

COHESIVE-ZONE MODELING OF DEBOND GROWTH AT ADHESIVELY BONDED INTERFACES IN AGGRESSIVE ENVIRONMENTS

Samit Roy*, D. Nagendra*, and K.M. Liechti**

***Mechanical Engineering Department, Oklahoma State University**

****Engineering Mechanics Department, University of Texas-Austin**

Abstract

In this study, a node-release algorithm based on a linear traction separation law was implemented in a test-bed finite element code that was developed to simulate normal (Mode I) and tangential (Mode II) crack growth at the interface. The combined effects of nonlinear viscoelasticity, temperature cycles, and moisture diffusion in the adhesive layer and their influence on crack-growth rates are included in the model. The particular values of the parameters of the traction-separation law can be determined through comparison with crack opening displacement data from test specimens following an iterative procedure previously established. The effect of crack length on mode mix and the existence of asymmetric shielding mechanisms can be accurately assessed using this procedure. Some preliminary benchmark results are presented.

Bond Durability Modeling Approach

One of the primary objectives of the current study is to be able to model the synergistic bond degradation mechanisms at the adhesive-composite interface. The following sections describe the details of the synergistic modeling approach.

Diffusion Controlled Crack Growth

Environmental cracking in a polymer typically occurs in the presence of a penetrant, such as moisture, and stress. It has been postulated that the mechanism involved in environmental crack growth in a polymer involves a small zone of craze formation and/or plasticization at the crack tip due to stress-enhanced moisture ingress. For the case of craze formation, Darcy's law for diffusion in porous media can be used to predict crack (or craze zone) growth. However, for thermoset resins, such as epoxy, energy absorption at the crack tip is primarily by a shear yielding process and not by crazing. Consequently, for a thermoset epoxy, the zone of plasticization ahead of the crack tip must be determined using a diffusion law for non-porous media, such as Fick's law. In the event of synergistic interaction between several processes, a crack will grow at the rate determined by the slowest controlling process and when this is diffusion, then there is diffusion-controlled crack growth.

Free Volume Constitutive Model

The free volume constitutive model [1,2] is based on the premise that the mechanical response of a viscoelastic polymer is dependent on the ability of its molecular chains to accommodate imposed deformations. Free volume may be conceptualized as the volume that is not occupied by the molecular chains in the material. Free volume is typically considered an indicator of molecular segmental mobility, where greater free volume provides the extra mobility needed to accommodate imposed deformations quickly.

Studies of the variables influencing the time scale of viscoelastic materials have shown that temperature, solvent concentration and mechanical dilatation all influence the time scale of the material in a similar manner. Hence the shift factor $a(T, c, \theta)$ can be represented as a function of temperature (T), solvent concentration (c) and mechanical dilatation (θ). Doolittle [3] defined a shift factor relating the fractional free volumes of a material at the current and reference states through the expression,

$$\log_{10} a = \frac{B}{2.303} \left(\frac{1}{f} - \frac{1}{f_0} \right) \quad (1)$$

where, $B =$ a constant, $f =$ fractional free volume at the current state, $f_0 =$ fractional free volume at the reference state. Knauss and Emri [1,2] postulated the fractional free volume to depend on temperature (T), solvent concentration (c) and mechanical dilatation (θ). Therefore the fractional free volume can be expressed as,

$$f = f_0 + A \cdot \alpha * dT + B \cdot M(t) * \sigma_{kk} + C \cdot \gamma(t) * dc \quad (2)$$

where, $\alpha(t)$ and $\gamma(t)$ are the volume coefficients of thermal and moisture expansion. In general, $\alpha(t)$ and $\gamma(t)$ are functions of T , c , the creep compliance $M(t)$ is a function of $\theta(t)$, V_0 is a reference volume, σ_{kk} is the first stress invariant, and A , B , C are constants to be determined. Note that the (*) notation used in eqn. (2) denotes Stieltjes convolutions representing the time history of the respective variables. For small changes in variables below the glass transition temperature of the polymer and the boiling point of the penetrant, it is assumed that $\alpha(t)$, $\gamma(t)$ and $M(t)$ are constants with respect to time. Further under such conditions, simple multiplicative relations can replace the convolutions in eqn. (2), giving,

$$f = f_0 + \alpha \Delta T + \gamma \Delta c + \delta \theta \quad , \quad \text{where } \theta = \epsilon_{kk} \text{ , and } \delta \text{ is a material constant} \quad (3)$$

Substituting eqn. (3) in eqn. (1) gives the nonlinear shift factor,

$$\log a(T, c, \theta) = - \frac{B}{2.303 f_0} \frac{\alpha \Delta T + \gamma \Delta c + \delta \theta}{f_0 + \alpha \Delta T + \gamma \Delta c + \delta \theta} \quad (4)$$

For negligible solvent concentrations and dilatation eqn. (4) reduces to the WLF equation. It was found from experimental data [4] that the value of δ was very close to unity, so henceforth the model assumes that $\delta = 1$. In this model the nonlinear shift factor definition in eqn. (4) incorporates all the nonlinearity in the linear viscoelastic constitutive description of an isotropic solid under infinitesimal deformations. At reference conditions, the constitutive equations for a viscoelastic material are,

$$\begin{aligned}
 s_{ij} &= \int_{-\infty}^t 2\mu(t' - \tau') \frac{\partial e_{ij}}{\partial \tau} d\tau \\
 \sigma_{kk} &= \int_{-\infty}^t 3K(t' - \tau') \frac{\partial(\theta + \alpha\Delta T + \gamma\Delta c)}{\partial \tau} d\tau \\
 t' - \tau' &= \int_{\tau}^t \frac{d\xi}{a[T(\xi), c(\xi), \theta(\xi)]}
 \end{aligned} \tag{5}$$

where s_{ij} and e_{ij} are components of deviatoric stress and strain tensors. The nonlinear set of equations (3) - (5) account for the temperature, solvent concentration, and dilatation histories and essentially comprise the free volume constitutive model.

Cohesive Zone Model

The cohesive zone interface model was developed by Needleman [5] in order to provide a unified description of crack initiation from initial debonding through complete separation and subsequent crack growth. The interface constitutive equation developed in the model was such that, with increasing interface separation, the traction across the interface of the crack reaches a maximum, decreases, and eventually vanishes so that complete decohesion occurs. The subsequent mechanical response of the crack is dependent on the strength of the interface, which is specified by the critical stress measure near the tip of the crack, and the work of separation per unit area. This interface model is based on the cohesive zone model developed by Dugdale and Barenblatt. Needleman introduces a characteristic length in order to determine the size of the cohesive zone where the tractions are to be applied, the equivalent of which is defined as the crack tip opening displacement in the Dugdale-Barenblatt model. The tractions at the interface are therefore a function of the crack tip opening displacement. Further investigations of crack growth in thin film blistering of polyimide film on aluminum substrate by Shirani and Liechti [6] made use of a simplified version of the Needleman interface model. In this case, the decay of tractions with the result of the traction separation law was simulated as non-linear softening springs attached to the nodes of the crack interface in the finite element model. This method has been referred to as “nodal relaxation” by several authors [7,8,9] due to the gradual decrease in traction force rather than the immediate release of the node due to debonding. The dependence of the

tractions on the crack tip opening displacement is considered invariant with respect to quasi-static propagation in a controlled environment as specified by Ungsuwarungsri and Knauss [10]. The use of the traction separation law as improvised by Shirani and Liechti has been successfully incorporated into a test-bed (NOVA-3D) finite element code to analyze tensile decohesion for elastic structures in two and three-dimensional cases. In this model, attention is directed towards the interface close to the crack that supports a nominal traction field \mathbf{T} (force/unit reference area), which in general, has both normal and shearing components. Two material points A and B may be chosen which were initially on opposite faces of the interface and the interfacial traction is taken to depend only on the displacement difference vector across the interface, $\Delta\mathbf{u}_{AB}$. Thus at each point on the interface, we may define normal and tangential components of displacements and tractions,

$$u_n = \mathbf{n} \cdot \Delta\mathbf{u}_{AB}, \quad u_t = \mathbf{t} \cdot \Delta\mathbf{u}_{AB} \quad (6)$$

$$T_n = \mathbf{n} \cdot \mathbf{T}, \quad T_t = \mathbf{t} \cdot \mathbf{T} \quad (7)$$

where, T_n = normal component of traction, T_t = shear component of traction, and positive u_n corresponds to increasing interfacial separation. This dependence of the traction magnitude on the amount of the separation between the interfaces can be expressed in terms of a potential $\phi(u_n, u_t)$, which is defined as,

$$\phi(u_n, u_t) = -\int_0^{u_t} [T_n du_n + T_t du_t] \quad (8)$$

As shown in Fig. 1, Needleman defined the model in such a way that as the interface separates, the magnitudes of the tractions increases, achieves a maximum and ultimately falls to zero when complete separation occurs. The model shown is defined for pure normal tractions on the interface with u_t being zero. Needleman has proposed to define the traction-separation curve in terms of the potential as,

$$\phi(u_n, u_t) = \frac{27}{4} \sigma_{\max} \delta \left\{ \frac{1}{2} \left(\frac{u_n}{\delta} \right)^2 \left[1 - \frac{4}{3} \left(\frac{u_n}{\delta} \right) + \frac{1}{2} \left(\frac{u_n}{\delta} \right)^2 \right] \right\} \quad (9)$$

where, σ_{\max} = maximum traction carried by the interface undergoing pure normal separation, and, δ is a characteristic length. When $u_n > \delta$ then $\phi \equiv \phi_{sep}$, where ϕ_{sep} is the work of separation. The interfacial tractions for pure normal separation may be obtained by differentiating eqn. (9) and setting $u_t=0$ to give,

$$T_n = \frac{\partial \phi}{\partial u_n} = -\frac{27}{4} \sigma_{\max} \left\{ \left(\frac{u_n}{\delta} \right) \left[1 - 2 \left(\frac{u_n}{\delta} \right) + \left(\frac{u_n}{\delta} \right)^2 \right] \right\} \quad (10)$$

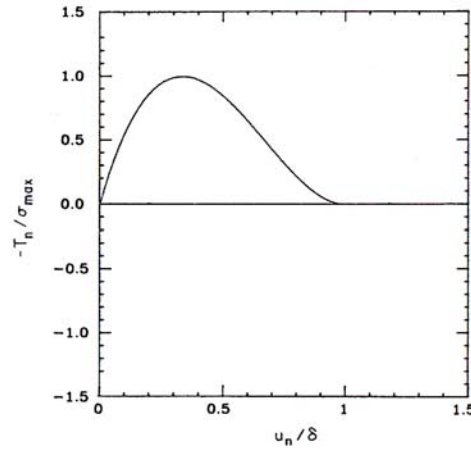


Figure 1. Normal tractions across the crack interface as a function of normal displacements

The fracture energy (work of separation) is defined as the area under the curve in Figure 1 and is given by,

$$\phi_{sep} = 9\sigma_{\max} \delta/16 \quad (11)$$

For a given fracture energy based on the material and stress at the crack tip, the value of δ may be computed using eqn. (11).

Preliminary Benchmark Results

Figure 2 depicts the strain energy release rate as a function of incremental crack length obtained from the analysis of an elastic Double Cantilever Beam (DCB) specimen employing the cohesive-zone crack growth model. The benchmark plot shows good agreement of the test-bed code (NOVA-3D) results when compared with crack growth data obtained from the commercial finite element code ABAQUS. Synergistic interfacial crack growth modeling in the presence of diffusing penetrants, material nonlinearities, and adhesive viscoelasticity is currently underway.

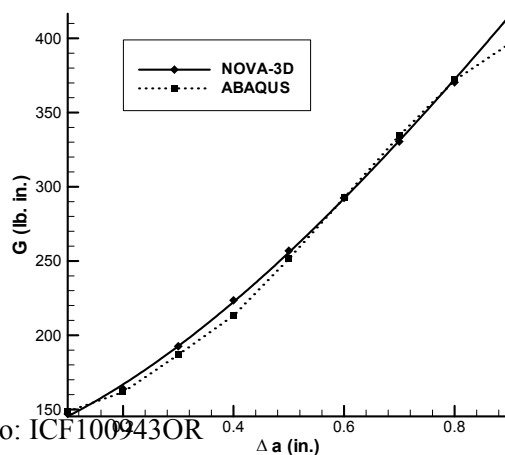


Figure 2. Strain energy release rate vs. incremental crack length, DCB steel specimen, constant load test, $P = 600$ lb.

Acknowledgement

The authors would like to thank the Automotive Composites Consortium, and the CMS Division of the National Science Foundation for supporting this research.

List of References

1. Knauss, W.G. and Emri, I., Non-Linear Viscoelasticity based on Free Volume Consideration, *Computers and Structures*, V.13, pp. 123-8, 1981.
2. Knauss, W.G. and Emri, I., Volume Change in the Nonlinearly Thermo-Viscoelastic Constitution of Polymers, *Polymer Engineering and Science*, V.27, pp. 86-100, 1987.
3. Doolittle, A.K., Studies on Newtonian Flow. II. The Dependence of the Viscosity of Liquids on Free-Space, *Journal of Applied Mechanics*, V.22, pp. 1471-5, 1951.
4. Knauss, W.G. and Kenner, V.H., On the Hygrothermomechanical Characterization of Polyvinyl Acetate, *Journal of Applied Physics*, V.51, pp. 5131-6, 1980.
5. Needleman, A., A Continuum Model for void Nucleation by Inclusion Debonding. *Journal of Applied Mechanics*, Vol. 54, pp. 525-531, 1987.
6. Shirani, A. and Liechti, K. M., A Calibrated Fracture Process Zone Model for Thin Film Blistering. *International Journal of Fracture*, Vol. 93, pp. 281-314, 1998.
7. Malluck J. F. and King W. W., Fast Fracture Simulated by Conventional Finite Elements: A Comparison of Two Energy-Release Algorithms, *Crack Arrest Methodology and Applications*, ASTM STP 711, G. T. Hahn and M. F. Kanninen, Eds., American Society for Testing and Materials, pp. 38-53, 1980.
8. Malluck J. F. and King W. W., Fast Fracture simulated by a Finite Element Analysis which accounts for crack tip energy dissipation. *International Conference on Numerical Methods in Fracture Mechanics*, pp. 648-659, 1978.
9. Rydholm G., Fredriksson B. and Nilsson F., Numerical investigations of rapid crack propagation. *International Conference on Numerical Methods in Fracture Mechanics*, pp. 660-672, 1978.
10. Ungsuwarungsri, T. and Knauss, W. G., The Role of Damage-Softened Behavior in the Fracture of Composites and Adhesives. *International Journal of Fracture*, Vol. 35, pp. 221-241, 1987.