MODELIZACIÓN DE MATERIALES CERÁMICOS Y POLIMÉRICOS MEDIANTE EL MODELO DE GRIETA COHESIVA: RELACIÓN ENTRE LA CURVA DE ABLANDAMIENTO Y EL CAMPO DE DESPLAZAMIENTO EN LA ZONA DE PROCESO

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Resumen. En este trabajo se presenta el estudio del comportamiento a fractura y modelización por el modelo de grieta cohesiva de dos materiales semi-frágiles: un polímero granular y una cerámica refractaria. En primer lugar se estudia un polímero consistente en microesferas de polimetilmetacrilato polimerizadas en una matriz de polimetilmetacrilato formando una estructura de porosidad abierta; estos materiales se ensayan tanto en seco a temperatura ambiente como en agua a 45 ºC. Durante la fractura de estos materiales, los desplazamientos alrededor de la zona de procesos de la fractura se miden mediante una técnica de correlación digital de imágenes. Finalmente el comportamiento de este material se modela con el método de grieta cohesiva empleando una curva de ablandamiento bilineal cuyos parámetros se fijan mediante ajuste numérico con las curvas experimentales. A continuación se modela la cerámica refractaria con el mismo método de grieta cohesiva, pero en este caso los parámetros de la curva de ablandamiento se obtienen a partir de consideraciones microestructurales y se comparan con modelizaciones por ajuste numérico efectuadas por otros autores. En ambos casos, la modelización se ajusta satisfactoriamente a los resultados experimentales.

Abstract. The modelling with the fictitious crack model of two materials, a granular polymer and a refractory ceramic, is presented in this work. The granular polymer is made of polymethyl methacrylate beads polymerised together in a polymethyl methacrylate matrix, forming an open pore microstructure. This material is tested in dry, room temperature conditions and submerged in water at 45 ºC. During fracture, the displacements around the fracture process zone are measured with a digital image correlation technique. The mechanical behaviour of this material is modelled with the fictitious crack model with a bilinear tension-softening curve, whose parameters are obtained with a fitting procedure. The refractory ceramic is also modelled with the fictitious crack model, but in this case the parameters of the tension-softening curve are obtained through experimental considerations. The results obtained in this way agree with the experimental force-displacement curves, and are also compared with previous modelling done by other authors with numerical fitting procedures.

1. INTRODUCTION

Quasi-brittle fracture is, nowadays, one of the hottest topics in fracture mechanics. Specially, the relationship between the energy dissipative mechanisms in the fracture process zone and the macroscopical mechanical behaviour of the quasi-brittle materials is not yet fully understood. This type of quasi-brittle fracture can be found in a variety of materials, like: concrete, refractory ceramics, toughened technical ceramics, rocks, composites and some metals and polymers under certain conditions [1]. This behaviour is due to the existence of a number of different types of toughening mechanisms that shield the growth of the crack inside the fracture zone. Among all of them, microcracking and bridging are the most important mechanisms in this type of fracture [2].

Applications of linear elastic fracture mechanics and small-yielding fracture mechanics to understand these materials were made since 1950, but with limited success. This is due both to the complex fracture process zone and to the scale of the problem (meso-scale). In 1976 by Hillerborg et al. [3] proposed the fictitious crack model (also known as cohesive crack model) based on a Dugdale-Barenblatt model with a tension-softening curve, which successfully describes the fracture of these materials. This model takes into account the various shielding mechanisms present in the fracture process zone modelling them by a tension-softening curve, which acts between the faces of the crack with decreasing stress as the crack opens. Figure 1 presents a sketch of the modelling process.

However, the correspondence between the physical parameters of the material and the numerical parameters chosen for modelling that material is still not clear. In fact, it is not clear if any relationship exists at all. The choice of a suitable softening curve is also an open question, as often in literature different softening curves for describing the same material are encountered. The softening curve parameters are normally determined through fitting procedures and a correlation with the physical material is seldom given.

In this paper we present the mechanical testing and fictitious crack modelling of two quasi-brittle materials: a porous granular polymer and a refractory ceramic. First, we characterize and model the polymer in two conditions: at room temperature and immersed in water at 45 ºC. The modelling is done through a numerical fitting procedure yielding very good fitting for different geometries and length scales. The refractory ceramic, on the other hand, is modelled after microstructural considerations with also relative good results.

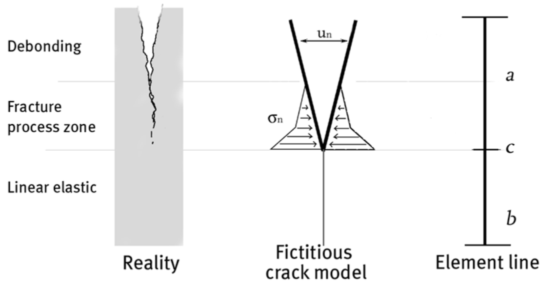

Fig 1. - Sketch of the fictitious crack concept. At the left is the real crack, in the middle is the fictitious crack modelling, and at the right is the element line with its three different labelled regions. In the computation, three regions are differentiated: before the crack tip (b), the crack tip (c) and after the crack tip (a)

2.- MATERIAL DESCRIPTION AND MECHANICAL TESTS

2.1 Polymer

The studied polymer consists of polymethyl methacrylate (PMMA) beads polymerized together in an open-pore polymethyl methacrylate matrix. This material is widely in the ceramic industry as a replacement of Gibson moulds for ceramic components, especially whiteware. This polymeric mould has shorter drying times, larger number of cycles, is easily produced and machined and has improved mechanical properties.

The procedure to manufacture this material [4, 5] is as follows: First, a water-in-oil emulsion of a polymeric resin (oil phase), consisting of poly- ethyleneoxide - *block*- methyl methacrylate (PEO-PMMA), with molecular weight (Kg/mol) 10-*b*-10, and water is repared. This resin is dissolved in a mixture of styrene and methyl methacrylate in a weight ratio of 1:9, with 2% weight emulsifier and surfactant agents. Then 100 µm (48.5 wt %) and 1 mm (8.7%wt) polymethyl methacrylate beads, together with tap water (32 wt %) and dibenzoylperoxide as initiator (1 wt %) are added to the emulsion, resulting in a viscosity of 5000 cP at 25 °C. Once this is achieved, a regulator, disodium tetraborate decahydrate [$Na_2B_2O_4 \cdot 10H_2O$], and a polymerization regulator [dimethyl-p-toluidine, 10 % concentration] is added. The reaction is carried out at 17 °C for about 30 min. The resulting material is washed three times with warm water (60 °C) and dried subsequently. The yield is close to 100 %. Figure 2 presents a picture of the microstructure of this material.

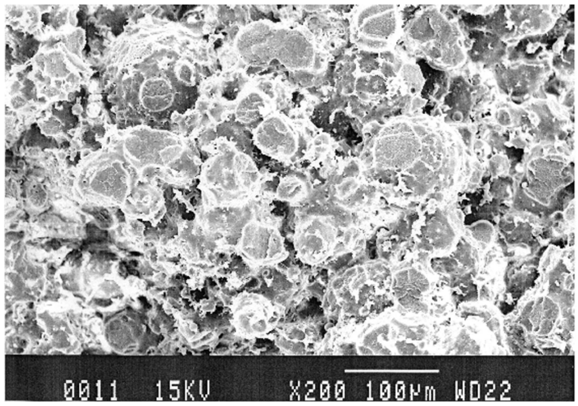

Fig 2. - Microphotograph of the NZS material, where it is seen the PMMA beads bonded together.

Samples were tested both in dry, room temperature conditions and immersed in water at 45 ºC (in order to replicate the working conditions when this material is used as white ware moulds). Two geometries were used in both conditions: Wedge Opening Load (WOL) samples with dimensions 150×120×30 mm and notch length *a*, equal to 60 and 90 mm and single-edge notched beams (SENB) samples with dimensions 20×20×80 mm and notch length, *a*, equal to 5 mm, which corresponds to ¼ of the sample height, and 10 mm, which corresponds to ½ of the sample height, tested in four point bending (l_1= 5 mm; l_2= 60 mm).

In all cases the notch was finalized with a razor blade and diamond paste of 1 µm to produce a notch width of 0.5 mm, which is smaller than the largest microstructural feature assuring that fracture will start from the notch tip. All the tests were carried on in a universal test machine at a constant cross head speed of 5 mm/min. The displacements were measured with an extensometer attached to the load cell, measuring the displacement of the sample and the machine. The stiffness of the machine and jigs was measured before experiments, and recorded displacements subsequently corrected for this extra compliance.

During the mechanical tests of the WOL geometries the displacements around the crack tip were recorded and measured with a digital image correlation technique [6, 7]. This technique allows measuring precisely the displacement field of a solid, with accuracy and without the attachment of markers to the solid surface. In our case, our system consisted in a CCD camera (1024*1024 pixel resolution) connected to a PC through a frame grabber card and a dedicated software to calculate these displacement fields. The software that implemented the image correlation method was Veddac (Vector Displacement and Deformation Analysis by means of Correlation) originally developed by the Fraunhofer Werkstofmechanik from Germany [8]. This program is able to determine displacement fields with an accuracy of 0.1 pixels.

The observation window was placed 45 mm away from the crack tip. Comparable results were obtained for all the samples of the same geometries and conditions. Another two samples for every material were observed 15 mm and 60 mm away from the crack tip producing again, comparable results.

2.2.-Refractory ceramic

The refractory ceramic is composed of alumina (Al_2O_3, 56 wt%) and mullite ($3Al_2O_3 \cdot 2SiO_2$, 43.5 wt%) grains, with a crystalline phase present at the grain boundaries and some traces of iron oxide (Fe_2O_3, 0.1 wt%) [9]. This ceramic is normally used for producing kiln furniture for supporting and protecting ceramic products during firing, such as tiles, table ware, sanitary ware or technical ceramics as ferrites.

The same geometries and dimensions as used for the PMMA materials were employed to test the ceramic materials, with the exception of the SENB samples with notch lengths of 10 mm, due to the limitations of the fictitious crack model with small ligament lengths. In this case, much better modelling is obtained through improved models as the gradient-enhanced fictitious crack model [10, 11, 12].

3. DESCRIPTION OF THE FICTITIOUS CRACK MODEL

In this model a process-zone of finite size is taken into account that moves with the crack in front of the crack tip and in which the material shows a softening type of behaviour: the stress on the faces decreases with increasing crack opening.

To avoid possible numerical instabilities the inverse flexibility method, first introduced by Carpinteri et al. [13], is used. This method uses the superposition principle and is valid for small deformations and rotations (outside the crack) assuming that the material, outside the crack path, behaves in a linear elastic manner.

Because the parameters of the FC model will be estimated using the force - displacement curves of the geometries tested, the stresses and strains in the interior of the structure are not required in this procedure. The crack is modelled through interface elements at the crack line, whose length should be smaller than the characteristic length of the fracture process zone. The length of the finite elements l_e is identical for all geometries and equal to 0.1 mm.

On the crack line the regions before and after the crack tip and the crack tip itself, are labelled separately for latter partition of the matrices, as it is shown in figure 1, where label *a* stands for after the crack tip, label *c* stands for crack tip and label *b* stands for before the crack tip.

The solid is modelled by the finite element method and the problem to be solved is expressed as:

$$\boldsymbol{f} = \boldsymbol{H}\boldsymbol{u} + \boldsymbol{l}p \qquad (1)$$

where $\boldsymbol{f}$ is the column matrix with the (cohesive) nodal forces acting along the crack line, $\boldsymbol{u}$ is the column matrix describing the nodal (crack opening) displacements, p is the scalar external force and $\boldsymbol{H}$ and $\boldsymbol{l}$ are matrices obtained by substructuring (for details of substructuring, see [12]).

This equation can be partitioned by considering nodes in front ($\boldsymbol{u_b}$), at (u_c) and behind the crack tip ($\boldsymbol{u_a}$).

The displacements in front ($\boldsymbol{u_b}$) of the crack and the displacements at the crack tip (u_c) are equal to zero, and therefore the elements in the second and third column of the matrix $\boldsymbol{H}$ are not relevant. The elements f_c, u_c and l_c are one element column matrixes. After multiplication to obtain three equations and after eliminating p we can express $\boldsymbol{f_a}$ as:

$$\boldsymbol{f_a} = \boldsymbol{H_{aa}} \cdot \boldsymbol{u}_a + \frac{\boldsymbol{l}_a}{l_c}\left(f_c - \boldsymbol{H_{ca}}\boldsymbol{u_a}\right) \qquad (2)$$

The relationship between the stresses along the crack line and the crack opening is given by a softening model. In this case a bilinear curve was chosen. The parameters of this bilinear model are f_t, α, β and u_{cr}. The relationship between σ_n (the cohesive stress) and u_n (the crack opening) can then be expressed as:

$$\sigma_n = \begin{cases} f_t\left(1 - \dfrac{1-\beta}{\alpha}\dfrac{u_n}{u_{cr}}\right) & if \quad 0 \le u_n \le \alpha u_{cr} \\ \dfrac{\beta}{1-\alpha} f_t\left(1 - \dfrac{u_n}{u_{cr}}\right) & if \quad \alpha u_{cr} \le u_n \le u_{cr} \\ 0 & if \quad u_n > u_{cr} \end{cases} \qquad (3)$$

and the fracture energy as:

$$G_f = \frac{f_t u_{cr}(\alpha + \beta)}{2} \qquad (4)$$

The nodal forces are computed from the cohesive stress by means of numerical integration. In this case nodal lumping was applied.

With the relationship $\sigma_n = \sigma_n(u_n)$ given in the softening model, the problem can be solved by iteration. This is not done by prescribing a value of the external load p in the incremental process but by prescribing the position of the fictitious crack tip at the end of the process zone and obtaining p as a result. That is, in successive steps the position of the crack tip is shifted one node simulating a propagating crack

4. FITTING PROCEDURE

4.1 Polymeric material

In order to find an optimal solution for the softening curve parameters a local minimum fitting algorithm (Nelder-Mead simplex direct search method [14]) was also implemented for the PMMA-based materials. This algorithm compares the experimental peak force and energy values with the peak forces and energy obtained with a given set of parameters. If the difference between both is larger than a given amount, a step change is made to the parameters until an optimal solution for all four parameters, f_t, u_{cr}, α, β is found. The softening curves obtained are presented in figure 3.

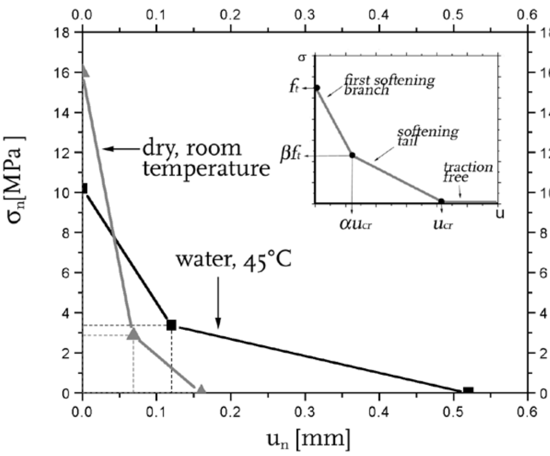

Fig 3.- Softening curves of the FC simulation for the two conditions of the PMMA-based materials

The force-displacement curves obtained for the WOL geometries of the PMMA-based materials are presented in figures 4 and 5. SENB geometries are also successfully modelled, although not shown here. Figures 6 and 7 present the crack profile measured experimentally with the digital correlation technique and the simulated crack profile with the fictitious crack model.

4.2 Ceramic material

Although it is acknowledged that the fictitious crack model is a phenomenological model with some limitations (as ligament length, straight crack, quasi-static load…), if softening curve parameters that resemble the real stress transfer state in the material are chosen, it may be possible to produce a good fitting of the experimental force-displacement curve.

As it was said before, microcracking and bridging are identified as the main shielding mechanisms in this type of material. Microcracking is essentially short-range, high stress transfer mechanism, while bridging is long range, low stress transfer mechanism. Therefore a bilinear softening curve may resemble the real stress transfer state. The parameters of this bilinear softening cure are then chosen according to the following criteria:

1. The f_t parameter has the approximate value of the strength of the material
2. The product of the parameters α by u_{cr} parameter is the transition between microcracking and bridging (in a large sample away from the boundaries)
3. The first softening branch simulates the microcracking and the softening tail simulates the bridging of the material.

By inspecting (with digital image correlation) the fracture process zone area we can estimate the transition from microcracking to bridging and the approximate contribution of both mechanisms. This observations, together with the knowledge of the experimental fracture energy, which is set equal to (4), leads us to propose a set of softening curve parameters based on experimental observations [15].

This set of parameters is compared with both the experimental results and the numerical results obtained by van Gils et al [12, 16] using the same material and the numerical fitting procedure of the PMMA-based materials described in the previous part. The two set of parameters are presented in table 1 and force displacement graphs are presented in figures 8 to 10.

	van Gils et al	this work
f_t	5.5 MPa	7.5 MPa
u_{cr}	0.23 mm	0.067 mm
α	0.18	0.06
β	0.10	0.5
G_f	175 J/m^2	141 J/m^2
$\alpha\, u_{cr}$	0.0414 mm	0.0040 mm

Table 1 – FC model parameters: the first column presents the parameters obtained form van Gils et al [12, 16] and the second column presents the FC parameters estimated through experimental observations.

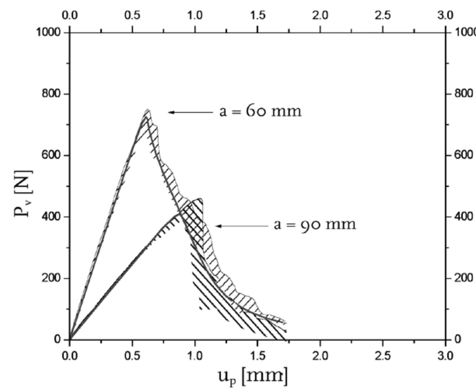

Fig. 4 –Experimental data and fictitious crack fitting of WOL samples at room conditions with two different notch lengths

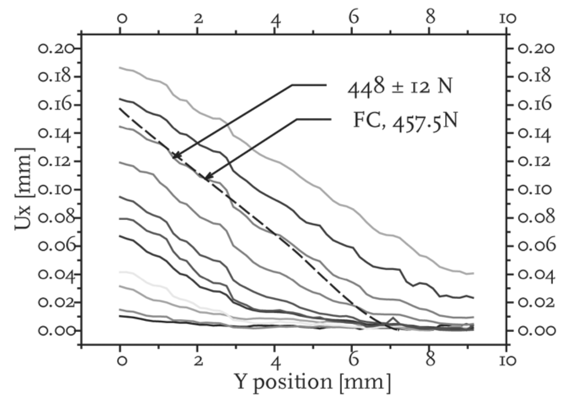

Fig. 7 – Experimental data and fictitious crack fitting of the crack profile of samples in water at 45 °C

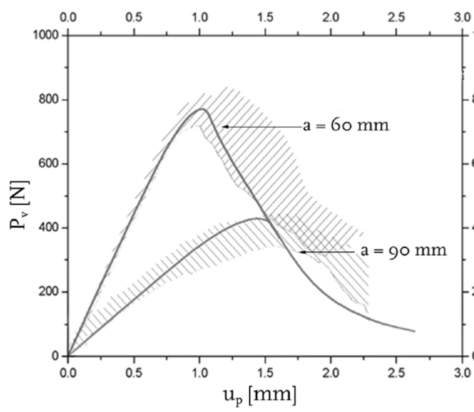

Fig. 5 – Experimental data and fictitious crack fitting of WOL samples in water at 45 °C with two different notch lengths

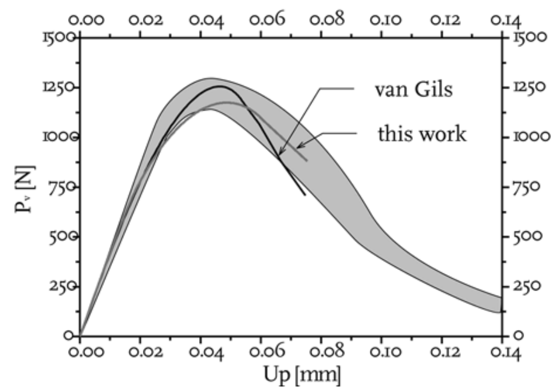

Fig 8 –Force –displacement plot of a WOL sample with notch length a = 60mm.

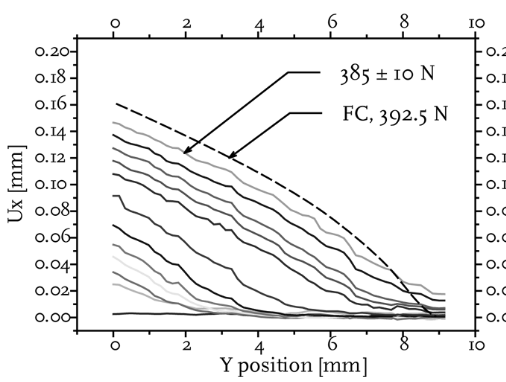

Fig. 6 – Experimental data and fictitious crack fitting of the crack profile of dry samples at room temperature

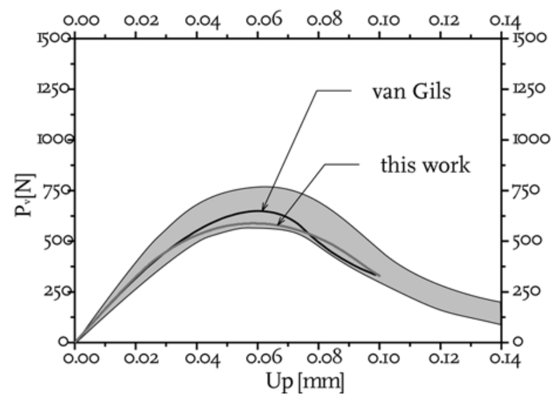

Fig 9– Force –displacement plot of a WOL sample with notch length a = 90mm.

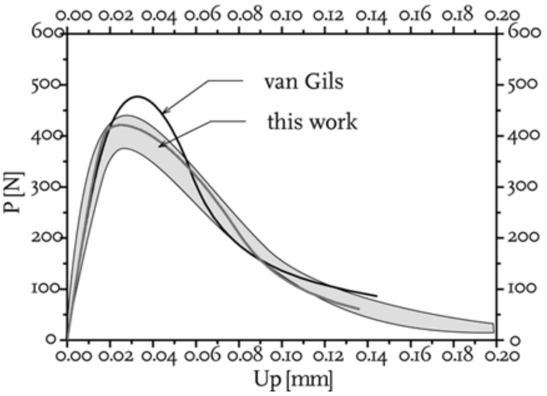

Fig 10 – Force –displacement plot of a SENB sample with notch length a = 5 mm.

4. DISCUSSION

The results obtained after modelling of the PMMA-based material show that the fictitious crack model is a successful model for describing the fracture of this material. For all geometries and conditions the agreement with the experimental curves is good. Moreover, the correct modelling of the crack profile is also good, indicating that modelling of other (more complex) geometries under the same conditions using the same parameters will probably be successful.

The modelling of the refractory ceramic also agrees with the experimental data, despite the fact that the parameters were set not by numerical fitting of the force-displacement curves, obtaining results that are, at least, as good as the obtained through numerical fitting by van Gils et al.

This good agreement shows that a softening curve that resembles the real stress transfer state of the solid is able to produce a fair fitting. However, it is important not to forget that the fictitious crack model is a phenomenological model and there is no univocal relationship between the material parameters and the softening curve parameters. The fictitious crack is a very simplified model that summarizes all the fracture processes, which are three-dimensional, into a single line (fracture line). Furthermore this model losses validity when small ligament lengths are considered, because the fracture energy is reduced, or when the crack tip is close to a sample boundary. In addition, the softening curve is also a simplification of the mechanisms happening in the real material, which are far more complex and stochastic.

Taking into consideration these limitations, it seems possible to set up some initial values of the softening curve parameters base on material parameters, which may yield a fair modelling. Of course, better modelling will be obtained after fitting procedures are applied, and more sophisticated softening curves will improve the results, but the use of the values obtained as described above as initial values for fitting algorithms, may shorten the computation times and increases the chances of an optimal solution.

6. CONCLUSIONS

It has been shown that both the granular polymer, under two ambient conditions, and the refractory ceramic are modelled successfully with the fictitious crack model. In both cases, a bilinear softening curve was used. In the PMMA-based material the parameters of the softening curve were found through a numerical fitting procedure, while in the refractory ceramic the parameters were set after micromechanical considerations. The success of this fitting shows that using a softening curve that resembles the real stress transfer between faces of the crack may produce satisfactory results.

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