Fracture assessment of graphite V-notched and U-notched specimens by using the cohesive crack model

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Received Date: 28 August 2014; Accepted Date: 25 October 2014; Published Online: 21 November 2014

ABSTRACT
This article explores the capability of the Cohesive Zone Model in predicting the critical load of blunt notched specimens made of coarse-grained polycrystalline graphite, a brittle material that has gained the attention of researchers because of its favourable properties for protection against thermal loads. To that aim, 39 different tests on U-notched and V-notched specimens made of this material, with loading modes raging from mode I to mixed mode I/II, have been modelled by using the Cohesive Zone Model. The model has been implemented through the embedded crack approach, avoiding thus the necessity of defining the crack trajectory prior to the simulation because it is automatically generated once the maximum principal stress overcomes the tensile strength of the material. The numerical predictions obtained show good agreement with the experimental results.

Keywords brittle fracture; cohesive zone model; embedded crack; notched components.

NOMENCLATURE

\[ a = \text{notch depth} \]
\[ D = \text{diameter of semi-circular bending and Brazilian disk specimens} \]
\[ D = \text{fourth order elastic moduli tensor} \]
\[ d = \text{notch length in U-notched Brazilian disk specimens} \]
\[ E = \text{Young’s modulus} \]
\[ f_t = \text{tensile strength} \]
\[ f() = \text{softening curve} \]
\[ G_F = \text{specific fracture energy} \]
\[ K_{IC} = \text{fracture toughness} \]
\[ L = \text{length of three-point bending specimens} \]
\[ l_{ch} = \text{characteristic length} \]
\[ n = \text{unitary vector normal to the maximum principal stress} \]
\[ P = \text{load} \]
\[ S = \text{span between supports of specimens} \]
\[ t = \text{traction vector} \]
\[ W = \text{specimen width (three-point bending specimens)} \]
\[ w = \text{mode I crack opening} \]
\[ w = \text{crack opening vector} \]
\[ \bar{w} = \text{equivalent crack opening} \]
\[ u() = \text{displacements field} \]
\[ u_i = \text{nodal displacements of node } i \]
\[ N_i() = \text{shape function associated to node } i \]
\[ H() = \text{heaviside function} \]
\[ b_i = \text{gradient vector of the shape function associated to node } i \]

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**Greek**

\[2\alpha = \text{notch opening angle}\]
\[\beta = \text{notch angle in U-notched Brazilian disk specimens}\]
\[\varepsilon = \text{strain tensor}\]
\[\sigma = \text{mode I stress}\]
\[\sigma = \text{Cauchy’s stress tensor}\]
\[\rho = \text{notch root radius}\]
\[\nu = \text{Poisson’s ratio}\]

**INTRODUCTION**

Failure assessment in presence of stress concentrators can be considered a challenging task that strongly depends on the macrostructural and microstructural aspects of the material considered.

In the case of brittle materials under mode I loading conditions, when the stress concentrators are cracks, the analysis through the stress intensity factors (SIFs) provided by the Linear Elastic Fracture Mechanics (LEFM) has proven to be a satisfactory approach. However, when the stress concentration is caused by notches, the analysis becomes more complex and a different framework must be used, even if the material is of the linear elastic type. Within the framework of the LEFM, some authors have opted for the generalization of the SIF through the notch SIF concept.\(^1\)–\(^5\) This approach can be used for sharp notches (zero radius at the notch tip) as well as blunt notches (non-zero radius) but only up to a certain value of the notch tip radius, which depends on the material properties.\(^6\)

When the loading conditions differ from the mode I ones, the problem becomes even more complex and the extrapolation of the LEFM framework comprises several difficulties as shown, for example, in Refs. [7–9]. Because of these reasons, different alternatives have been proposed during the last decades for the analysis of the critical load for notched brittle materials, such as those based on critical virtual cracks,\(^10,11\) the Strain Energy Density,\(^12–14\) the Theory of Critical Distances\(^15–17\) or the Cohesive Zone Model (CZM).\(^18–21\)

Focusing on the CZM, it was firstly proposed by Hillerborg \textit{et al.}\(^22\) based on the seminal works from Dugdale and Barenblatt. One of its main advantages is that it postulates that a crack may form anywhere at the continuum and not only ahead of a pre-existing crack or stress concentration. Therefore, it can be applied for the critical load assessment of brittle materials with different geometries, ranging from sharp-notched to plain unnotched specimens, and loading modes, spanning from pure mode I to different mixed mode combinations. For further information about the CZM, the reader is addressed to Refs. [23,24].

One of the main ingredients of the CZM is the softening curve, which is assumed to be a material property. Hence, in order to obtain satisfactory results by using this model, the precise shape of the softening curve must be obtained for the material under analysis. Unfortunately, this is not an easy task, especially for those materials with a small characteristic length.\(^23\)

The purpose of this article is to explore the applicability of the CZM to mixed mode I/II fracture of polycrystalline graphite, a material whose fracture properties have gained the interest of many researchers during the last years (see, for example, Refs. [24,25]). To this end, a large set of fracture tests under mode I and mixed mode I/II (117 tests) previously performed\(^26,27\) with the aforementioned material were checked against numerical predictions using the CZM. In order to set the softening function, a simple iterative process was used, given that a general procedure to obtain it from experimental tests is not yet available.

The article is structured in four main sections. First, the experimental data are summarized; four specimens were tested providing 117 test results. The second section provides the main details about the implementation of the CZM through the embedded crack approach.\(^28,29\) The third section is devoted to numerical predictions achieved with the CZM; to this end, the softening function is deduced, and the used FE procedure is explained. Finally, experimental and numerical results are compared and discussed.

**EXPERIMENTAL DATA**

In this section, a series of experimental data published in the open literature (Refs. [26,27]) dealing with brittle fracture in V-notched and U-notched graphite specimens.
under mode I and mixed mode I/II loading conditions are described. It is attempted to predict such data in the forthcoming sections by means of the cohesive crack model.

Material

The material properties of the coarse-grained polycrystalline graphite studied in Refs. [26,27] are presented in Table 1.

Specimens

**V-notched specimens under mode I loading**

In Ref. [26], three different geometries of blunt V-notched specimens where tested under pure mode I loading: three-point bending blunt V-notched specimen, semi-circular bending blunt V-notched specimen and the blunt V-notched Brazilian disk specimen. The geometry and dimensions of these specimens are schematically shown in Fig. 1. Three notch angles of 30°, 60° and 90° and also three notch tip radii of 1, 2 and 4 mm were tested. Three specimens have been tested for each of the 27 geometries, making a total of 81 test results.26 The thickness for all specimens was equal to 8 mm. The geometry of all specimens is summarized in Tables 2–4. Table 5 provides the failure loads of all tested specimens.

**Table 2** The three-point bending blunt V-notched specimen dimensions26

<table>
<thead>
<tr>
<th>Specimen</th>
<th>$\rho$ (mm)</th>
<th>$a$ (mm)</th>
<th>$L$ (mm)</th>
<th>$S$ (mm)</th>
<th>$W$ (mm)</th>
<th>$2\alpha$ ($^\circ$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>RV-TPB</td>
<td>1, 2, 4</td>
<td>10, 16</td>
<td>100, 160</td>
<td>60, 96</td>
<td>20, 32</td>
<td>30, 60, 90</td>
</tr>
</tbody>
</table>

RV-TPB, three-point bending blunt V-notched.

**Table 3** The dimensions of the semi-circular bending blunt V-notched specimen26

<table>
<thead>
<tr>
<th>Specimen</th>
<th>$a$ (mm)</th>
<th>$D$ (mm)</th>
<th>$\rho$ (mm)</th>
<th>$2\alpha$ ($^\circ$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>RV-SCB</td>
<td>15</td>
<td>60</td>
<td>1, 2, 4</td>
<td>30, 60, 90</td>
</tr>
</tbody>
</table>

RV-SCB, semi-circular bending blunt V-notched.

**Table 4** The dimensions of the blunt V-notched Brazilian disk specimen26

<table>
<thead>
<tr>
<th>Specimen</th>
<th>$a$ (mm)</th>
<th>$D$ (mm)</th>
<th>$\rho$ (mm)</th>
<th>$2\alpha$ ($^\circ$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>RV-BD</td>
<td>15</td>
<td>60</td>
<td>1, 2, 4</td>
<td>30, 60, 90</td>
</tr>
</tbody>
</table>

RV-BD, blunt V-notched Brazilian disk specimen.
U-notched specimens under mode I and mixed mode I/II loading

Recently, Torabi et al.\textsuperscript{27} have published experimental results for U-notched Brazilian disk (UNBD) specimens subjected to mode I and mixed mode I/II loading. The material used was the same graphite from Ref. [26] (V-notched specimens under mode I loading section). The geometry of the specimens and the loading conditions are shown in Fig. 2.

In Fig. 2, \(\beta\) is the angle between the notch bisector line and the loading direction. \(D\) and \(P\) are the disk diameter and the applied load, respectively. The degree of mode II loading in these specimens can be adjusted by varying the angle \(\beta\). For \(\beta=0\), the specimens are tested under pure mode I, and the contribution of mode II loading is augmented as the angle \(\beta\) increases. In the tests conducted in Ref. [27], three loading angles of 0°, 10° and 20° were used (\(\beta=0^\circ\) for mode I and \(\beta=10^\circ, 20^\circ\) for mixed mode I/II).\textsuperscript{27} The diameter, the overall slit length (i.e. the distance between the U-ends) and the thickness of the UNBD specimens were equal to 60, 18 and 10 mm, respectively. The notch tip radii (\(\rho\)) were set equal to \(0.5, 1, 2\) and \(4\) mm.\textsuperscript{27} Table 6 summarizes the experimental fracture loads reported in Ref. [27] for the UNBD graphite specimens.

### MATERIAL MODEL FOR THE COHESIVE ZONE MODEL

The material model used is based on the one presented in Ref. [30] but adapted for quadrilateral and brick elements. It can be summarized as a linear elastic material model, plus a cohesive crack that is inserted in the finite element once the maximum principal stress reaches the tensile strength. The cohesive crack is inserted through the embedded crack approach.\textsuperscript{28,29}

### The cohesive crack model

The cohesive crack model, or fictitious crack model, is based on the assumption that a fracture process zone develops prior to the formation of a physical crack in
the material. In this fracture process zone, the material suffers a progressive degradation from the intact condition under low stresses or no stresses at all, to the fully damaged condition when a crack has been fully created. From a mechanical point of view, this progressive degradation is characterized by a decrease of the material strength as the strain in the material increases.

The cohesive crack model postulates that this fracture process zone can be lumped into a single line in 2D problems (coincident with the crack trajectory) or a surface in 3D problems. The material degradation is modelled through the softening curve, which relates crack opening in a certain point on the crack line with the stress transferred between crack lips. The cohesive crack model also assumes that the fracture process zone develops once the stress in the material exceeds the tensile strength, $f_t$, which is equivalent to set the tensile strength as the value of the softening curve when crack opening is equal to zero. Moreover, because the softening curve sets the transition from the intact condition to a fully developed crack, the area under the curve represents the energy necessary to create a unit area of crack in the material, which is equivalent to the specific fracture energy, $G_F$. Figure 3 illustrates these concepts.

Besides the tensile strength and the fracture energy, the shape of the softening curve plays also a paramount role in the cohesive crack model. In principle, each material must have its own softening curve. However, for some materials, standard types of softening curves have been proposed (Fig. 4): rectangular for steel\textsuperscript{31} and PMMA\textsuperscript{20} bilinear for concrete\textsuperscript{32,33} exponential also for concrete\textsuperscript{23,34} and linear.\textsuperscript{23} Unfortunately, up to date, no general procedure has been established to measure the actual shape of the softening curve for any given material.

The embedded crack approach

The cohesive crack model has been implemented in the simulations through the embedded crack approach\textsuperscript{28,29} which allows for the insertion of a jump in the displacements field of a given finite element once a certain criterion has been satisfied. In the simulations presented here, the model presented in Ref. [30] has been adopted. The model can be summarized as a linear elastic material model in which a crack is inserted once the maximum principal stress overcomes the material tensile strength. The crack, which is oriented perpendicularly to the direction of the maximum principal stress, behaves according to the cohesive crack model approach.
At initial stages of the loading process, when the maximum principal stress has not reached the value of the tensile strength, the material behaves as a linear elastic one. Therefore, the stresses are evaluated through

$$\sigma = D \varepsilon, \quad (1)$$

where $\sigma$ is the Cauchy’s stress tensor, $\varepsilon$ is the strain tensor and $D$ is the fourth order elastic moduli tensor.

Once the principal stress in the element reaches the value of the tensile strength, a crack is inserted in the element in the direction normal to the maximum principal stress, $n$. Crack opening is characterized through the vector $w$, and we will assume it to have a constant value along the crack. Figure 5 illustrates these concepts.

As Fig. 5 shows, the insertion of the crack defines two regions in the element, the lower one $A^-$ and the upper one $A^+$. The nodes that belong to the $A^+$ region are referred to as solitary nodes. The jump in displacements created by the crack modifies the displacements field that now reads

$$u(x) = \sum_{\alpha \in \mathcal{A}^- \cup \mathcal{A}^+} N_{\alpha}(x) u_{\alpha} + \left [ H(x) - \sum_{\alpha \in \mathcal{A}^+} N_{\alpha}(x) \right ] w, \quad (2)$$

where $u(x)$ is the displacement field, $N_{\alpha}$ is the shape function associated to the node $\alpha$, $u_{\alpha}$ is the nodal displacements for the node $\alpha$ and $H(x)$ is the Heaviside function, having a null value in the region $A^-$ and a value of 1 in the region $A^+$.

The strain field in the continuum is obtained by taking the symmetric part of the gradient to the displacement field expressed by Eq. 2:

$$\varepsilon'(x) = \sum_{\alpha \in \mathcal{A}^- \cup \mathcal{A}^+} [b_{\alpha}(x) \otimes u_{\alpha}]^S - \left [ \sum_{\alpha \in \mathcal{A}^+} b_{\alpha}(x) \right ] \otimes w w, \quad (3)$$

where $b_{\alpha}(x)$ is the gradient of the shape function associated to node $\alpha$. The symbol ‘$\otimes$’ expresses the tensorial product. According to the finite element method theory, the first summation represents the strain field the element would have if no crack was present in it. From now on, we will refer this term as apparent strain,

$$\varepsilon'^a(x) = \sum_{\alpha \in \mathcal{A}^+} [b_{\alpha}(x) \otimes u_{\alpha}]^S. \quad (4)$$

Therefore, Eq 4 can be expressed as

$$\varepsilon'(x) = \varepsilon'^a(x) - [b^I(x) \otimes w]^S, \quad (5)$$

being $b^I(x) = \sum_{\alpha \in \mathcal{A}^+} b_{\alpha}(x)$. Equation 5 represents the strain field of the continuum of an element with a crack embedded in it. Because in the continuum the material behaves as linear elastic, the stress tensor can be obtained through:

$$\sigma(x) = D \left [ \varepsilon'(x) - [b^I(x) \otimes w]^S \right ]. \quad (6)$$

Inside the crack, however, the stresses are governed by the softening curve according to the cohesive crack model. To take into account that crack may open in different modes, ranging from mode I to mode II, in this work, a central forces model has been used:

$$t = f(\tilde{w}) \frac{w}{w}, \quad (7)$$

being $t$ the traction vector transferred across the crack and $f()$ the softening curve. The variable $\tilde{w}$ represents an equivalent crack opening defined as the historical maximum value of the Euclidean norm of the crack opening vector. According to Eq. 7, the traction forces vector is parallel to the crack opening vector, and its modulus is given by the softening curve. It must be noted that, also according the equation, the softening curve unloads to the origin. Figure 6 illustrates these concepts.

The last step is to prescribe equilibrium between the traction forces vector in the crack and the stresses in the continuum. However, by comparing Eqs. 6 and 7, we find that the traction forces vector in the crack has a constant value, while the stresses in the continuum are a tensorial field. This issue can be circumvented by restricting this methodology only to constant stress elements, as it has been made in this work. Therefore, by prescribing equilibrium between the traction forces vector and the projection in the $n$ direction of the stress tensor in the continuum, we find

Fig. 5 Insertion of an embedded crack inside a finite element and identification of the solitary nodes.
In Eq. 8, the only unknown is the \( w \) vector, being possible to solve it by numerical methods.

\[
(D [\varepsilon'(x) - [b'(x) \otimes w]^N]) n = f(|w|) \frac{w}{|w|}.
\] (8)

In Eq. 8, the only unknown is the \( w \) vector, being possible to solve it by numerical methods.

**NUMERICAL SIMULATIONS**

**Material parameters**

All material parameters used in the simulations were taken from Table 1, except for the fracture energy. As explained in the previous section, the cohesive crack model needs the fracture energy instead of the fracture toughness. Being polycrystalline graphite a brittle material, the fracture energy was estimated through Irwin’s equation:

\[
G_F = \frac{K_{IC}^2}{E(1-\nu^2)}
\] (9)

Leading to a value of 129.40 N m\(^{-1}\).

**Shape of the softening curve**

While in the case of some materials, such as concrete, the shape of the softening curve has been deeply analysed,\(^{23,32,33}\) in the case of the material addressed here, to the authors’ knowledge, no study about the shape of the softening curve has been carried out up to date. Moreover, neither a general procedure for setting the softening curve for a given material has been proposed yet. For this reason, in this work, it was decided to obtain a *tailored* softening curve through an iterative process, starting with the simplest possible shapes of softening curve, and modifying them until achieving good agreement between numerical and experimental results. This process was applied to a single mode I geometry (semi-circular bending blunt V-notched specimens, with V-notch angle \( 2\alpha = 60^\circ \)), and the resulting softening curve was then applied to the whole set of simulations presented in this article.

The iterative process started by performing two numerical simulations using two different softening curves: the rectangular and the linear ones. As shown in Fig. 7, the predictions achieved by using the linear softening curve were clearly below the maximum loads obtained in the experiments, while the predictions with the rectangular one were above the experimental results. Therefore, it was decided to interpolate a curve in between these two extremes, by the use of a trapezoidal softening curve that provides a smooth transition between the rectangular and the linear softening curves, as shown in Fig. 7b, preserving the same specific fracture energy. The interpolation procedure consisted on increasing

![Fig. 6 Central forces model applied to the embedded crack and illustration of the unloading-reloading path in the softening curve.](image)

![Fig. 7 (a) Maximum load predictions achieved for the semi-circular bending blunt V-notched specimens (\( 2\alpha = 60^\circ \)); (b) softening curves used.](image)
progressively the slope of the initial descending branch of the trapezoidal curve, until a good agreement was achieved between the numerical predictions and the experimental results. The resulting softening curve is the trapezoidal one depicted in Fig. 7b. It is important to remind that no procedure for the accurate determination of the softening curve for a given material has been set up to date. Therefore, the softening curve proposed here can be only considered as a simplification of the actual softening curve of the material. Further research is necessary to explore other possibilities for the softening curve of this kind of materials.

It is important to note that the shape of the softening curve was tailored for a single geometry, and thereafter, the same curve was applied for the rest of the specimens, achieving a good level of prediction for all geometries as shown later.

**Simulation details**

The simulations were run using the LS-DYNA 971 software (Livermore Software Technology Corporation, Livermore, California, USA). This is a finite element commercial code with explicit time integration, originally intended for highly dynamic events, such as impacts or explosions. The use of an explicit code presents the advantage that because no static equilibrium is prescribed, convergence issues are avoided. This is especially convenient when multiple cracks may propagate within the same mesh. On the other hand, because this kind of numerical codes require small time integration steps, load was applied considerably quicker than in the actual tests, but controlling that inertial effects were kept negligible.

According to the cohesive crack model approach, the element size must be limited by the characteristic length in order to achieve representative simulations. According to the CZM, the characteristic length, which is related with the size of the fracture process zone, can be obtained through Ref. [23]:

$$l_{ch} = \frac{G_F}{f^2} \frac{E}{f}$$  \(10\)

According to the material parameters of the material considered here, this leads to a characteristic length of 1.377 mm. For this reason, the element size in the notch tip was limited to 0.1 mm. Figure 8 shows, as an example, a detail of the mesh of one UNBD specimen ($\rho = 4$ mm).

Unlike in previous works that also used the cohesive crack model in combination with the embedded crack for the study of notched specimens failure loads,\(^5\) the characteristic length of this material allows the use of an homogeneous mesh at the crack tip, without the need of setting a special region around the point of the highest values of maximum principal stress, to enforce crack generation at this area.

The resulting load–displacement curves showed a behaviour close to the linear one up to failure, with small oscillations because of the propagation of small amplitude-elastic waves within the continuum, which is modelled given the explicit character of the simulations (Fig. 9). The peak loads of the load–displacement defined the maximum loads reported in the following section. It is important to note that because of the quasibrittle nature of the material, the maximum loads are achieved after the cohesive cracks have propagated up to a certain extension that depends on the specimen geometry. When the ligament has been weakened enough because
of the crack propagation, the specimen is no longer capable to withstand the load level applied and the crack propagates in an unstable manner, causing a sudden drop in the load registered, which defines the maximum load as shown in Fig. 9.

RESULTS

V-notched specimens

Figures 10–12 show the numerical predictions of the maximum loads compared with the experimental results obtained for the V-notched specimens with $2\alpha = 30^\circ$, $60^\circ$ and $90^\circ$, respectively. In the authors’ opinion, a good level of agreement between the experimental results and the numerical predictions has been achieved.

U-notched specimens

U-notched specimens were loaded under mode I and mixed mode (I + II) conditions. Figures 13–15 show the numerical predictions compared with the experimental results for the loading angles $\beta = 0^\circ$, $10^\circ$ and $20^\circ$, respectively. The numerical simulations succeed in reproducing the experimental trend found for the notch tip radii of 1, 2 and 4 mm, according to which the critical load decreases as the notch radius increases. In opinion of the authors, the reason for such behaviour can be found in the increasing notch width with the notch tip radius. As shown in Fig. 16, wider notches induce higher values of tensile stresses in the mid plane of the specimens, because of the higher values of the angle between the compressive stresses created between both loading points.
For the lower value of notch radius (0.5 mm), although the tensile stresses induced in the mid plane are lower, the stress intensity created by the small radius increases the stress levels at the notch tip, leading to crack initiation at lower levels of load. This is the reason why the experimental critical loads for the smaller radius (0.5 mm) show a decreasing trend. This trend for the lower radius size is not accurately reproduced by the numerical predictions provided by the CZM, probably because for this notch tip size, the radius is of the same order of magnitude than the grain size. Given that the CZM averages the damage processes at a mesoscale, it is not able to capture accurately the fracture processes that develop between a small amount of grains around the notch tip.

**CONCLUSIONS**

This work shows the capability of the cohesive crack model in predicting the failure load of notched brittle materials loaded under mixed mode. To this aim, 39 different geometries of notched specimens made of polycrystalline graphite have been modelled.

The shape of the softening curve has proved to be of paramount importance in the prediction of the critical loads obtained for this particular material. Therefore, it has been necessary to fit the shape of this curve by using the experimental data obtained for a certain geometry, and then, it has been used for the simulation of the entire experimental campaign.

Except for some singular cases in which the notch radius was of the order of magnitude of the grain size where the behaviour of the monocrystalline material may differ from the polycrystal, the model has been able to provide good predictions of the failure loads for different notch geometries, under mode I loading in the case of V-notched specimens and under mixed mode (mode I + II) loading in the case of U-notched specimens.

Unlike previous works based also in the cohesive crack model in combination with the embedded crack approach, the characteristic length of this particular material has made possible to use a homogeneous element size at the crack tip, avoiding the need of setting preferential mesh areas for crack initiation. This enhances the predicting capabilities of this approach, because crack is initiated and propagated as a result of the simulation.

**REFERENCES**

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