<table>
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<th>Title</th>
<th>Micro-Mechanical Modelling of Void Growth, Damage and Fracture of Nano-Phase Structural Adhesives Using the Finite Volume Method</th>
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<tbody>
<tr>
<td>Authors(s)</td>
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<tr>
<td>Publication date</td>
<td>2011</td>
</tr>
<tr>
<td>Conference details</td>
<td>6th International Conference on Fracture of Polymers, Composites and Adhesives, September 11-15, 2011, Les Diablerets, Switzerland</td>
</tr>
<tr>
<td>Publisher</td>
<td>The European Structural Integrity Society Technical Committee</td>
</tr>
<tr>
<td>Item record/more information</td>
<td><a href="http://hdl.handle.net/10197/4766">http://hdl.handle.net/10197/4766</a></td>
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1. Introduction

Significant toughening of structural adhesives is attainable with the addition of nano and/or micro particles. A deep understanding of the effect of particle de-bonding and subsequent void growth to coalescence is key to evaluating the strengthening and failure mechanisms occurring in the damage and fracture of these adhesives. Tapered Double Cantilever Beam (TDCB) experiments, conducted at University College Dublin (UCD), have observed a significant dependence of the fracture toughness of these adhesives on bond gap thickness. In conjunction with this change in fracture toughness, scanning electron-microscopy (SEM) of the fracture surface has also revealed corresponding changes in void evolution as the bond gap is varied. Classical analysis suggests the change in toughness may be attributed to a physical constraint of the size to which the plastic zone around a crack tip may develop. However, simulation of these TDCB tests using finite volume stress analysis has found that little plasticity develops in the bulk adhesive layer and is instead concentrated in the fracture process zone. The change in fracture toughness and void evolution present can be attributed to the change in triaxiality at different bond gap thicknesses and the results agree quite well with the void growth model of Rice & Tracey. The variance of void growth with triaxiality is investigated here.

The initial work considered here concerned 3D modelling of a void in an elastic perfectly plastic material with a view to verifying exponential dependence of void growth on the macroscopic stress triaxiality in the system in accordance with the Rice & Tracey model. The model examines void growth rate dependence on the stress triaxiality, for a given effective strain.

2. Rice & Tracey model

Rice & Tracey considered a spherical void in a rigid, perfectly plastic solid and derived an exponential dependence of void growth on stress triaxiality or constraint defined as:

\[ D = 0.283 \exp(1.5H), \quad H = \frac{\sigma_{\text{hyd}}}{\sigma_{\text{eq}}}, \quad D = \frac{R}{\epsilon_{\text{eq}} R_0} \]  \hspace{1cm} (1)

\[ \sigma_{\text{hyd}} = \frac{\sigma_{11} + \sigma_{22} + \sigma_{33}}{3}, \quad \sigma_{\text{eq}} = \sqrt{\frac{2}{3}} s, \quad s = \sigma - \sigma_{\text{hyd}} \]  \hspace{1cm} (2)

where \( D \) is the dilatational amplification factor, \( H \) is the constraint, \( \epsilon_{\text{eq}} \) is the equivalent macroscopic strain, \( R \) is the average void radius and \( R_0 \) is the initial void radius.

This exponential dependence of the void growth amplification factor with constraint is investigated subsequently with numerical simulations to determine its appropriateness and validity in this case.

3. Numerical Model

Simulations were conducted with the open source finite volume package OpenFOAM (Open Field Operation And Manipulation) and compared to Abaqus Finite Element predictions where appropriate. OpenFOAM is a general 3D based, object-oriented C++ computational continuum mechanics library. A unit cell consisting of a single void is considered. Due to three planes of symmetry, only one eighth of the geometry is modelled. The ratio of the void radius to the outer dimension of the cell is 1 : 15, which was considered a suitable approximation to the infinite domain considered by Rice & Tracey. A hexahedral mesh is constructed in Gambit, exported as a Fluent mesh file and then imported into OpenFOAM using the OpenFOAM utility fluentMeshToFoam, see Figure 2(a).

The material was modelled using a homogeneous isotropic elastic-plastic constitutive model given by:

\[ \sigma = \begin{cases} E\epsilon & \text{for } \epsilon < \epsilon_\sigma, \\ \sigma_0\left(\epsilon_\sigma\right)^n & \text{for } \epsilon \geq \epsilon_\sigma, \quad n = 0, 0.1, 0.2, 0.3 \end{cases} \]  \hspace{1cm} (3)

where \( E \) is Young’s Modulus, \( \epsilon \) is strain, and \( \sigma_0 \) and \( \epsilon_\sigma \) are the stress and strain at yield, respectively, with values of 8.4 GPa and 28 MPa being used for Young’s Modulus and yield stress, respectively.
With reference to Figure 2(b), a normal displacement is applied to the top patch, patch 1 (shown in blue), with unit normal in the x direction and a normal stress is applied to patches 2 & 3, with unit normals in the y and z directions, respectively (red patches), with the void surface set as traction free. The value of the normal stress applied on patches 2 & 3 is calculated as a function of the traction on patch 1 resulting from the prescribed displacement in each time step giving a constant value of macroscopic constraint throughout the simulation.

By writing the constraint, H, in terms of the principal stresses, an expression for $\sigma_2$ can be derived in terms of $\sigma_1$ as follows:

$$H = \frac{\sigma_{bud}}{\sigma_{eq}} = \frac{\sigma_1 + 2\sigma_2}{3}\sqrt{(\sigma_1 - \sigma_2)^2}, \sigma_3 = \sigma_2$$

$$= \frac{\sigma_1 + 2\sigma_2}{3(\sigma_1 - \sigma_2)}, \text{assuming } \sigma_1 > \sigma_2 \quad (4)$$

Rearranging, $\sigma_2 = \sigma_3 = \left(\frac{3H - 1}{2 + 3H}\right)\sigma_1 = \lambda\sigma_1 \quad (5)$

When calculating $\sigma_2$ (and thus $\sigma_3$), the value of $\sigma_1$ from the previous time step was used in order to reduce the numerical overhead with a negligible effect on the solution as the loading rate was sufficiently small.

4. Void Volume Measurement

Void Volume Measurement was implemented by writing a post processing OpenFOAM utility which moves the case mesh by the displacement field, U, calculated at each time step. A trapezoidal rule was then used to calculate the void volume. At each time step, after the mesh had been moved, the x component of the area vector, dA, of each face on the void surface was found. This was then multiplied by the average distance in the x direction of the four vertices which make up the face from a plane with unit x normal going through the centre of the void. This step was completed for each face on the void surface to give the total void volume at each time step. This method can be seen schematically in Figure 3.

For cases run in Abaqus, the same method was used to evaluate the equivalent void radius, however, the method used to calculate the void volume was different. In the Abaqus simulations, the void volume was meshed also, allowing the output of the displacements of each vertex. As simulations were conducted using small strain analysis, it was not possible to calculate the void volume by summing the Abaqus EVOL variable for each cell considered. Instead, a Abaqus script was written in python which would automate the process of reading in the results file and outputting the displacement of each vertex of the void mesh for each time step.

A C++ program was then written to read in the Abaqus mesh and script displacement output file and displace the mesh by the calculated displacements for each time step. Each cell in this hexahedral mesh was then split up into 6 polyhedrons composed of the four vertices of each face and the geometric centre of the hexahedral cell. These polyhedrons were then split into 4 further tetrahedrons composed of two vertices of each face, the geometric centre of the face and the geometric centre of the hexahedral cell. The relative locations of three of the tetrahedrons vertices were found with respect to the fourth vertex, which is the point corresponding to the geometric centre of the original cell. Getting the triple product of these three position vectors gives the volume of that tetrahedron and thus calculating the volume of the remaining 23 tetrahedrons in the same way, the volume of the original hexahedral cell was calculated. The volume of each cell was calculated in this way as it was demonstrated to be numerically efficient by Grandy\textsuperscript{1}.

5. Results

For direct comparison with the Rice & Tracey model, initial cases use a perfectly plastic material model (strain hardening exponent, n = 0) with values of macroscopic constraint achieved ranging from $\frac{1}{3}$ to 3. It was observed that the computed void growth rates did not agree well with the Rice & Tracey model, with significantly larger values of void growth present for all values of triaxiality compared to the analytical solution as seen in Figure 4.

Dependence of void growth on stress triaxiality for different material models was also investigated. Stress hardening exponents, n, equal to 0.1, 0.2 and 0.3 were considered. As seen in Figure 4, increasing plastic modulus acts to suppress void growth, as void growth for a particular value of constraint, H,
decreases with increasing strain hardening exponent, \( n \). However, a significant dependence of void growth on constraint can be seen in all cases. A typical distribution of the equivalent stress can be seen in Figure 5.

To verify the conflict between the numerical results and the analytical model of Rice & Tracey, the mesh was exported in Abaqus format. The same cases were then conducted in Abaqus using the same material model and boundary conditions. Agreement between Abaqus and OpenFOAM was excellent confirming the disparity between the numerical and analytical results.

6. Conclusions

It is evident from the numerical results that the analytical void growth model of Rice & Tracey doesn’t agree well with numerical simulations for a perfectly plastic material model considered here. However, good agreement is obtained using a power-law hardening material which is more similar to real world materials.

References