues a decrease in fatigue strength with increasing binder content (Sailer et al. (2001)), besides, according to other researchers, there is no evident influence of the binder content on the fatigue behaviour (Kursawe et al (2001)). All these contradictory observations can be related to the varying grades of WC/Co investigated in different studies. However, most recent studies devoted to the fatigue crack propagation in WC/Co claim a strong relation between time dependent toughening of the binder phase and fatigue susceptibility in this material (Tarrago et al. (2013)).

To authors' knowledge, numerical studies evaluating the micro crack initiation and propagation in WC/Co consider explicitly the monotonic loading conditions (Fischmeister et al. (1988), McHugh and Connolly (2003), Debski and Sadowski (2014)). Whereas studies evaluating the fatigue crack are not common in literature. The scarcity of numerical studies in this respect, on one hand, can attribute to the experimental complexity and on the other hand to the limitations on the computational capacity.

The main focus of present study is to simulate the microscale crack propagation in WC/Co under cyclic loads using finite element (FE) method. In this study, both binder and the carbide phases subject to fundamental continuum mechanics principles, and within this context, a damage model based on a continuum damage mechanisms (CDM) approach was used to model the crack propagation in the material. In this respect brittle and ductile damage laws were implemented for the WC and the Co phases respectively.

The material parameters for the WC are taken from literature. Meanwhile, to determine the material parameters for the binder, a particular model alloy has been produced to represent the composition of the binder based on the works of Almond and Roebuck (1988). Experimental investigations are carried out with this binder alloy to identify parameters for more accurate plasticity and damage models.

In order to evaluate the performance of the approach a numerical model based on a real damaged microstructure is generated and the results of the two studies were compared.

Nomenclature

$\boldsymbol{\sigma}$	stress	$\tilde{\boldsymbol{\sigma}}$	effective stress
σ_I	maximum principal stress	σ_{eq}	equivalent stress
D	damage parameter	$\boldsymbol{\sigma}^D$	deviatoric stress tensor
D_c	critical damage parameter	p	equivalent plastic strain
UTS	ultimate tensile strength	$\dot{p}$	accumulated plastic strain rate
c	kinematic hardening modulus	s	unified damage law exponent
r	dynamic rate of back stress	S	energetic damage law parameter
Y	energy density release rate	$\boldsymbol{U}$	displacement
R_v	triaxility function	$\boldsymbol{\Sigma}$	effective stress
E	elastic modulus		
υ	Poisson's ratio		
σ_H	hydrostatic stress		

2. Material Method

2.1. Macroscopic Simulation

The experimental model used for the comparison in this study is introduced by Keusemann et al. (2011). In this prior study the authors investigated the fatigue crack propagation mechanisms of various industrial grades and particularly studied the fatigue crack evolution of a 20 wt. % Co grade with detailed scanning electron microscope (SEM) imagery. Average carbide grain size for this particular grade was reported as 2.18 µm.

As an initial phase of the current study a macroscopic numerical model was generated based on the experimental specimen described in the aforementioned work. Keusemann et al. (2011) indicated that this experimental specimen was subjected to cyclic loading for 857200 cycles until a microcrack of 900 µm was generated. Then the specimen was investigated in SEM for crack path evolution. The microcrack was observed to be emanating from the center of the notched region over the planar surface. Based on this information the model was modelled in the exact dimensions and analogous loading conditions were implemented. Since the model consists of a symmetric structure, the numerical model was simplified accordingly. In fatigue experiments, the samples are submitted to very low external loads and the stress caused by these loads do not exceed the macroscopic yield limit at any material point. Therefore in the numerical study of the fatigue the plasticity was neglected. Exact values for the elastic properties of the component were not provided in the early study; therefore those properties were derived from literature based on a similar grade (Table 1).

To expel the influence caused by discretization, first a mesh convergence study was conducted on the macroscopic model. The results of the convergence study illustrates that the magnitude of global stress components observed in the single element converges after the number of elements exceeds a certain threshold (Fig. 1b). Based on the convergence study, the eventual macro model took first order hexahedral and tetrahedral elements with reduced integration and the entire FE model was composed of 650198 such elements.

The relationship between models in macro- and microscale is provided in Fig.1a. As it is seen from the figure the stress state from a particular hexahedral element is observed to be critical, and thus is mapped to the micro model to study the material's response. Because the out-of-plane components of this stress tensor are quite trivial, the microstructural model adopts a plane stress idealization. In current case, this simplification is sufficient to capture the material behavior of interests.

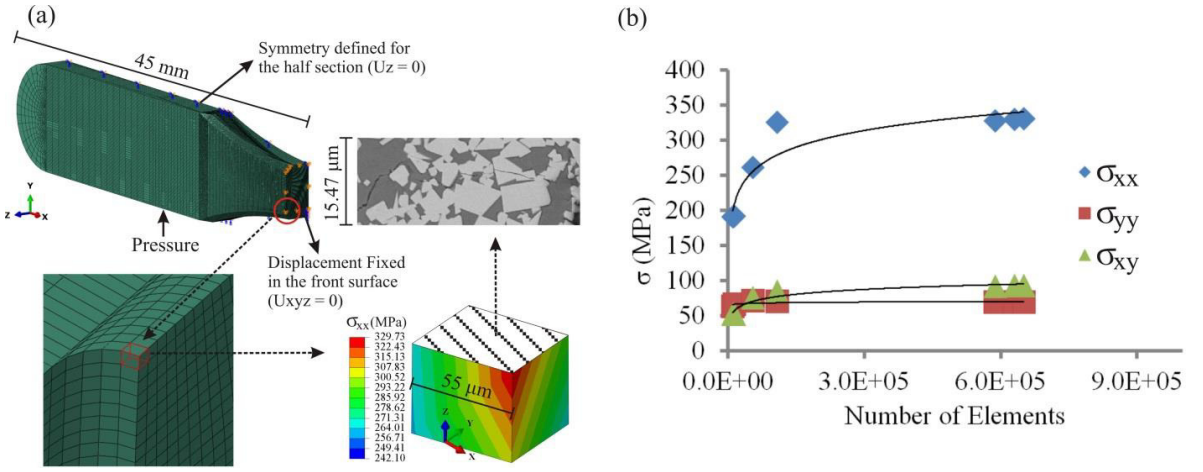

Fig. 1. (a) macroscopic FEM model and its relation to the microstructural model; (b) results of the convergence study.

Table 1. Mechanical properties of the materials used for microscopic and macroscopic simulation.

Material	Elastic Modulus (GPa)	Poison's Ratio (-)	Yield Strain (%)	Yield Stress (MPa)	Kinematic Hardening Modulus (GPa)	Dynamic Rate of Back Stress (-)	Ultimate Tensile Strength (MPa)	Critical Damage Parameter (-)
WC	700.00 *	0.24 *	-	-	-	-	4000	-
Co	227.28	0.30	0.3	683.07	52.379	151.638	-	0.3 (-) [+]
WC/Co [#]	600.00	0.22	-	-	-	-	-	-

[#] Aoki et al. (1996), [+] Lemaitre and Desmorat (2005), * Sadowski and Nowicki (2008)

2.2. Microscopic Simulation

Similar to the macroscopic model a microstructural model was generated based on the work of Keusemann et al. (2011). The model considers only a small section of the fractured area. The FE model attempts to represent the microstructure within a component before it completely fails, thus only elements at certain locations are deleted to represent preexisted local cracks. In this respect elements in two critical positions were deleted as observed from the micrograph (Fig 2).

Both phases of the material were modeled based on a CDM approach with distinctive damage laws. Based on this approach elements are removed from the model as soon as certain damage criteria are met. The remove of failed elements will lead to a degradation of global stiffness. Similar techniques are applied in the works of Mishnaevsky et al. (1999, 2003). To realize this technique, material models for both phases were developed as user defined material subroutine (VUMAT) in commercial software Abaqus 6.11 (2011), and the solutions were calculated in the FEM solver Abaqus using an explicit scheme.

A relatively simple damage law based on the maximum principal stress (σ_I) was implemented for the brittle carbide phase. In this scenario WC grains fail once the critical failure stress value is achieved. To authors' knowledge, among existing literature, an exact value of this parameter for a single carbide grain is still missing. Since WC/Co composites with very high carbide content (90-95 wt. % WC) can obtain transverse rupture strength of up to 5000 MPa, a reasonable value is adopted for the *UTS* of WC phase (Table 1).

For the binder phase, a non-linear damage law based on the accumulated plastic strains is defined. The elasto-plastic material parameters for the model were experimentally determined. In reality, the behavior of the cyclic plastic deformation of a material cannot be explained precisely either by isotropic or linear kinematic hardening law. Therefore, a non-linear kinematic law characterized by both kinematic hardening modulus *(c)* and dynamic rate *(r)* of back stress were used for the Co phase (Dunne and Petrinic, 2005). All of the measured values are provided in Table 1. The full damage constitutive equation for cobalt is derived from Lemaitre and Desmorat (2005) and defined in the user subroutine as follows:

$$\dot{D} = \begin{cases} \left(\frac{Y}{S}\right)^{s} \dot{p}, & if\ p > 0 \\ 0, & if\ not \end{cases} \tag{1}$$

Where

$$\begin{cases} Y = \frac{\tilde{\sigma}_{eq}{}^{2} R_v}{2E}, \\ R_v = \frac{2}{3}(1+\nu) + 3(1-2\nu)\left(\frac{\sigma_H}{\sigma_{eq}}\right)^{2} \end{cases} \tag{2}$$

Where Y is the energy density release rate, R_v is the triaxiality function, E is the elastic modulus, ν is the Poisson's ratio, σ_H is the hydrostatic stress, $\tilde{\boldsymbol{\sigma}}_{eq}$ is the effective stress, σ_{eq} is the equivalent stress, $\boldsymbol{\sigma}^D$ is the deviatoric stress, p is equivalent plastic strain and $\dot{p}$ is the accumulated plastic strain rate. Here the two variables s and S, as defined in Lemaitre and Desmorat (2005), are two material parameters which are functions of temperature.

Since temperature has no effect on the current study, both parameters are unit values. Based on this relationship damage in the element is removed when damage parameter $D = D_c$.

The loading applied to the model is the effective stress ($\boldsymbol{\Sigma}$) retrieved from the macroscopic simulation. Note due to the conversion from 3D to 2D, only in-plane components are reserved. A unit thickness is assumed for the model and the model is constrained by the boundary conditions indicated in Figure 2. The model is composed of 5601 first order linear elastic and elasto-plastic elements.

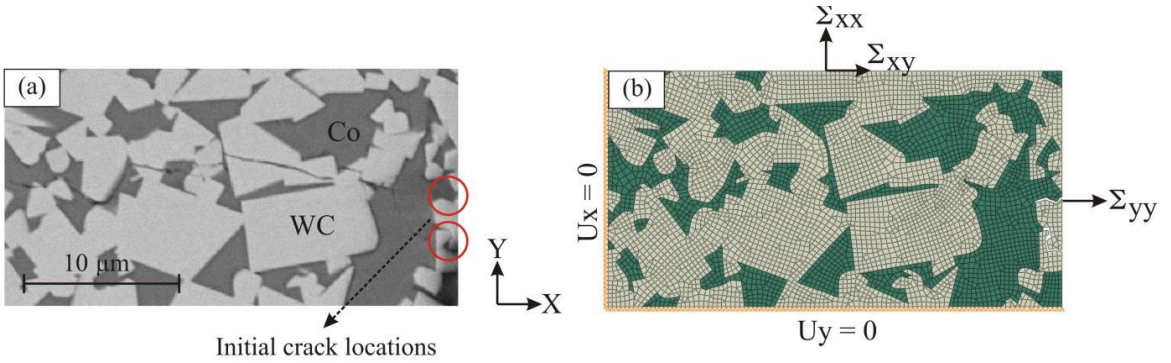

Fig. 2. (a) micrograph of the damaged microstructure; (b) FE model generated based on the micrograph.

3. Results and Discussion

A result was recorded after each 10th increment in order to avoid excessive memory usage. The results of the simulation exhibit a cyclic evolution of the crack path. As observed in Fig.3, the crack initially develops at location where predefined initial crack exists. However after certain number of cycles, damaged elements appear as well on elsewhere distant from this initial region (Fig.3.c). On regions where such secondary damage occurs, significant accumulated plasticity can be observed, and according to (1), such plasticity eventually leads to damage. The results of the simulation reflect strong agreement with the experimental observation. However it has to be indicated that the number of cycles to the failure should not be considered in a quantitative manner since those values are strongly affected by the element size and the overall size of the model. Nevertheless the model does qualitatively capture a similar fracture pattern as observed in a real experiment subjected to cyclic loading.

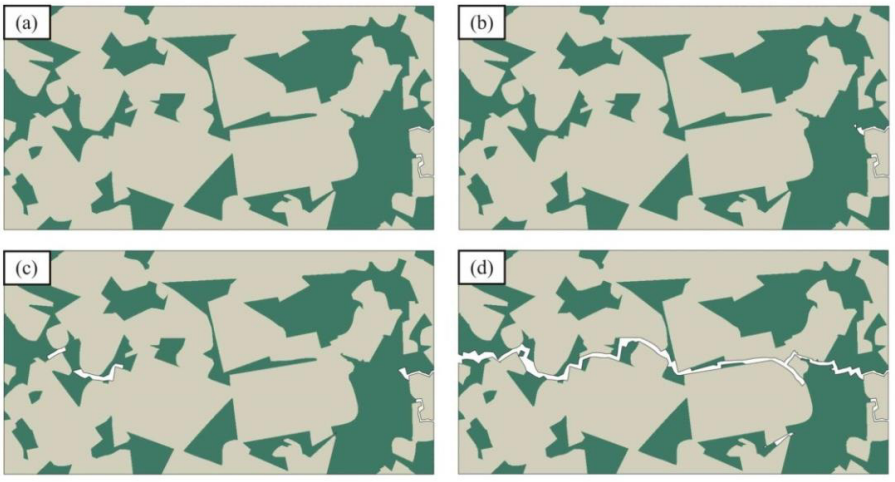

Fig. 3. Evolution of damage in the FE model at (a) 0 cycles; (b) 1000 cycles; (c) 1800 cycles; (d) 1860 cycles.

4. Conclusion

In this study a numerical model based on a real experimental study was generated in order to simulate the microscale evolution of a fatigue crack in WC/Co. In this respect a FEM model based on a continuum damage mechanical approach was implemented in commercial solver Abaqus/Explicit for simulating the crack propagation in the material. Separate damage laws based on brittle failure and fatigue are implemented for the WC and the Co phases, respectively.

Although a small section of the experimental model was considered, the results of the study indicated strong agreement to the real crack evolution in this material. In addition, results of this study also show a strong dependence of the fatigue crack pattern on accumulated plasticity of the binder phase. The study provides a novel perspective of the fatigue damage evolution for this material and it is a basis for larger microstructural models which will be studied in future.

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