

BRIDGING THE GAP BETWEEN PHYSICS AND LARGE-SCALE STRUCTURAL ANALYSIS: A NOVEL METHOD FOR FATIGUE LIFE PREDICTION OF COMPOSITES

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ABSTRACT

The need for the capability to apply physics-based theories and principles to composite materials has been widely recognized. Efforts to develop this capability for analysis of large structures have been hindered by excess computational time or the inability to separate differences in the physical behavior exhibited by each constituent material in the composite. In this work, a new approach is proposed for composite fatigue life prediction. The stresses and strains of the composite constituents are calculated using multicontinuum theory, which requires negligible additional computation time beyond that of standard finite element analysis of a homogenized material. The constituent stresses are used in combination with kinetic theory to predict fatigue life in large-scale composite structures under a variety of complex load states. This method is easily adapted to existing finite element analysis tools and requires minimal composite fatigue characterization. The approach provides the needed bridge between physics and large-scale structural analysis.

1. INTRODUCTION

Fatigue of composite materials has been studied for four decades [1,2]. But in spite of numerous research efforts, agreement regarding methods to predict fatigue life in composites has yet to emerge. Most predictive theories pertain to a specific load history at a specific temperature and are not easily generalized to capture multiaxial load states, variable amplitude or spectral loading, temperature changes, or environmental effects. In addition, any general solution must be able to be implemented into design codes, such as finite element analysis software, with computational efficiency.

This goal is unlikely to be achieved as long as composite fatigue predictions are based on purely empirical relationships. Physics-based concepts must be applied to the composite in order to use a minimal amount of characterization data to predict the fatigue life of a composite under a variety of loading and environmental conditions. But applying physics-based theories requires knowledge of constituent-level behavior. Using multicontinuum theory [3], however, constituent level stresses and strains can be exactly determined with simple equations. Moreover, this technique has already been implemented in Helios:MCT™ [4], which integrates with existing finite element software to allow constituent-level stress and strain resolution with negligible additional computation time.

In this paper, we combine the constituent-level stresses calculated using multicontinuum theory with the well-established kinetic theory of fracture to produce a novel physics-based, multiscale method for predicting fatigue life in composite materials. This method is validated against published off-axis fatigue data at different temperatures [5,6]. Because the method is physics-based it provides a framework to predict fatigue life under any loading condition or environment, and it requires a minimal amount of composite characterization data.

2. THEORETICAL DEVELOPMENT

One crucial observation regarding the character of composite fatigue failure is that, with the exception of nearly perfect axial loading, fatigue failure is a matrix-dominated event [5,7,8]. This means that the kinetics of the polymer matrix is the physics-based ingredient needed to predict fatigue. The physical mechanism of fatigue failure in polymers is outlined in the following subsection. Incorporation of this physical mechanism in a composite material is then discussed in the next two subsections on multicontinuum theory and effective matrix stress, respectively.

2.1 Fatigue failure of polymers

The relationship between polymer kinetics and mechanical behavior was developed more than five decades ago by Zhurkov [9,10] and Coleman [11-13] in parallel efforts. Zhurkov used experimental observations to show that conceiving of strength in terms of molecular kinetics was well-founded. Most importantly, Zhurkov showed that the bond rupture rate determines the fracture strength of a polymer and the time to failure under a creep load, where the bond rupture rate K_b under a tensile load σ has the form

$$K_b = \nu_0 \exp\left(-\frac{U - \gamma\sigma}{kT}\right). \quad [1]$$

In Equation (1), U is an activation energy that is closely related to bond energy, γ is an activation volume, and k is the Boltzmann constant. (Note that this is the Eyring equation, as discussed by Ward [14].) Approaching the problem from statistical mechanics, Coleman developed a similar equation and noted that it could also be used to predict polymer fatigue life [13]. ν_0 is the oscillation frequency of the atom, which should be proportional to kT/h , where h is Planck's constant; at room temperature $kT/h = 6.105 \times 10^{12} \text{s}^{-1}$. Zhurkov [9] reports a value of 10^{13}s^{-1} for this term, while Coleman [11] reports a value of $1.84 \times 10^{12} \text{s}^{-1}$. As a first-order approximation, we simply use kT/h for ν_0 such that Equation (1) becomes

$$K_b = \frac{kT}{h} \exp\left(-\frac{U - \gamma\sigma}{kT}\right). \quad [2]$$

Hansen and Baker-Jarvis [15] combined these earlier works to develop a rate-dependent kinetic theory of fracture for polymers, which successfully predicted the strength of polymers subjected to a wide range of stress rates. In their formulation, they introduced a differential equation for the evolution of a damage variable n with time t , where the evolution of the damage variable is directly related to the bond rupture rate as:

$$\frac{dn}{dt} = (n_0 - n)K_b \quad [3]$$

where $n_0 = \frac{e}{e-1}$

The damage variable, which represents the fraction of microcrack density required for fracture, is zero initially and unity at failure. Combining Equations (2) and (3) gives the starting equation for determining the fatigue life of a polymer.

$$\frac{dn}{dt} = (n_0 - n) \frac{kT}{h} \exp\left(-\frac{U - \gamma\sigma(t)}{kT}\right), \quad n(0) = 0 \quad [4]$$

For the work reported here, we derived the equation for fatigue life cycles to failure assuming a sawtooth-shaped load history with frequency f , maximum stress σ_{max} , and minimum stress σ_{min} . As a first-order approximation, we assume that the stiffness properties do not degrade with increasing n , as has been observed in some experimental work on composites [16]. Using these assumptions and solving Equation (4) gives the number of cycles to failure N_f .

$$N_f = \frac{f\gamma(\sigma_{max} - \sigma_{min})}{h} \exp\left(\frac{U}{kT}\right) \left[\exp\left(\frac{\gamma\sigma_{max}}{kT}\right) - \exp\left(\frac{\gamma\sigma_{min}}{kT}\right) \right]^{-1} \quad [5]$$

2.2 Multicontinuum theory for unidirectional composites

In order to apply kinetic theory to composite structures, the stress in the fiber and matrix constituents must be determined. Multicontinuum theory, as developed for two-constituent composite materials by Garnich and Hansen [3,17], provides an elegant and computationally efficient method to determine volume-averaged stresses of the matrix and fiber. Here we are interested in matrix-dominated fatigue failure, so the average matrix stress is the physically relevant parameter. The exact value of average stress in the matrix σ_m can be written as

$$\sigma_m = Q_m \sigma_c - \psi_m (\Delta T) \quad [6]$$

where

$$\begin{aligned} Q_m &= C_m \{C_c (\phi_m I + \phi_f A)\}^{-1} \\ \psi_m &= C_m \left\{ \phi_f [(C_c - C_f)(\phi_m I + \phi_f A)]^{-1} a + \eta_m - (\phi_m I + \phi_f A)^{-1} \eta_c \right\} \\ A &= -\frac{\phi_m}{\phi_f} (C_c - C_f)^{-1} (C_c - C_m) \\ a &= C_c \eta_c - \phi_f C_f \eta_f - \phi_m C_m \eta_m \end{aligned} \quad [7]$$

In Equations (6) and (7), σ_c is the six-component composite stress vector; ΔT is the temperature change from the stress-free state; C_i ($i = c, f, m$) are the reduced stiffness matrices for composite, fiber, and matrix, respectively; ϕ_f and ϕ_m are the fiber and matrix volume fractions, respectively; and η_i ($i = c, f, m$) are the thermal expansion coefficients of the composite, fiber, and matrix, written as six-component strain vectors where the shear components are zero.

2.3 Determination of an effective matrix stress

Given a composite stress state or stress history, Equation (6) can be used to determine the average matrix stress, which can then be used to predict fatigue life according to Equation (5). But one obvious challenge in this process is determining how to represent the matrix stress tensor as an effective scalar stress that can be used in Equation (5). Several researchers have shown that an appropriate parameter for predicting fatigue life is the fatigue strength normalized by the static strength under the same load condition [7,5,18]. Thus, we use the functional form of static failure criteria for determining an effective stress.

In considering the form of the failure criterion, it is useful to consider the failure modes observed in experiment. It has been widely reported that in unidirectional composites fatigue failure often occurs via cracking parallel to fibers [8,19]. Thus, it is expected that tensile forces perpendicular to the fibers will play a substantial role in fatigue as well as the shear stresses on these planes. Taking the axial direction of the fiber to be the 1-direction, we propose an *in situ* matrix failure criterion in the form of transversely isotropic invariants of the matrix stress tensor that takes the form

$$B_t \{I_t\}^2 + \frac{1}{\left(1 - \frac{\beta}{\tau_0} \{-I_h\}\right)} [B_{s1} I_{s1} + B_{s2} I_{s2}] = 1 \quad [8]$$

where

$$\begin{aligned}
I_t &= \frac{\sigma_{22} + \sigma_{33} + \sqrt{(\sigma_{22} + \sigma_{33})^2 - 4(\sigma_{22}\sigma_{33} + \sigma_{23}^2)}}{2} \\
I_{s1} &= \sigma_{12}^2 + \sigma_{13}^2 \\
I_{s2} &= \frac{1}{4}(\sigma_{22} - \sigma_{33})^2 + \sigma_{23}^2 \\
I_h &= \sigma_{22} + \sigma_{33}
\end{aligned} \tag{9}$$

and the $\{\}$ denote Macaulay brackets such that the value is zero if the encompassed quantity is negative. The values of B_i are determined from three composite static failure tests: transverse tension, transverse compression, and in-plane shear, all of which involve failure of the matrix constituent. Dividing Equation (8) by B_{s1} gives a form for an effective stress σ_{eff}

$$\frac{B_t}{B_{s1}} \{I_t\}^2 + \frac{1}{\left(1 - \frac{\beta}{\tau_0} \{-I_h\}\right)} \left[I_{s1} + \frac{B_{s2}}{B_{s1}} I_{s2} \right] = \sigma_{eff}^2, \tag{10}$$

where β is a pressure strengthening coefficient and τ_0 is the matrix shear strength with no pressure strengthening. Taking the square root of Equation (10) gives an effective stress for predicting fatigue life according to Equation (5).

$$\sigma_{eff} = \sqrt{\frac{B_t}{B_{s1}} \{I_t\}^2 + \frac{1}{\left(1 - \frac{\beta}{\tau_0} \{-I_h\}\right)} \left[I_{s1} + \frac{B_{s2}}{B_{s1}} I_{s2} \right]}. \tag{11}$$

3. RESULTS

In the following two sections, we discuss the results of static and fatigue failure as predicted by the model described in the previous section. The static failure results demonstrate that our representation of failure is adequate. The fatigue failure results demonstrate that our model correctly capture the relevant physics of the matrix.

3.1 Static failure predictions

In order to validate that Equation (8) correctly predicts static failure, failure coefficients were calculated from test data shown in Table 1, which were reported by Kawai *et al.* [5]. Compressive strengths for the same material were reported in a later paper by Kawai and Suda [6], but some significant deviation appears. Nevertheless, in the absence of other data the

reported value of $^{-}S_{22} = -68$ MPa was used for room temperature compressive strength. Thermal expansion properties of the composite were assumed to be similar to other carbon/epoxy composites as reported elsewhere [20]: in the longitudinal direction $\alpha_{11} = -1 \times 10^{-6}/^{\circ}\text{C}$ and in the transverse direction $\alpha_{22} = 26 \times 10^{-6}/^{\circ}\text{C}$.

Table 1. Composite properties reported by Kawai *et al.* [5].

	Room Temperature Properties	100°C Properties
E_{11} (GPa)	159	156
E_{22} (GPa)	8.45	6.32
G_{12} (GPa)	4.78	3.01
ν_{12}	0.357	0.338
$^{+}S_{22}$ (MPa)	48.5	25.6
S_{12} (MPa)	77.8	43.1

Fitting the failure coefficients in Equation (8) required matrix stresses to be determined. As shown in Equations (6) and (7), the elastic properties of the constituent are required in order to determine matrix stresses. To produce the reported temperature-dependent properties of the composite, fiber properties were assumed to be temperature invariant and matrix properties were assumed to be temperature dependent. Both fiber and matrix properties were chosen such that a micromechanical model yielded the reported composite stiffness. The elastic constituent properties determined using this process is shown in Table 2.

Table 2. *In situ* constituent elastic properties used in analysis

	Fiber	Matrix (RT)	Matrix 100°C
E_{11} (GPa)	248	4.01	2.45
E_{22} (GPa)	12.8	3.93	2.20
G_{12} (GPa)	15.0	1.49	0.812
ν_{12}	0.276	0.46	0.436
α_{11} ($10^{-6}/^{\circ}\text{C}$)	-1.307	26.7	27.4
α_{22} ($10^{-6}/^{\circ}\text{C}$)	13.04	38.1	39.1

The pressure strengthening coefficient β was taken to be 0.35 based on reported strengthening parameters for epoxy and other polymers [21]. This value was assumed to be isothermal. At room temperature, the value of $\tau_0 = 33.5$ MPa was calculated from the average matrix stress at failure in a longitudinal composite shear test. At high temperature, the value of $\tau_0 = 15.1$ MPa was calculated using the composite static shear test.

For room temperature failure, all three coefficients in Equation (8) were determined using average *matrix* stresses in the composite. For composite failure at 100°C, the matrix stresses induced by thermal expansion mismatch between the fiber and matrix were highly compressive. The magnitude of the compressive stresses were such that the reported transverse “tensile” strength of 25.6 MPa, did not produce a positive tensile stress in the matrix at all. Rather, it induced a shear failure. Thus, for the 100°C failure, the two shear coefficients were fitted using the matrix stresses that were determined at the composite transverse tensile and shear strengths. Table 3 shows the values of the coefficients.

Table 3. Failure coefficients determined from matrix stresses at reported composite failure loads

	Room temperature	100°C
B_t (Pa ⁻¹⁵)	0.824	N/A
B_{s1} (Pa ⁻¹⁵)	0.894	4.07
B_{s2} (Pa ⁻¹⁵)	6.94	51.9

Using the coefficients reported in Table 3, off-axis static failure predictions were generated for loading at both room temperature and 100°C. The comparison of these predictions with the experimental data given by Kawai *et al.* [5] is shown in Figure 1. The squares and circles correspond to experimental failure points at room temperature and 100°C, respectively. The solid and dashed curves correspond to failure predictions at room temperature and 100°C, respectively. The predicted values are in good agreement with experimental results, both quantitatively and qualitatively. This indicates that the failure criterion proposed in Equation (8) adequately captures the failure modes of matrix constituent. Thus, Equation (11) is deemed an acceptable measure of effective stress for use in the kinetic theory of composite fatigue.

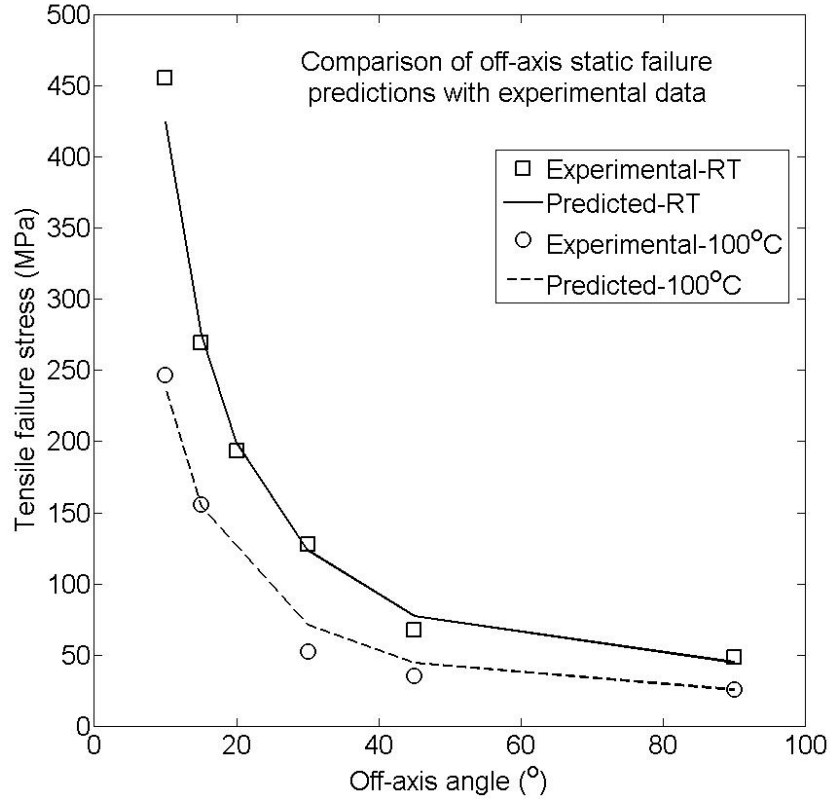


Figure 1. Off-axis static failure as predicted using Equation (7) compared with experimental data from Kawai *et al.* [5]

3.2 Fatigue life predictions

In the following two subsections, we apply the model described above to off-axis fatigue of unidirectional T800H/2500EP carbon/epoxy composites. We compare our model with experimental data reported by Kawai *et al.* [5] at both room temperature and 100°C. This is a particularly challenging problem for two reasons: the failure mode of the matrix changes and the properties of the matrix change. The failure mode changes because of thermally-induced compressive stresses that arise on heating the composite to 100°C. We show that our model can be used for prediction of both types of failure and can be used to infer changes in the physical properties of the polymer, namely, activation energy and activation volume.

3.2.1 Room temperature fatigue

Having demonstrated that our failure criteria is adequate to describe the static failure of composites, we now use our representation of effective stress coupled with Equation (5), derived from kinetics, to model composite fatigue life at room temperature. Only two additional parameters beyond static failure data are needed: activation energy U and activation volume γ . Using off-axis room temperature fatigue data reported by Kawai *et al.* [5] for T800H/2500EP, we determined a best fit of $U = 110.0$ kJ/mol and $\gamma = 1.312$ kJ/MPa-mol. The results of these model predictions are shown in Figure 2, where the markers depict experimental data and the dashed lines indicate model predictions.

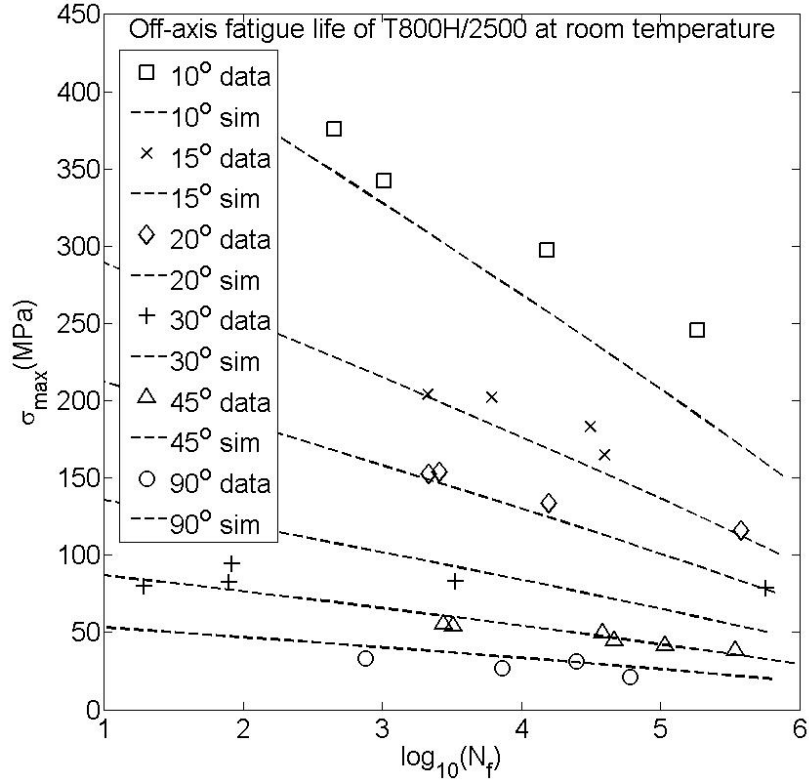


Figure 2. Off-axis composite tension-tension fatigue life predictions at room temperature (dashed lines) compared with experimental data (markers) from Kawai *et al.* [5].

3.2.2 High-temperature fatigue

The high-temperature fatigue case presents a unique challenge in that the nature of the matrix loading changes from the room temperature case. At room temperature, the matrix shear stresses are coupled with tensile stresses; in fact, at an angle of 90° the matrix stresses suggest a tensile failure. In contrast, at 100°C the matrix stresses are always a combination of shear and compressive stresses, so that fatigue failure will be shear-dominated with a pressure-strengthening component. Despite this change, we apply the methodology described above to the high-temperature fatigue problem. The model predictions are shown in Figure 3 by the dashed lines, while the markers denote experimental data from Kawai *et al.* [5]. For these data, the best fits of the activation energy and activation volume were $U = 146.8$ kJ/mol and $\gamma = 3.82$ kJ/MPa-mol. As was observed in the room-temperature case, excellent agreement between the model and experimental results was obtained.

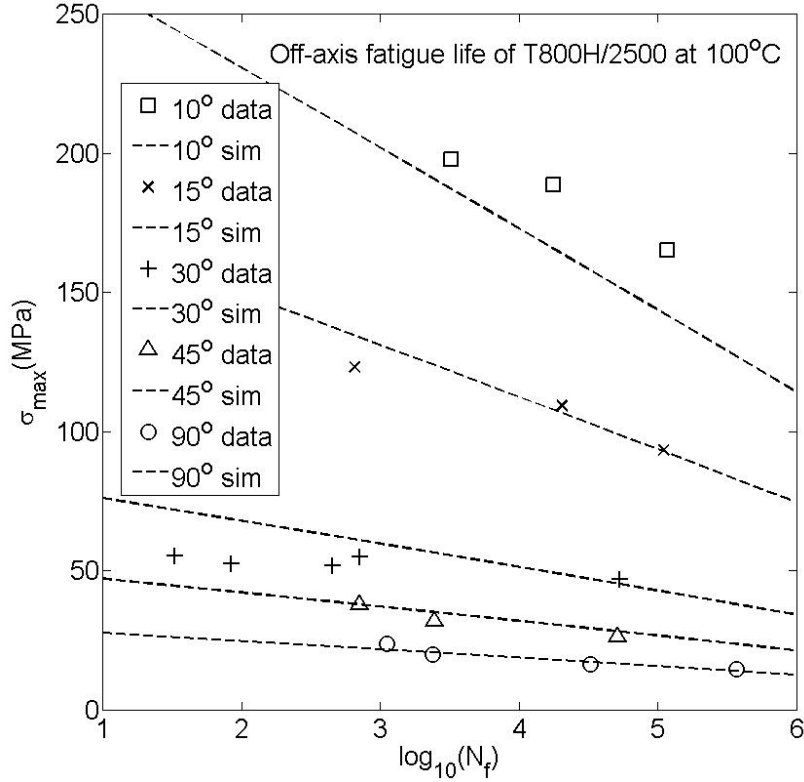


Figure 3. Off-axis composite tension-tension fatigue life predictions at 100°C (dashed lines) compared with experimental data (markers) from Kawai *et al.* [5].

Despite the good agreement observed in Figure 3 between the experimental data in our model, several features warrant discussion. First, the value of the activation volume γ is nearly three times larger than the activation volume observed at room temperature. This is consistent with experimental work on polymer relaxation at a variety of temperatures. Cook *et al.* [22] reported that activation volume in several epoxy resins, with glass transition temperatures similar to the one used as a matrix material in this study (130°C [6]), increased nearly 400% over a temperature range of 140°C. Thus, our observation that the activation volume increases by 300% over a temperature range of 80°C appears reasonable.

The second feature we observe is an increase in the activation energy U of roughly 30% with increasing temperature change. Isothermal measurement of epoxy activation energies have been shown to vary by 10% in the same material [23]. But a strong temperature dependence has been observed in epoxy resins such that activation energy increases with increasing temperature and can increase by as much as 100% over a 100°C temperature range [24]. Again, our observation of an increase in activation energy is entirely consistent with observed polymer physics.

Finally, as in the room temperature case, the 30° off-axis case was least well approximated with our model. And as with the room temperature results, this is believed to be because the composite nonlinearity was largest at 30°, which means that the elastic constants used in this analysis were likely to be artificially high. A more refined model that captures elastic nonlinearity would likely capture the fatigue response better.

4. CONCLUSIONS

We have outlined a physics-based model for fatigue life prediction in composite materials based on physically relevant parameters at the constituent level. The model requires four fundamental steps. (1) Using multicontinuum theory, we determine the average constituent stresses—without resorting to a finite element micromechanics model. (2) The matrix stress tensor is mapped to an effective stress for use in the equations of kinetic theory. (3) Kinetic parameters of the matrix constituent are determined from a minimal set of fatigue data. (4) Kinetic theory applied to *matrix* stresses is used to predict *composite* fatigue life under *any* loading condition, including multiaxial load states and varying load histories. Our results demonstrate that, using multicontinuum theory, kinetics can be applied to composite materials at the constituent level to predict fatigue life from fundamental physical properties of the polymer matrix.

4.1 Scalability

The use of multicontinuum theory to extract the matrix stresses allows this theory to be utilized in large-scale analyses. In a conventional finite element analysis, multicontinuum theory as used by Helius:MCT™ adds only about 3% to the computational time required for a large-scale structural analysis. Given the simple nature of the model proposed, we expect a similar computational burden implement this fatigue life prediction model into existing finite element software. This would permit rapid, robust fatigue life analysis of large-scale structures.

4.2 Future work

The ability to incorporate physics into large-scale analyses of composite materials has far-reaching implications. The framework outlined here can be readily extended to model the effects of harsh environments on the mechanical behavior of composites. This is simply because a changing environment changes the bond activation energies and volumes, the effects of which can be captured with minor modifications to Equation (1). But perhaps the most important implications is that using a physics-based approach like the one proposed here allows the designer to more accurately estimate the effects of conditions and events for which the composite was not tested. This not only means that physical intuition can play a larger role, but that composite behavior can be modeled with minimal characterization and testing.

5. ACKNOWLEDGEMENTS

The research was sponsored by the Air Force Research Laboratory Space Vehicles Directorate under contract number FA 9453-07-C-0191 under the direction of Dr. Thomas Murphey.

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