Proceedings of IMECE04 2004 ASME International Mechanical Engineering Congress and Exposition November 13-20, 2004, Anaheim, California USA



DAMAGE IN SHORT-FIBER COMPOSITES: FROM THE MICROSCALE TO THE CONTINUUM SOLID

Ba Nghiep Nguyen, Brian J Tucker, Mohammad A Khaleel Pacific Northwest National Laboratory P.O. Box 999, Richland, WA 99352, USA

Tel: (509) 375 3634, Fax: (509) 375 6736, Email: Ba.Nguyen@pnl.gov

ABSTRACT¹

This paper proposes a multiscale mechanistic approach to damage in short-fiber polymer composites (SFPC). At the microscale, the damage mechanisms are analyzed using micromechanical modeling, and the associated damage variables are defined. The stiffness reduction law dependent on these variables is then established. The macroscopic response is determined using thermodynamics of continuous media, continuum damage mechanics and finite element analysis. Final failure resulting from saturation of matrix microcracks, fiber/matrix debonding, fiber pull-out and breakage is modeled by a vanishing element technique. The model was validated using the experimental data and results from literature, as well as those obtained from a random glass/vinyl ester system.

INTRODUCTION

The word "short-fiber composite" used in this paper is to exclude continuous fiber composites but not to restrict consideration to fiber lengths lower than some arbitrary value. Damage in short-fiber polymer composites is a very complex phenomenon. At the *microscale*, damage can start with the occurrence of matrix microcracks that propagate and weaken the fiber tow/matrix and fiber/matrix interfaces and lead to debonding of fiber tows and fibers. Also, it can begin with the debonding mechanism at weakened interfaces, which will in turn induce matrix cracking. Excessive matrix cracking and fiber/matrix decohesion at higher loading levels will engender fiber pull-out and breakage. These damage mechanisms strongly affect the homogenized behavior of the composite layer or of the composite representative volume element (*mesoscale*). Finally, accumulation of damage leads to initiation and propagation of a macroscopic crack, and the composite structure (*macroscale*) will fail. Fig. 1 gives a schematic descriptions of different scales considered in the analysis.





In this paper, a *multiscale mechanistic* approach to damage in SFPC is developed based on *micromechanical* and *continuum damage mechanics descriptions* to determine the

¹ This manuscript has been authored by Battelle Memorial Institute, Pacific Northwest Division, under Contract No. DE-AC06-76RL0 1830 with the U.S. Department of Energy. The United States Government retains and the publisher, by accepting the article for publication, acknowledges that the United States Government retains a non-exclusive, paid-up, irrevocable, world-wide license to publish or reproduce the published form of this manuscript, or allow others to do so, for United States Government purposes.

macroscopic response of these materials suffering from matrix cracking and fiber/matrix debonding. Modeling matrix cracking coupled with fiber/matrix debonding starts from the modified Eshelby-Mori-Tanaka formulation [1, 2] by Qu [3] applied to a three-phase composite. In this formulation, imperfect fiber/matrix interfaces are accounted for using the concept of a "spring layer" of vanishing thickness surrounding the fiber. Matrix microcracks parallel to each other and to the fibers are modeled as the second inclusion phase with zero stiffness. Such a composite containing aligned fibers, matrix microcracks and imperfectly bonded interfaces is defined as a reference composite. From this micromechanical analysis, two damage variables are defined. The first variable is the crack density while the second one is linked to the compliance of the spring layer representing the weakened interface. Next, the stiffness of the random fiber composite containing random matrix microcracks and degraded interfaces is calculated from the stiffness of the reference composite averaged over all possible orientations and weighted by an orientation distribution function. Since matrix cracking and fiber/matrix debonding are not independent mechanisms, the relationship between the corresponding damage variables needs to be identified experimentally. This relationship expresses how fiber/matrix debonding can evolve with matrix cracking.

Finally, the macroscopic response is determined by means of a *continuum damage mechanics* formulation similar to that used by Nguyen and Khaleel [4, 5], which extends the Renard et al.'s [6] damage model formulation for continuous fiber composites to randomly oriented short-fiber composites. In this formulation, the damage evolution law is obtained using a damage criterion and the concepts of thermodynamics of continuous media. Failure as a result of excessive matrix cracking, fiber/matrix debonding, fiber pullout and rupture leading to initiation and propagation of a macroscopic crack is modeled by a *vanishing element technique*.

The model was validated using the experimental data and results by Meraghni and Benzeggagh [7] as well as those obtained from a random glass/vinyl ester system.

PROBLEM FORMULATION

Micromechanical modeling. Consider a short fiber composite in which the fiber tows and fiber-shape matrix microcracks are unidirectional. In addition, this composite contains imperfect fiber/matrix interfaces. The as-defined composite serves as the reference composite. Due to degradation at the interface, the fiber/matrix bonding becomes imperfect. It is assumed that interfacial deterioration has not led to fiber pull-out yet so that the concept of a spring layer of vanishing thickness used by Qu [3] can still be applied to characterize the imperfect bonding. In such a case, the interfacial tractions are still continuous, but a displacement discontinuity may happen at the interface. Qu modified the structure of the Mori-Tanaka solution to fully account for the existence of weakened interfaces. Accordingly, the stiffness of a composite containing n aligned ellipsoidal inclusion phases (of volume fractions f_i) with weakened interfaces is given by:

$$\boldsymbol{C} = \left(f_{\mathrm{m}} \boldsymbol{C}_{\mathrm{m}} + \sum_{i=1}^{n} f_{i} \boldsymbol{C}_{i} : \boldsymbol{A}_{i} \right) : \left(f_{\mathrm{m}} \boldsymbol{I} + \sum_{i=1}^{n} f_{i} \boldsymbol{A}_{i} + \sum_{i=1}^{n} f_{i} \boldsymbol{H}_{i} : \boldsymbol{C}_{i} : \boldsymbol{A}_{i} \right)^{-1} (1)$$

where $C_{\rm m}$ and C_i (i = 1,...,n) are the stiffness tensors of the matrix and inclusions, respectively. A_i denote the fiber concentration matrices given by

$$\mathbf{A}_{i} = \left[\mathbf{I} + \mathbf{S}_{i}^{*} : \mathbf{C}_{m}^{-1} : (\mathbf{C}_{i} - \mathbf{C}_{m}) \right]^{-1}$$
(2)

with the modified Eshelby tensor defined by Qu [3] in terms of the Eshelby tensor *S* and the interface compliance *H* as:

$$S_{i}^{*} = S_{i} + (I - S_{i}): H_{i}: C_{m}: (I - S_{i})$$
(3)

To obtain the solution for a composite containing imperfect fiber/matrix interfaces and a given volume fraction of matrix microcracks, we consider a *hybrid inclusion* system in which the microcracks are the second inclusion phase of zero stiffness. Consequently, the stiffness of such a composite reads: $C = \lim_{n \to \infty} (f_n C_n + f_1 C_1; A_1 + f_2 C_2; A_2);$

$$(f_{\rm m} I + f_1 A_1 + f_2 A_2 + f_1 H_1 : C_1 : A_1 + f_2 H_2 : C_2 : A_2),$$

$$(f_{\rm m} I + f_1 A_1 + f_2 A_2 + f_1 H_1 : C_1 : A_1 + f_2 H_2 : C_2 : A_2),$$

$$C_2 \to 0$$
(4)

Next, it is necessary to define the damage variables associated with the governing damage mechanisms. Prior to final failure, these mechanisms can be classified into two categories [7]. The first category is related to matrix cracking and subsequent growth of microcracks between fiber tows while the second one corresponds to decohesion between fiber tows and fiber/matrix debonding. In this analysis, the matrix microcrack volume fraction f_2 is used as the damage variable describing matrix cracking, and it is renamed as α while a parameter governing the compliance of the fiber/matrix interfaces is used as the second damage variable. Before total failure, relative sliding between fibers and matrix without separation is considered. In addition, the compliance of the interface should be comprised between two limiting values. The first value is infinite and corresponds to a complete debond while the second one is zero, which is the case of a perfectly bonded interface [3]. Therefore, the interface compliance can be expressed in terms of the parameter β defined as:

$$\beta = \beta(r, E_{\rm m}, \beta^*) = \frac{r\beta^*}{E_{\rm m}} \tag{5}$$

where *r* is the fiber radius, and $E_{\rm m}$ the matrix elastic modulus. β^* is linked to the participation rate of fiber/matrix debonding in the damage process and is taken as the damage variable associated with this mechanism. β^* varies from 0 to $\beta_{\rm L}^*$. The 0 value represents a perfectly bonded interface while advanced stages of degradation approaching complete debonding is characterized by $\beta^* = \beta_{\rm L}^*$. Since matrix cracking is coupled with interfacial debonding, it is necessary to identify the relationship: $\beta^* = \beta^*(\alpha)$ experimentally.

The stiffness of the random fiber composite containing random matrix microcracks is computed from the stiffness of the reference composite given by Equations (4), which is averaged over all possible orientations and weighted by an orientation distribution function [4, 5]:

$$\overline{C}(\alpha) = \frac{\int_{-\pi/2}^{0} \mathbf{R}(\alpha,\theta) \lambda e^{-\lambda(-\theta)} d\theta + \int_{0}^{\pi/2} \mathbf{R}(\alpha,\theta) \lambda e^{-\lambda\theta} d\theta}{2 \int_{0}^{\pi/2} \lambda e^{-\lambda\theta} d\theta}$$
(6)

where $R(\alpha, \theta)$ is the global stiffness matrix of the reference composite, which is obtained by transforming $C(\alpha)$ into the global coordinate system. This coordinate system is defined such that the fibers are assumed in the layer plane 1-2 with the orientation angle measured relative to the 1-axis. Karcir et al.'s [8] orientation distribution function dependent on parameter λ is used in Eq. (6). The analysis presented here considers random orientations of fibers and microcracks; hence λ is rather small and tends to zero when the fibers and microcracks are completely random.

Meso modeling. The damage evolution law in terms of the local strains ε_i can be obtained using thermodynamics of continuous media and a continuum damage mechanics formulation similar to that used by Renard et al [6] for continuous fiber composites subject to transverse matrix cracking. Such a formulation was extended by Nguyen & Khaleel [4, 5] to random short-fiber composites containing random matrix microcracks. It relies on the use of a thermodynamic potential (which is the elastic deformation energy), Clausius-Duhem's inequality (dissipation criterion) and a damage criterion. Only *independent state variables* are retained in the dissipation criterion, which are α and ε_i in this analysis. Using the damage criterion and the consistency conditions, the damage evolution law is obtained as

$$d\alpha = -\frac{\frac{d\overline{C}_{ij}}{d\alpha}\varepsilon_i d\varepsilon_j}{\frac{1}{2}\frac{d^2\overline{C}_{ij}}{d\alpha^2}\varepsilon_i \varepsilon_j - \frac{dF_c}{d\alpha}}$$
(7)

where $F_c(\alpha)$ is the damage threshold function that is identified using the experimental data providing the crack density as a function of the applied stress or strain [4, 5]. Such data can be obtained by an amplitude analysis of acoustic emission signals (see e.g. [7, 9]).

Macro modeling. The stiffness reduction law, constitutive relation and damage evolution equation established at the micro and meso scales can be introduced into a finite element formulation for the analysis of a composite structure. To this end, considering kinematically admissible finite elements under small strain assumption, the discretization of the displacement field $q^{(n)}$ allows computation of the strain increment as

$$\Delta \boldsymbol{\varepsilon}^{(n)} = [\boldsymbol{B}_0 + \boldsymbol{B}_{nl}(\boldsymbol{q})] \Delta \boldsymbol{q}^{(n)}$$
(8)

at each iteration *n* of the Newton-Raphson procedure. B_0 and $B_{nl}(q)$ are the linear and nonlinear deformation matrices dependent on the derivatives of the interpolation functions. The damage increment is computed in terms of the strain increment using Equation (7), which can be rewritten as:

$$\Delta \alpha^{(n)} = G(\alpha^{(n-1)}, \varepsilon^{(n)}) . \Delta \varepsilon^{(n)}$$
(9)

The equilibrium equations obtained from the virtual work principle leads to:

$$\boldsymbol{K}_{\mathrm{T}}^{(n)} \Delta \boldsymbol{q}^{(n)} = \boldsymbol{R}^{(n)} \tag{10}$$

where $K_{T}^{(n)}$ is the tangent stiffness matrix, and $R^{(n)}$ is the global residual load vector. The iterative procedure converges if the norm of $R^{(n)}$ is smaller or equal to a prescribed precision.

When the damage variable α attains the maximum value $\alpha_{\rm lim}$ corresponding to the highest crack density, *total failure* occurs, and consequently the material can no longer carry load. Total failure is modeled here using a *vanishing element technique* that consists of reducing the local stiffness and stresses to zero in a certain number of steps in order to avoid numerical instability [4, 5]. To create a computational tool for the damage analysis of SFPC structures, the damage model has been implemented into the ABAQUS finite element code (version 6.4) by means of user-subroutines.

EXPERIMENTAL IDENTIFICATION OF DAMAGE

When composite materials are subjected to continuously increasing loads until failure, microstructural damage occurs in the material releasing energy in the form of mechanical sound waves. These sound waves known as acoustic emissions (AE) can be detected with sensors and recorded for later analysis. Previous work by Meraghni & Benzeggagh [7] and by Barre & Benzeggagh [8] revealed that the type of damage mechanisms occurring during loading could be correlated with the amplitudes of AE signals. A test setup based on these references was developed for the acquisition of AE signals from random glass/vinyl ester specimens during tensile loading to failure. Amplitude information was calculated from each acquired waveform and was used to construct a histogram showing the number of events versus amplitude. This enabled the participation of a given mechanism to the damage process to be identified. The participation rates have allowed the crack density and the matrix cracking/fiber-matrix debonding relationship $\beta^* = \beta^*(\alpha)$ to be determined.



Figure 2. Cumulative amplitude distribution during a tensile test for a random glass/vinyl ester specimen.

Figure 2 shows the number of events versus the amplitude (dB) of AE signals obtained for a random glass/vinyl ester specimen, in which the fiber volume fraction is about 30%, and the average fiber tow aspect ratio is of 34. The data in Fig. 2 enable the determination of the participation rates as follows. First, based on Refs [7, 9], AE techniques and scanning electron microscopy (SEM) were used to verify that the range of amplitudes between 30 and 55dB were attributed to matrix cracking and growth of microcracks between the fiber bundles. Second, the events recorded within this range during a tensile test occurred mostly uniformly over the sample volume (Fig. 3) used for strain measurement (extensometer gage length). This reflects the random damage distribution due to matrix cracking.

As a consequence, this range is adopted in this paper to determine the participation of matrix cracking in the damage process. Higher amplitude levels are associated with fiber/matrix debonding. However, high load levels leading to fiber pull-out, rupture, and damage localization were excluded from the final damage analysis. Input for the computer models did not include participation rates for crack density calculations at the load levels leading to failure.

AE Events up to 110 MPa

90

80 70

60

50

30

10

AE Event Amplitude (dB)



Distance along Gage (mm)

20

The participation rates of matrix cracking, P_i^m and of both matrix cracking and fiber/matrix debonding, P_i at a given applied stress level, *i*, are defined respectively as:

$$P_i^{\rm m} = \frac{a_i^{\rm m}}{A_{\rm tot}}; \qquad P_i = \frac{a_i}{A_{\rm tot}} \tag{11}$$

30

where $a_i^{\rm m}$ is the area bounded by the events versus amplitude curve up to 50 dB for a given load level (Fig. 2) and a_i is the total area under the number of events versus amplitude curve for a given load level. $A_{\rm tot}$ is the total area of the distribution of amplitudes at the ultimate stage prior to final failure characterized by the onset of damage localization and instabilities. Based on Ref. [7], the microcrack volume fraction (crack density) is given by:

$$\alpha = P_i^{\rm m} f_{\rm m} = \frac{P_i^{\rm m}}{1 + P_i^{\rm m}} (1 - f_{\rm b})$$
(12)

where f_{b} is the fiber tow volume fraction in the composite.

The damage variable β^* associated with fiber/matrix debonding can be expressed in terms of the participation rate related to fiber/matrix debonding as:

$$\beta^* = c \left(P_i - P_i^{\mathrm{m}} \right) \tag{13}$$

where *c* is an interface property parameter. It can be identified knowing the maximum participation rate of fiber/matrix debonding, which corresponds to $\beta^* = \beta_L^*$. β_L^* was taken to be equal to 1 in this analysis. Finally, the relationship between the damage variables α and β^* is obtained from Eqs. (12) and (13). Figures 4 and 5 respectively show the participation rates of the damage mechanisms and the evolution of β^* as a function of α for the glass/vinyl ester samples.

NUMERICAL APPLICATIONS

The damage model was implemented into the ABAQUS finite element code by means of user subroutines. In particular, the subroutine UMAT was used for the implementation of the constitutive relations. This section presents the simulations of the tensile stress/strain responses for the random 1200tex glass/epoxy and glass/vinyl ester systems. In the former case, the material properties and crack density data were taken from Ref. [7]. The crack density data were used to identify the damage threshold function in the damage model (Eq. (7)). This enabled the simulation of the tensile stress/strain response of the glass/epoxy material using the damage model.



Figure 4. Participation rates of the damage mechanisms versus the applied stress.



Figure 5. Evolution of the damage variable β^* as a function of the crack density α .

Figure 6 shows the predicted stress/strain response compared with the experimental results in [7]. Due to the lack of information about the participation rate for fiber/matrix debonding, only matrix cracking was considered in the analysis. Taking into account of the significant scatter in the experimental values, the matrix cracking model provided a fair prediction of the experimental results. The predicted crack density versus applied stress curve is presented in Fig. 7 which shows a very good agreement with the experimental data also illustrated in the same figure.



Figure 6. Tensile stress/strain responses for the random 1200tex glass/epoxy specimens. The values denoted by the symbols were extracted from the experimental curves in [7].



Figure 7. Applied stress versus crack density for the random 1200tex glass/epoxy specimens. The experimental values denoted by the symbols were from [7].

Next, the damage model was used to compute the tensile stress/strain responses for the random glass/vinyl ester specimens. The participation rate (Fig. 4) for matrix cracking obtained from the analysis of acoustic emission signals was converted into crack density versus applied stress data to determine the damage threshold function for this material. Also, the relationship $\beta^* = \beta^*(\alpha)$ identified through the participation rates (Fig. 5) was also used in the damage model to account for matrix cracking coupled with fiber/matrix debonding. Figures 8 and 9 present the tensile stress/strain responses and the applied stress versus crack density for these specimens. On the same figures are also shown the experimental values. Figure 8 shows a better agreement with the experimental curves when both matrix cracking and fiber/matrix debonding were accounted for in the analysis. The evolution of the crack density with the applied stress was very well captured by the model both in tendency and numerical values (Fig. 9).



Figure 8. Predicted and experimental tensile stress/strain responses for the random glass/vinyl ester specimens.



Figure 9. Applied stress versus crack density for the random glass/vinyl specimens

CONCLUSION

A micro-macro mechanistic approach to damage in shortfiber polymer composites has been developed in this paper starting from the microscale related to the constituents, microcracks and interfacial defects to the scale of a macroscopic composite structure. Before final failure, matrix cracking and interfacial decohesion responsible for the reduction of the composite stiffness have been accounted for. The elastic and reduced properties of the composite have been obtained from micromechanical modeling based on the modified Mori-Tanaka model. Two damage variables have been defined: one variable is the crack density, and the other describes the deterioration of the fiber/matrix interface. The continuum composite obtained through this homogenization (mesoscale) has been used to establish the constitutive relation and the damage evolution law. Finally, the implementation of the damage model into the ABAQUS finite element code has enabled structural analyses (macroscale) using this model. Different scales in modeling have then been bridged. Numerical tests have shown that the model provided good predictions of the tensile stress/strain responses and the crack density versus applied stress for the random glass/epoxy and glass/vinyl ester specimens. The model can be used to assist the damage assessment for SFPC structures subjected to quasistatic loading.

ACKNOWLEDGEMENT

The support of Pacific Northwest National Laboratory's Computational Science and Engineering Initiative is gratefully appreciated.

REFERENCES

 [1] Eshelby, J.D., 1957, "The Determination of The Elastic Field of An Ellipsoidal Inclusion and Related Problems," Proceedings of the Royal Society London, A 241, pp. 376-396.
 [2] Mori, T., Tanaka, K., 1973, "Average Stress in Matrix and Average Elastic Energy of Materials with Misfitting Inclusions," Acta Metallurgica, 21, pp. 571-574.

[3] Qu, J., 1993, "The Effect of Slightly Weakened Interfaces on The Overall Elastic Properties of Composite Materials," Mechanics of Materials, **14**, pp. 269-281.

[4] Nguyen B.N., Khaleel M.A., 2003, "Prediction of Damage in A Randomly Oriented Short-Fiber Composite Plate Containing A Central Hole," Proceedings, The Second M.I.T. Conference in Computational Fluid and Solid Mechanics, Bathe, K.J., Editor, Elsevier, pp. 519-522.

[5] Nguyen, B.N., Khaleel, M.A., 2004, "A Mechanistic Approach to Damage in Short-Fiber Composites Based on Micromechanical and Continuum Damage Mechanics Descriptions," Composites Science and Technology, **64**, pp. 607-617.

[6] Renard, J., Favre, J.-P., Jeggy, T., 1993, "Influence of Transverse Cracking on Ply Behavior: Introduction of A Characteristic Damage Variable," Composites Science and Technology, **46**, pp. 29-37.

[7] Meraghni, F., Benzeggagh, M.L., 1995, "Micromechanical Modeling of Matrix Degradation in Randomly Oriented Discontinuous-Fibre Composites," Composites Science and Technology, **55**, pp. 171-186.

[8] Karcir, L, Narkis, M, Ishai O., 1975, "Oriented Short Glass-Fiber Composites: I Preparation and Statistical Analysis of Aligned Fiber Materials," Polymer Engineering Sciences, **15**, pp. 525-531.

[9] Barre, S., Benzeggagh, M.L., 1994, "On the Use of Acoustic Emission to Investigate Damage Mechanisms in Glass-Fibre-Reinforced Polypropylene," Composites Science and Technology, **52**, pp. 369-376.