Mesomechanical simulation of crack propagation through graded ductile zones in hardmetals
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Abstract
The influence of Co-islands with graded surface zones on the crack resistance of WC/Co hardmetals is addressed. The hardmetal is modelled as a stiff elastic matrix with discontinuously distributed ductile Co-islands. The islands are elliptic in shape and are surrounded by a graded layer of finite thickness with spatially varying properties. A cohesive surface type model is applied to study the crack propagation along a prescribed path through the graded ductile zone. The formulation used here is based on a variational principle with constraints and differs essentially from other proposed cohesive models. The correctness of the posed mathematical problem is discussed. An important feature of this concept is that quite general constitutive relations characterising the material behaviour, on one hand, and the cohesive surface, on the other, can be incorporated into the formulation. In the present study the decohesion criterion is defined as a function of the spatial position in order to capture the variation of the cohesive toughness in the graded zone and the coating. The role of the inclusion thickness, residual stresses and the local decohesion criteria on the crack propagation, retardation and arrest is investigated. © 1998 Elsevier Science B.V. All rights reserved.

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1. Introduction
Fracturing in hardmetals has been of considerable interest over the recent years. A more complete understanding of the nature of crack propagation will contribute towards an accurate description of the fracture mechanism as well as to further material improvement. The paper aims to give a phenomenological basis for an improved model based on a cohesive surface concept. It focuses on the different mechanisms of cracking in the individual phases – unstable and stable crack propagation as well as crack blunting and arrest within Co-rich zones.

The present paper examines the fracture process in WC–Co alloys with up to 25 vol% Co. The considered composite consists of a stiff elastic matrix containing separated elastic–plastic Co-rich inclusions. These ductile islands are assumed to be large enough so that the analysis can be performed based on a continuum plasticity theory.

The shape of the inclusions is taken to be ellipsoidal. This simplification is based on the widely used assumption for an equivalent ellipsoidal
inclusion which allows the main effects of the composite behaviour to be modelled without extensive computations [1]. The Co-inclusions themselves can be heterogeneous due to the presence of non-uniformly distributed carbide particles. The binder rich regions are surrounded by a transition area where the phases interpenetrate [2]. For the purposes of our mesomechanical analysis, this area is modelled as an intermediate composite layer within which the properties are smoothly varied from the ductile inclusion material to the elastic matrix (Fig. 1).

The graded interlayer is modelled as a series of perfectly bonded sub-layers, to each of them being assigned slightly different properties. The $J_2$ deformation theory of plasticity with isotropic hardening is employed to characterise the inclusion material and the graded layer. The elastic behaviour of all constituents is assumed to be linear and is described by Hooke’s law. The flow curves used in the analyses (Fig. 2) are obtained after a best fit approximation of the experimental data reported by Poech et al. [3].

2. Cohesive surface model

The propagation of a vertical crack through a ductile island surrounded by a graded layer (Fig. 3) is simulated using a cohesive surface model. It allows the evolution of crack initiation from the free surface or from a pre-existing crack, crack growth and crack arrest to be described. It is worth noting that this model differs essentially from the so-called “cohesive zone models” (e.g. Needleman [4]) where the prescribed crack path has been characterised as a thin material layer with its own elastic or elastic–plastic constitutive relation (traction – separation law). These relations are such that, with increasing crack opening, the traction reaches a maximum, then decreases and eventually vanishes so that complete decohesion occurs.

In this work the following approach is used: it is postulated that a criterion for decohesion is controlled by the traction transmitted through the cohesive surface. For this purpose special interface elements that are provided in ABAQUS [5] were used. Decohesion under Mode I may occur if the normal traction reaches a critical value (cohesive strength of the material).

$$T_n(s) = \sigma_{n_j}(s)n_j(s) \geq T_n^{\text{critical}}(s),$$

where $s$ is a parameter co-ordinate on the curve along which the crack path is prescribed, $T_n(s)$ is the normal traction transmitted through the prescribed crack path at point $s$, $n_j(s)$ are the normal vector components to the crack path, and $\sigma_{ij}(s)$ are the local stress tensor components. The summation convention with respect to repeated indices is adopted throughout this paper.

It is clear that a key matter in our formulation is the correct calculation of the tractions along the
prescribed crack path (they are continuously distributed), or equivalently, the calculation of the discrete nodal forces. In the numerical solution procedures used here, the nodal forces are taken as primary unknowns. They are calculated by using the Lagrange multiplier method that allows the kinematic contact conditions to be enforced exactly. The decohesion criterion is defined in terms of tractions – they are to be recovered from the obtained nodal forces. The traction over a cohesive surface segment along the prescribed crack path can be obtained by interpolating the nodal tractions $T_n^k$, $k = 1, \ldots, m$ (where $m$ is the total number of contacting nodes) using the interface element shape functions, i.e.

$$T_n(s) = \phi_k(s) T_n^k, \tag{2}$$

In the finite element analysis, the tractions are transformed into equivalent nodal forces at the nodes of the contacting segment,

$$f^k = \int_{\gamma_k} \phi_k(s) T_n(s) \, ds = \int_{\gamma_k} \phi_k(s) \phi_j(s) T_n^j \, ds = H_{kj} T_n^j, \tag{3}$$

where $f^k$ is the nodal force at node $k$ due to the contact traction; $\gamma_k$ is the area of the segment and $H_{kj} = \int_{\gamma_k} \phi_k \phi_j \, ds$.  

It is to be noted that each nodal contact force contains contributions from all contact segments sharing the same node. Finally, the equation system which relates the nodal tractions and the nodal contact forces possesses the form:

$$\{f^k\} = [H] \{T_n^j\}, \tag{5}$$

where $[H]$ is a square matrix obtained after assembling the corresponding interface element matrices, $\{f^k\}$ and $\{T_n^j\}$ are vectors whose components are respectively the nodal forces and the tractions at the nodes along the prescribed crack path.

In such a way for each chosen FE mesh, the assumed decohesion criterion in terms of a critical normal traction can be transformed in an equivalent criterion for the nodal forces and the mesh-dependence of the solution is eliminated.

As noted by some authors (e.g. [6,7]), such stress based criteria seem to be adequate for the correct description of crack propagation. In our formulation the decohesion criterion is embedded
in the boundary value problem as an additional boundary condition along the prescribed crack path. It is not comprised as a constitutive law of a thin material layer joining the two parts of the system (as in the models of Needleman [4], Tvergaard [8] etc.). The addition of the non-overlapping condition: \( u_n \geq 0 \), where \( u_n \) is the relative normal displacement of the crack faces, leads to a variational formulation with inequalities [9]. Incremental solutions are obtained using a displacement based Finite Element method that incorporates additional contribution from the prescribed crack path integral to the right-hand side of the algebraic system of equations (and does not affect the global stiffness matrix). The rest is a standard elastic–plastic analysis. This formulation is quite different from the one used in the above mentioned models and leads to a mathematically well-posed problem.

The analyses were conducted within the framework of a plane strain formulation. The loading is applied by a prescribed horizontal displacement at the top edge. The Co-rich islands are elliptic in shape and their long axis is parallel to the top free surface. The thickness of the surrounding graded layer is set to 2 \( \mu \text{m} \). The variation of the thermo-mechanical properties with distance is assumed in such a way that a smooth transition from the matrix to the Co-island is assured.

The non-linear FE-analysis was performed within the framework of a semi-infinite representative volume element. The crack path is prescribed to run perpendicular to the top surface through the centre of the ductile island. Due to the symmetry only one half of the model needs to be considered. A rigid surface was defined along the symmetry line in order to simulate a symmetric Mode I crack. In such a way the crack propagation is simulated as decohesion along the prescribed crack path. The lower boundary is extended to infinity and was modelled by infinite elements (a sketch of the model as well as the loading and boundary conditions are shown in Fig. 3). The commercial code ABAQUS [5] was used for the FE-calculations.

In the present analysis the deformation theory of plasticity is employed to characterise the inclusion material and the graded interlayer. The deformation plasticity theory allows fully plastic analysis of ductile metals, usually under small displacement conditions, for fracture mechanics applications. The model is based on the Ramberg–Osgood relationship and has the form (in one dimension):

\[
E \varepsilon = \sigma + \alpha \left( \frac{\sigma}{\sigma_Y} \right)^{n-1} \varepsilon,
\]

where \( \sigma \) is the stress, \( \sigma_Y \) the yield stress, \( \varepsilon \) the mechanical strain, \( E \) Young’s modulus and \( \alpha \) and \( n \) are material parameters chosen to fit data. The material behaviour described by this model is nonlinear at all stress levels, but for commonly used values of the hardening exponent \( n \) (3 or more) the nonlinearity only becomes significant at stress magnitudes approaching or exceeding \( \sigma_Y \). Typical \( n \)-values range from 3 to 5 for materials with high hardening to as large as 20 for nearly perfectly plastic materials.

The model is generalized to multiaxial stress through the use of the Mises stress potential and associated flow law (for details see e.g. Hutchinson [6]). The multiaxial model relating stresses and strains is,

\[
E \varepsilon = (1 + \nu)S + (1 - 2\nu)\sigma_H I
\]

\[
+ \frac{3}{2} \alpha \left( \frac{\sigma_Y}{\sigma_Y} \right)^{n-1} \hat{S}, \tag{7}
\]

where \( \varepsilon \) is the strain tensor, \( \sigma \) the stress tensor, \( \sigma_H \) the hydrostatic stress, \( \sigma_Y = \sqrt{\frac{2}{3}S'} \) the Von Mises equivalent stress, \( \sigma_Y \) the equivalent yield stress, \( S = \sigma - \sigma_H I \) the stress deviator and \( \nu \) is Poisson’s ratio, and \( I \), the unit tensor.

The model is termed deformation plasticity because the stress is defined by the total mechanical strain with no history dependence. There is no “unloading” criterion (to allow recovery of the initial elastic stiffness immediately after a strain reversal), so that the model is useful as a plasticity model in cases of continuous flow under monotonic loading. It is, in fact, a nonlinear elastic model, but it is to be noted that solutions based on the deformation theory of plasticity coincide exactly with the solutions based on the \( J_2 \) (Von Mises) flow theory if proportional loading occurs.
everywhere, i.e. the stress components change in fixed proportion to one another. In general, the condition of proportionality is not always satisfied. However, it is worth noting that in the problem under consideration, the applied loading (prescribed displacement of the top edge) is monotonically increasing, on one hand, and the size of the ductile zone is small compared with the size of the representative volume element (Fig. 3). For this reason, following the suggestion of Hutchinson [10], we expect that under the assumed conditions the obtained solutions come sufficiently close to meeting proportionality in the fracture process zone near the crack tip, thus justifying the use of deformation theory.

An important feature of the cohesive surface concept is that quite general constitutive relations characterising the material behaviour, on one hand, and the cohesive surface, on the other, can be incorporated into the formulation. It allows the decohesion criterion to be defined as a function of the spatial position.

3. Cohesive strength

The cohesive strength was determined iteratively by numerical simulations of three-point bending tests of homogeneous specimens with different contents of cobalt.

The iterative procedure consists of the following steps:

(i) for an assumed value for $T^\text{critical}$, a finite element simulation is performed and the reaction force when fracture occurs is obtained;

(ii) from the reaction force, the corresponding bending strength (BS) is calculated by using the relation,

$$\sigma_{\text{BS}} = \frac{3}{2} \frac{F l}{b h^2},$$

where $F$ is the numerically determined reaction force and $l, b, h$ are length, thickness and height of the specimen respectively. The obtained value is compared with the available experimental data ([11,12]; see Fig. 4).

(iii) Steps (i) and (ii) are repeated until an acceptable fit with the test data is achieved.

Fig. 4. Experimental data for the bending strength of WC–Co alloys as a function of the Co volume fraction.

Due to the fact that experimental data were available for volume fractions of Co less than 40%, it was possible to identify in a realistic way the cohesive strength in this range (these values are plotted by a solid line in Fig. 5). For volume fractions of Co up to 100%, a parametric study was performed in order to determine the values for which the crack propagates in a brittle or stable manner, or stops due to blunting within the islands. For this purpose the model shown in Fig. 3 (but without coating) was used. It was found that after the crack initiates at the top surface it propagates in a brittle manner through the elastic.
hardmetal matrix. An essential retardation occurs when the crack tip reaches the graded layer. Further propagation depends strongly on the stress state within each sublayer, the yielding of the material there and the assumed local fracture criterion. The upper dashed line in Fig. 5 denotes the lower bound of the cohesive strength for which the crack crosses the graded interlayer but stops in the Co-island. A zone of rapidly increasing plastic strain appears near the crack tip leading to crack blunting and arrest. For higher values of the cohesive strength the crack stops within some sublayer of the graded zone. The lower dashed line corresponds to the upper bound of the cohesive strength for which a brittle crack propagation through the Co-islands occurs (see Fig. 6).

The performed calculations demonstrate that for lower values of the cohesive strength all the constituents (except Co) remain in the elastic regimes and the crack propagates in a nearly brittle manner. Just a small retardation is observed within the Co islands due to yielding. For values between the two dashed curves the crack propagation is stable. It is accompanied by small scale yielding of the inclusion material that retards essentially the crack advance but does not arrest it. For values higher then the upper dashed line, the crack stops within the islands.

4. Coating and residual stresses

After determining the cohesive strength as a function of the Co volume fraction, the failure analyses can be carried out in order to examine the strength behavior of the considered RVE (representative volume element).

As a next step of the analyses, the presence of a graded surface layer at the top free surface was assumed (Fig. 3). Its Young’s modulus varies linearly with position from 450 to 600 GPa (the Young’s modulus of the substrate) over a range of 5 μm. The role of residual mismatch stresses due to cooling-down from 600°C to room temperature was investigated with this model. The differences in the thermal expansion coefficients lead to the development of relatively high tensile hydrostatic stresses within the inclusions and the coating. In addition, stress concentrations are observed in the matrix at the inclusion-matrix interface near the end of the inclusion. In Fig. 7(a) the distribution of the $\sigma_{xx}$-component of the stress tensor after cooling is shown. It is reasonable to expect that high tensile stresses that arise near the top surface will facilitate the crack propagation when additional mechanical tensile loading is applied after cooling.

Again the two limiting cases of crack arrest and propagation through the island are investigated with the help of the criteria denoted by the dashed lines in Fig. 5.

In both cases, after the crack initiates at the predefined location on the top surface it propagates in a brittle manner through the coating and the matrix and the crack tip reaches the graded layer (see Fig. 8). For this reason there arises a sharp peak and an abrupt drop in the force–displacement curve (Fig. 9). The presence of tensile residual stresses in the coating (Fig. 7(a)) facilitates crack initiation, resulting in a significant decrease of the peak loading value (of the order of 25–30% in comparison with the case without residual stresses) (Fig. 9).

With further loading increase, a retardation of the crack propagation through the graded layer and the Co-island is observed. The crack retardation in the graded layer can be explained, on one hand, with the increase of cohesive strength in the

Fig. 6. FE simulation of three-point bend tests: $\sigma_{xx}$ stress distribution before failure of WC–Co (40 vol% Co).
range of 0–40 vol% Co and, on the other hand, with the increasing role of plastic deformation in the range of 40–100 vol% Co even at decreasing cohesive strength (Fig. 5). After some amount of crack propagation a plateau in the force–displacement curve is attained. The plastic deformation that occurs near the crack tip is the major energy consuming process. Due to the small strain

Fig. 7. (a) Residual stresses distribution after cooling-down from 600°C ($\sigma_{xx}$ component). (b) $\sigma_{xx}$ stress distribution when crack blunting occurs.

Fig. 8. Two stages of crack propagation through a ductile Co island ($\sigma_{xx}$ component).

Fig. 9. Influence of residual stresses on the crack propagation (Co island thickness 2 μm).
hardening of cobalt the crack extension is very sensitive with respect to the decohesion criterion and the island thickness. It was found that relatively small changes in the island thickness influence significantly the crack resistance (Fig. 10). Crack blunting occurs again when the criterion with the higher critical value (upper curve in Fig. 5) is applied (Fig. 7(b)). When the criterion with the lower value is applied, the crack propagates through the island easier than in the case without residual stresses (two stages of crack propagation through the island are shown in Fig. 8). This fact is well illustrated by the corresponding force–displacement curves (Fig. 9) where the plateau is shorter, showing that a smaller amount of applied loading is required for the crack to propagate.

5. Conclusions

The developed Finite Element models have the potential to provide quantitative understanding and qualitative estimation of the composite response near aligned isolated Co-islands under thermo-mechanical loading when residual stresses due to cooling are present. The process of crack propagation is described with the help of a cohesive surface model. It provides a unified description of crack initiation from the top free surface to complete propagation or blunting and arrest within the Co-islands. The numerical simulations show that the cohesive surface model is a workable computational model which involves the material cohesive strength as a phenomenological parameter. Moreover, the model was extended in order to allow the cohesive strength to be defined as a function of the spatial co-ordinates thus making possible the simulation of crack propagation through graded zones.

It can be concluded that the main aspects of the inelastic and fracture behaviour of WC-Co alloys with low volume fraction of Co (25 vol% Co) can be captured by the chosen approach. It was found that the fracture strength, due to the presence of residual stresses, crack blunting and with decreasing island thickness significantly decreases.

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