PREDICTION OF FATIGUE FAILURE IN FIBROUS COMPOSITES USING THE REDUCED-ORDER MULTISCALE DISCRETE DAMAGE THEORY

Zimu Su, Caglar Oskay

Civil and Environmental Engineering Department
Vanderbilt University
Nashville, TN

ABSTRACT

We propose a physics-based, multiscale computational modeling framework for prediction of damage accumulation and failure in fiber-reinforced polymer composites subjected to fatigue. The proposed framework is multiscale in space and in time; and employs the principles of the mathematical homogenization theory. The spatial multiscaling is introduced to model the progressive damage accumulation at the scale of the composite constituents, and to bridge the damage information to the scale of a structural component. In order to alleviate the outstanding issues related to multiscale modeling of fracture processes (i.e., computational cost, mesh objectivity, existence of RVE), we propose the reduced order multiscale discrete damage theory (MDDT). MDDT tracks the evolution of failure at microscale at a set of potential “failure paths” and consistently bridges the failure information to the structural scale using length scale-dependent operators. The temporal multiscaling is introduced to efficiently describe the long-term evolution of damage under cyclic loading conditions, leveraging the time scale disparity between a single characteristic load cycle and the overall life of a structural component. The efficacy of the multiscale framework is demonstrated in the context of prediction of fatigue crack initiation in unnotched and open-hole specimens subjected to fatigue loading.

1. INTRODUCTION

Current design strategies for composites rely on conservative knock-down factors to account for the long-term degradation of properties under sustained cyclic loading. This is generally due to the lack of comprehensive understanding of the consequences of the presence and evolution of damage within the composite structure as a function of the cyclic loading. In particular, fatigue damage signatures that ultimately lead to catastrophic failure in composite structures may not always be apparent. Achieving a comprehensive understanding and predictive capabilities for fatigue damage evolution would allow leveraging the full capabilities (i.e., the high specific strength, stiffness, durability, etc.) of composite materials in the aerospace, automobile and many other industries. Progressive damage analysis (PDA) modeling for long-term failure prediction under cyclic loading offer a paradigm to achieve the aforementioned capabilities.
Significant developments are being made in the area of PDA modeling of composite structures subjected to a range of loading and environmental conditions. The predictive capabilities for many of the modeling approaches have improved rapidly in the past several years. Of particular note is PDA models that rely on multiscale principles to describe the progressive degradation of properties in composite structures. Composites naturally exhibit response at multiple length scales due to the disparity between the scale of a structural component and the heterogeneous microstructure of the material, especially as it pertains to the loading direction. In the context of multiscale modeling, a range of computational difficulties exist, including (1) high computational cost of evaluating coupled problems posed at the scale of the representative volume element (RVE) or a unit cell, and at the scale of the structure; and (2) Mesh sensitivity observed at both scales especially when continuum damage mechanics models are used to track progressive failure. Eigendeformation-based reduced order homogenization method (EHM) [1,2] is a multiscale approach based on the principles of the mathematical homogenization theory [3] that alleviates the issue of computational cost by approximating the microscale problem with a reduced-basis approximation. This approach has been demonstrated to accurately capture composite behavior under a range of loading conditions including static loading [4], blast loading [5], bearing problems in bolted joints [6] and fatigue loading [7-9]. A key shortcoming of EHM has been the mesh sensitivity at the coarse scale.

In addition to multiple length scales, damage accumulation under cyclic loading also introduces multiple time scales. This is due to the disparity between the time scale of a single load cycle and the time scale associated with slow damage growth in the composite. Leveraging homogenization principles, Crouch et al. (2013) [8] proposed a multiple space-time fatigue life prediction framework for composites, employing the EHM approach to efficiently describe the failure process. This framework was then enhanced with accelerated multiscale time integration schemes for faster predictions, leveraging model order reduction in time [7].

In this study, we propose a physics-based, multiscale computational modeling framework for prediction of damage accumulation and fatigue failure initiation in fibrous composites. The proposed framework extends the aforementioned multiple space-time framework. In order to alleviate the outstanding issue of mesh objectivity, we propose the reduced order multiscale discrete damage theory (MDDT) [10]. MDDT tracks the evolution of failure at the microscale using a set of potential “failure paths” and consistently bridges the failure information to the structural scale using length scale-dependent operators. This approach effectively eliminates the mesh size sensitivity observed at the coarse scale in the EHM formulation. This paper extends the applicability of MDDT to fatigue initiation predictions, by integrating it with the multiple time scale framework. The efficacy of the multiscale framework is demonstrated in the context of prediction of fatigue crack initiation in unnotched and open-hole laminated composite specimens subjected to fatigue loading.

2. MULTISCALE DISCRETE DAMAGE THEORY

MDDT approach builds on the EHM approach. In contrast to the EHM approach, which relies on continuum description of failure at the scale of the material microstructure, the MDDT formulation considers a discrete description of failure in a discrete fashion. The general idea of the MDDT approach is illustrated in Figure 1 in the context of a unit cell representing a square-packed unidirectionally reinforced composite microstructure. In the proposed approach, the failure processes are computed and tracked at the scale of a unit cell or an RVE associated with each
integration point of the discretized macroscopic structural domain. The microstructural problem is approximated using a reduced basis, leveraging the ideas of the EHM theory. The key concept in MDDT is to describe a set of “potential failure paths” – discrete surfaces within the microstructure which could form a crack under favorable loading conditions.

Figure 1: Discrete multiple “potential” failure path in microstructure.

The morphologies of the failure paths are pre-determined according to the expected failure modes. The determination of the failure paths can be performed either numerically (by computational analysis at the microstructure scale) or based on experimental observations of fracture patterns in the composite material. For example, in Figure 1, the failure paths within the unit cell include transverse matrix cracking, delamination and fiber fracture. The progressive failure within each failure path is expressed in terms of a cycle-sensitive traction-separation law described by a scalar damage parameter. While not included in the current study, it is also possible to introduce nonlinear material behavior for the constituent materials (e.g., to account for the shear nonlinearity of the matrix phase) by leveraging the EHM formulation [11]. This capability will be included in the proposed formulation in the near future as the role of shear nonlinearity is critically important in capturing behavior in laminates rich in off-axis plies.

Consider $m$ potential failure paths within the microstructure morphology associated with an arbitrary material point, $x$. Following the ideas of mathematical homogenization with multiple scales and the EHM-based model reduction, MDDT expresses the microstructural equilibrium along each failure path of the microstructure as:

$$t^{(\alpha)}(x,t) - C^{(\alpha)} : \tilde{\varepsilon}(x,t) + \sum_{\beta=1}^{m} D^{(\alpha\beta)} \cdot \delta^{(\beta)}(x,t) = 0; \quad \alpha = 1, 2, ..., m$$

where $\tilde{\varepsilon}$ stands for the macroscopic strain tensor at the material point, $x$, $t^{(\alpha)}$ and $\delta^{(\alpha)}$ respectively denote the average traction and average displacement jump vectors over the failure path, $\alpha$. $C^{(\alpha)}$ and $D^{(\alpha\beta)}$ are “coefficient tensors”. Coefficient tensors are integral expressions of characteristic influence functions (i.e., numerical Green’s functions) over the microstructure and
the failure path morphologies. They are evaluated a-priori to the multiscale analysis using a series of linear elastic analyses performed over the microstructure and treated as constitutive tensors within the multiscale analysis. These tensors introduce the micromorphological information to the reduced order equilibrium equations that define the progressive failure at the microscale (i.e., Eq. (1)). The average tractions and displacement jumps are related to each other by defining a traction-separation relationship in the form:

\[ t^{(a)} = \left(1 - \omega^{(a)}\right)K^{(a)} \cdot \delta^{(a)} \]  

(2)

where \( K^{(a)} \) stands for cohesive stiffness, which is a second order diagonal tensor, and \( \omega^{(a)} \in [0,1] \) indicates damage variable in the failure path. \( \omega^{(a)} = 0 \) and \( \omega^{(a)} = 1 \) respectively denote the intact state and fully formed crack along the failure path. The damage evolution equation is described as the function of displacement jumps with fatigue sensitivity \( \gamma \):

\[ \dot{\omega}^{(a)} = \Phi\left(\delta^{(a)}\right)/\omega^{(a)} \gamma \left( \Phi\left(\delta^{(a)}\right) \right) \]  

(3)

where \( \Phi\left(\delta^{(a)}\right) \) is also the function of fracture properties: critical strain energy release rate \( G_c \) and ultimate traction \( t_{ult} \) in the cohesive relationship.

Equations (1)-(3) constitute a set of \( 3m \) nonlinear algebraic equations that are evaluated using the Newton-Raphson method to compute the state of traction and displacement jumps for a prescribed macroscopic strain, which serves as the forcing function.

The MDDT formulation is regularized for mesh size sensitivity based on the idea of effective adjustment of the size of the microstructure. The idea employed in this study is similar to that proposed in Ref. [12]. Following the crack band regularization approach in Ref. [13], damage (that describes the cohesive relationships along the failure paths) at the macroscopic scale is allowed to localize. Mesh size consistency is achieved by ensuring that the dissipated energy at macroscopic element through the microscale failure processes depends on the size of the macroscopic element. The relationship between the dissipated energy and the element size is chosen such that the overall fracture energy remains independent of the mesh size. The key idea that distinguishes the proposed approach from the crack band method is that the energetic consistency is achieved by adjusting the size of the microstructure, rather than by adjusting the material parameters. In order to ensure that this relationship is obtained in a computationally efficient manner, we established analytical relationships between the coefficient tensors of the reduced order model and the macroscopic element size. The detailed analytical relationships are not included for brevity. The formulation of these relationships will be provided in a separate journal publication that is currently in preparation.

3. MULTIPLE TIME SCALE HOMOGENIZATION FOR FATIGUE DAMAGE PREDICTION

Predicting fatigue damage evolution using direct cycle-by-cycle simulation with the multiscale models, where each load cycle is resolved and time integrated, is clearly computationally prohibitive even when reduced order representation of the microscale problem is
employed. The so-called cycle-jump approaches rely on resolving a small subset of load cycles throughout the life of the structural component. The proposed multiple time scale homogenization approach provides a rigorous mathematical basis for the cycle-jump methods and allows the prediction of damage evolution under high-cycle fatigue. The idea is illustrated in Figure 2. Mathematical homogenization principles are applied at the time domain, employing two time scales. *Micro-chronological* time scale refers to the resolution of the unit load cycle applied to the composite, whereas *macro-chronological* time resolves the slow time scales through which damage slowly evolves in the structure. Asymptotic analysis of the governing equations of the PDA model results in a coupled system of governing equations. The micro-chronological problem provides the response of the composite structure subjected to a single load cycle, whereas the macro-chronological problem is evaluated to predict the long-term damage accumulation. Similar to the spatial homogenization principles, the coupled system requires the evaluation of a micro-chronological problem at each time step of the macro-chronological problem.

Figure 2: Multiscale modeling in time for fatigue damage prediction in the composite.

In order to ensure computational efficiency, we employ two ideas: (1) adaptive macro-chronological time stepping to evaluate as small number of micro-chronological problems as possible within a desired error tolerance; and (2) quasi-linear approximation of the micro-chronological problem where the equilibrium is strictly satisfied at the macro-chronological problem alone. In the adaptive strategy, the size for the macro-chronological time step (and expressing macro-chronological time in terms of load cycles) is computed based on the following condition:

$$
\Delta N_i = \Delta \omega \rho / \| \omega'(x, N_i) \|_{\infty}
$$

where $\Delta N_i$ is the macro-chronological time step size, $\omega'(x, N_i)$ is the change in the vector of damage variables associated with all failure paths at all integration points in the current micro-chronological load cycle. $\| \cdot \|_{\infty}$ denotes the infinity norm, which implies that the macro-
chronological time step size is chosen based on the maximum value of accumulated damage across all material points within the structure and among all failure paths. $\Delta \omega_p$ stands for the tolerance parameter for allowable damage accumulation across the macro-chronological time step. A tradeoff exists between prediction accuracy and computational efficiency in choosing $\Delta \omega_p$: smaller value leads to higher accuracy but requires more macro-chronological time steps that reduces the efficiency of the approach.

The MDDT approach has been implemented within the multiple time scale homogenization framework. The evaluation of the two-scale problems is performed using the commercial finite element package, Abaqus. MDDT has been incorporated into Abaqus using the user supplied subroutine capabilities. The information transfer between the two scale problems and the computation of the adaptive macro-chronological time step size is performed using a Python script that allows straightforward integration with the Abaqus solvers at both scales.

### 4. Model Verification

#### 4.1 Unnotched lamina configuration

The MDDT approach for fatigue damage prediction is first verified using simple unnotched lamina configurations subjected to cyclic loading. The unit cell and the potential failure paths employed at the microstructure scale is shown in Figure 3a. The microstructure is of a unidirectional graphite fiber reinforced epoxy with 65% fiber volume fraction. The failure modes that are considered in this study are fiber fracture, delamination and matrix cracking. The elastic and failure properties of the matrix and fiber phases are shown in Table 1. The matrix is assumed to be isotropic, whereas the fiber is considered transversely isotropic. In the configurations considered in the unnotched and open hole cases, delamination has not been observed. The geometry, discretization, loading and boundary conditions considered at the macroscale is shown in Figure 3b. Symmetry boundary conditions are employed to reduce edge effects. Strain-controlled loading is applied to a $90^\circ$ lamina with an amplitude of 1% and R-ratio of 0. The loading configuration is expected to naturally activate the matrix cracking mode, while the fiber damage is expected to remain near zero.

| Table 1: Elastic and damage properties of the composite constituents. |
|-----------------|--------|--------|---------|---------|---------|
| Matrix properties |         |         |         |         |         |
| $E$ [GPa]       | $\nu$  | $\gamma$ | $G_{IC}$ [MPa mm] | $G_{IIC}$ [MPa mm] | $t_{ult}$ [MPa] |
| 3.55            | 0.35   | 2.5     | 0.27    | 0.95    | 83      |
| Fiber properties |         |         |         |         |         |
| $E_1$ [GPa]     | $E_2$ [GPa] | $\nu_{12}$ | $\nu_{23}$ | $\gamma$ | $t_{ult}$ [MPa] |
| 263             | 27.5   | 0.32    | 0.2     | 25      | 3,917   |
Figure 4 shows the evolution of matrix cracking damage as a function of load cycles as predicted by the proposed MDDT with multiple time scaling (referred to as MDDT-F in what follows) approach along with the reference model. The reference simulation also employs the MDDT approach but consider direct cycle-by-cycle time integration. Two MDDT-F simulations with adaptive macro-chronological time step tolerance values of $\Delta \omega_p = 0.5\%$ and $1\%$ are presented in the figure. The curves predicted by MDDT-F approach compares well with the reference simulation. MDDT-F with $\Delta \omega_p = 1\%$ and $0.5\%$ required 24 and 48 macro-chronological time steps (hence micro-chronological load cycles), whereas the reference simulation resolves all 1,930 cycles needed to break the matrix at this load amplitude. MDDT-F with the tighter tolerance of $\Delta \omega_p = 0.5\%$ has a closer match with reference case compared with MDDT-F with $\Delta \omega_p = 0.1\%$, indicating the convergent trend of the proposed approach with smaller step size tolerance.

Figure 3: Verification study on unnotched lamina configuration: (a) The unit cell and the potential failure paths included in the model (b) Geometry, discretization and loading conditions at the macroscale.

Figure 4: Transverse matrix damage evolution in the 90° unnotched lamina.
4.2 Open-hole configuration

The performance of proposed multiscale approach is further assessed by open-hole 90° lamina and [0°/90°]s laminate configurations.

Figure 5a shows the geometry, discretization, boundary and loading conditions for the 90° lamina specimen. The specimen dimensions are 38 mm, 80 mm and 0.125 mm in width, length and thickness, respectively. The discretization of the specimen is performed using 8-noded hexahedral elements with tri-linear shape functions. Reduced integration (C3D8R in Abaqus) elements are used. A structured mesh is employed near the hole, where the fracture processes are expected. The mesh in the structured region aligns with the fiber orientation. The size of elements is approximately 0.25 mm near the notch area. One element along the ply thickness is considered. Symmetry boundary conditions along three sides are employed to model eighth of the full specimen geometry. The specimen is subjected to displacement-controlled cyclic loading in the tension direction with an amplitude of 0.02 mm and R-ratio of 0. The microstructure, potential failure paths, and the material parameters employed for the composite constituents are identical to the unnotched example. The simulations were performed using the MDDT-F approach and the reference cycle-by-cycle approach until the onset of fatigue crack. The analysis therefore focuses on the fatigue crack initiation regime.

Figure 5: Model verification for notched 90° lamina. (a) Geometry, discretization and loading conditions; Damage contours after (b) 195 cycles (c) 709 cycles (d) 1103 cycles of loading.

Figure 5b-d compares the damage contours around the notch computed by the MDDT-F model and cycle-to-cycle simulation at 195 cycles, 709 cycles and 1103 cycles. As expected, no significant fiber fracture or delamination damage is detected in the simulations and the damage contours in the figure are for the transverse matrix damage. The MDDT-F model in the plots
employ a macro-chronological time step size tolerance of $\Delta \omega_p = 1\%$. The damage contours predicted by the reference and the proposed approaches agree well with each other throughout the loading up to and including fatigue crack initiation.

Figure 6: Transverse matrix damage evolution in the first element that fails within the $90^\circ$ and $[0^\circ/90^\circ]$'s open-hole configuration.

For further comparison, Figure 6 shows the damage evolution within the first macroscale element that fails in the specimen. The figure compares MDDT-F model with tolerances of $\Delta \omega_p = 5\%$ and $\Delta \omega_p = 1\%$. Both models with large and small tolerances show a reasonable match with the reference simulation. The number of cycles to initial failure state is 1,103 predicted by MDDT-F model with the small step size tolerance. The fatigue crack initiation prediction error is 0.54% (1,109 cycles predicted with the reference model). The MDDT-F simulations require 18 ($\Delta \omega_p = 5\%$) and 90 ($\Delta \omega_p = 1\%$) resolved micro-chronological load cycles to predict fatigue initiation.

The results from the $[0^\circ/90^\circ]$ cross-ply lamina specimen are shown in Figure 7. The specimen differs from that of the $90^\circ$ lamina configuration only in that two plies are modeled along the thickness direction. The specimen is under displacement-controlled cyclic loading with an amplitude of 0.01 mm and R-ratio of 0. The simulation ends when the first element reaches completely failure. Figure 7b-d show the comparison of damage contours around notch at initial failure state computed by the MDDT-F model with $\Delta \omega_p = 2\%$. (1,902 cycles) and cycle-by-cycle simulation (1,911 cycles). Near the notch, fiber and matrix damage both exist in the $0^\circ$ ply, but fiber damage accumulation is much smaller than the matrix cracking. This is largely due to the fact that fiber is less sensitive to progressive cyclic damage. In $90^\circ$ ply, there is no fiber damage and matrix damage accumulates much faster than $0^\circ$ ply as load cycle increases. MDDT-F model and the reference simulations show good agreement with each other. The damage evolution within the element that fails first (located in $90^\circ$ ply layer) is also shown in Figure 6. Two cases with $\Delta \omega_p = 5\%$ and $\Delta \omega_p = 2\%$ are compared with the reference simulation. The number of cycles to initial
failure state is 1,902 predicted by the MDDT-F model with $\Delta \omega_p = 2\%$. The error is 0.47% compared with the reference one (1911 cycles). The MDDT-F model also shows great efficiency. Only 45 ($\Delta \omega_p = 2\%$) and 18 ($\Delta \omega_p = 5\%$) resolved cycles are required, while 1,911 cycles are resolved in the reference simulation.

Figure 7: Model and damage contour for [0°/90°]s lamina in initial failure state (a) Geometry, discretization and loading conditions; (b) Fiber damage state in 0° ply. (b) Matrix damage contour in 0° ply. (c) Matrix damage contour in 90° ply.

4.3 Sensitivity of fatigue initiation to element size

The sensitivity of fatigue initiation to element size in the MDDT-F model is investigated by comparing the failure initiation states of open-hole 90° lamina predicted with three different mesh configurations. Element sizes (denoted as $h$) of 0.25 mm, 0.125 mm and 0.0625 mm are used for the elements near the notch. Figure 8a shows the damage contours for $h=0.25$ mm and 0.125 mm at after approximately 1,100 cycles. At this stage, matrix cracking initiates at the most critical element in the $h=0.25$ mm case. There is a slight discrepancy in the damage contours between the two cases. In order to understand the source of the discrepancy, Figure 8b compares the initiation predictions between the two finer meshes. The damage contours in Figure 8b are at approximately 850 cycles, which corresponds to the first matrix crack occurrence in $h=0.125$ mm configuration. There is a much better fit between the two fine scale simulations. This indicates that the simulation with the coarse mesh ($h=0.25$ mm) may not be resolving the stress and deformation state around the notch with sufficient accuracy.
Figure 8: Damage contour in the initial failure state of (a). $h=0.25$ mm at 1103 cycles (left), compared to $h=0.125$ mm at 1105 cycles (right) (b). $h=0.125$ mm at 850 cycles (left), compared to $h=0.0625$ mm at 847 cycles (right)

5. CONCLUSIONS

This study proposed a new multiscale framework based on the ideas of multiscale discrete damage theory and the multiple time scaling (MDDT-F) for the prediction of fatigue crack nucleation in composite structures. The approach exhibits high computational efficiency and accuracy compared to the direct cycle-by-cycle simulations in the cases of laminate and specimen configurations investigated in this paper. The preliminary analyses shown here also demonstrate that fatigue initiation predictions are mesh size independent provided that sufficiently small elements are employed to accurately capture the stress and strain fields within the specimen. In the near future, we will extend the capabilities of the MDDT-F formulation to the crack propagation regime.

ACKNOWLEDGEMENT

The authors gratefully acknowledge the financial support of the Office of Naval Research Airframe Structures and Materials (Award No: N00014-17-1-2040, Program Manager: William Nickerson).

REFERENCES


