An Improved Fracture Mechanics-Informed Multiscale Thermomechanical Damage Model for Ceramic Matrix Composites

Travis Skinner, Jacob Schichtel and Aditi Chattopadhyay

Abstract This paper extends recent work done by the authors in modeling length scale-dependent damage behavior of ceramic matrix composites (CMCs) to include effects of local anisotropy introduced by matrix cracking. This model captures scale-dependent damage initiation and propagation behavior of the brittle matrix by employing internal state variable (ISV) theory within a multiscale modeling framework to obtain damaged matrix stress/strain constitutive relationships at each length scale. The damage ISV captures the effects of matrix cracking and growth by using fracture mechanics and the self-consistent scheme to determine the reduced stiffness of the cracked matrix. Matrix cracks, which activate when stress intensity factors near manufacturing induced cavities exceed the fracture toughness of the material, are assumed to be transversely isotropic in the plane of the crack, and matrix anisotropy occurs when the damaged stiffness tensor is rotated from the crack plane to the global axes. The crack progression and temporal evolution of the damage ISV are governed by fracture mechanics and crack growth kinetics. The model effectively captures first matrix cracking, which is the first significant deviation from linear elasticity. The nonlinear predictive capabilities of the material model are demonstrated for monolithic silicon carbide (SiC) and a 2D woven five-harness satin (5HS) carbon fiber SiC matrix (C/SiC) CMC.

Keywords Ceramic matrix composite · Multiscale · Damage · Fracture mechanics · Internal state variable

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Introduction

The low density, high strength and toughness, exceptional high-temperature performance, and gradual failure mechanisms of ceramic matrix composites (CMCs) grant CMCs a wide range of applicability and have made them the material of choice for many aerospace applications [1–4]. However, because of the difficulty of accurately modeling the complex multiscale thermomechanical behavior of CMC material systems under critical mechanical and environmental loading conditions, the inherent benefits of CMCs are not fully exploited. Modeling the complex damage behavior of CMCs requires a multiscale modeling framework that integrates physics-based thermomechanical constitutive models with scale-specific damage mechanisms.

Multiscale studies have shown significant potential for modeling scale-dependent material behavior and damage in heterogeneous composite material systems [5–7]. The strong length scale-dependent behavior of CMCs requires a multiscale modeling methodology to accurately model global material behavior and predict effective composite material properties. The generalized method of cells (GMC) developed by Aboudi et al. [8] can efficiently capture limited scale-dependent behavior and is well suited to model composite materials. GMC exploits the periodicity of a representative unit cell (RUC) to obtain the overall material response. The RUC consists of an arbitrary number of subcells which can be assigned different material properties to represent different composite constituents. Displacement and traction continuity conditions are enforced in an average sense between neighboring subcells, and localization/homogenization algorithms provide the relationship between the stress/strain in each subcell and the average RUC stress/strain. This methodology allows for an efficient and accurate semi-analytical solution, that links the behavior of the individual constituents to the overall material behavior. The GMC framework was extended by Liu et al. [9] into a multiscale GMC (MSGMC) framework that is well suited to capture material behavior in woven composites which consist of multiple length scales. In MSGMC, the GMC methodology is applied recursively to obtain the response of multiple relevant length scale models, thus enabling concurrent analysis of micro-, meso-, and macroscales, which is essential for an accurate analysis of realistic CMC weaves. This method is well suited to model CMC length scale-dependent behavior and can be used in conjunction with thermomechanical damage models to capture the effects of damage at each length scale.

ISV theory and continuum damage mechanics (CDM) can be used to describe material thermomechanical behavior by deriving constitutive laws based on the thermodynamics of deformation and damage. Researchers have applied ISV and CDM techniques to CMCs and have shown good agreement with experimental results [10–12]. However, these models are most often applied at the CMC macroscale, resulting in phenomenological and architecture-dependent models that have limited transferability to additional material systems and architectures. The definitions of the damage variables and other ISVs in these models satisfy thermodynamics, but they may not capture the actual physics of damage in CMCs because the evolution laws are often selected for mathematical tractability and to satisfy thermodynamics.

In order to better understand CMC thermomechanical response to critical loadings, the actual physics of scale-dependent damage in CMCs must be captured.

Most CMCs are manufactured through chemical vapor infiltration (CVI) or melt infiltration (MI) [13], which lead to a significant volume fraction of manufacturing induced cavities that detrimentally affects the integrity of the finished parts. Liu et al. [14] showed that accurately modeling the distribution of manufacturing induced cavities is critical to capturing CMC behavior. They proved that the physical distribution of cavities had a significant effect on CMC mechanical properties and concluded that localized cavity concentrations were necessary to accurately capture CMC deformation behavior. The authors previously made use of Liu's cavity distribution modeling methodology and derived a fracture mechanics-informed matrix damage model using an isotropic damage ISV to account for activation and growth of matrix cracks from cavities [15]. The model was implemented within the MSGMC framework to account for the multiscale nature of matrix damage initiation and propagation in CMCs and effectively captured nonlinearity in the macroscale composite response. A key drawback of the model is the assumption of an isotropic damage ISV; in reality, matrix cracking causes local anisotropy.

In this work, the previously mentioned fracture mechanics-informed damage model is improved to account for local anisotropy due to the formation and propagation of matrix cracks. The damage variable, which is a function of the crack density in the matrix, is determined using fracture mechanics and the self-consistent scheme [16]. The cracked matrix is assumed to be transversely isotropic in the plane of the crack, and matrix anisotropy occurs when the damaged stiffness tensor is rotated from the crack plane to the global axes. Matrix cracking is activated when stress intensity factors exceed the fracture toughness of the material and crack growth kinetics govern the growth of cracks and the progression of damage in the matrix. The model is applied to monolithic SiC and a 5HS woven C/SiC CMC using literature values for SiC and carbon fiber material properties.

Description of Damage Model

The governing equations of the ISV approach are obtained by combining the first and second laws of thermodynamics to obtain a dissipation inequality (Clausius–Duhem inequality). The Helmholtz free energy, which is assumed to be completely described by the linear thermoelastic strain potential, is taken as the scalar state potential function. Thus, the dissipation inequality governs the evolution of internal state variables, which can be chosen to represent specific damage mechanisms. In this work, a damage variable, D, is chosen to represent the damaged state of the matrix material due to cracking. The variable D is computed in the crack plane and its temporal evolution is related to the volumetric crack density, which increases as matrix cracks near manufacturing induced cavities activate and grow. Unlike classical ISV methods, which propose an additional scalar potential function to derive the damage ISV evolution laws [17, 18], this approach is grounded in the actual physics of matrix damage by accounting for fracture mechanics and crack growth kinetics in the definition and evolution of the damage ISV. The stress/strain constitutive relationship is obtained using the principle of strain equivalence for a damaged medium and by taking the derivative of the Helmholtz free energy with respect to the elastic strain.

The damage ISV is obtained using the self-consistent scheme [16] to determine the change in mechanical properties due to matrix cracks, which occur primarily at manufacturing induced cavities. This methodology is applied within the MSGMC modeling framework to allow the simulations to capture the effects of matrix crack initiation and propagation at each length scale. The local stresses are determined using localization algorithms as discussed in the following section, and the stress intensity factor, K_I, due to the cavity is evaluated in the principal plane and compared to the critical stress intensity factor (fracture toughness), K_{IC}. When $K_I \geq K_{IC}$, a crack is activated and begins to propagate through the matrix. In multiaxial stress states, one would expect mode II and III stress intensity factors to play a role in crack nucleation and growth, however, due to the brittleness of the matrix material, modes II and III play a negligible role in the rate and direction of crack growth [19] and are not included in the model. The matrix crack is assumed to be transversely isotropic in the plane of the crack, and the effective modulus perpendicular to the crack face, $\tilde{E}_n$, is derived as described in Ref. [20]:

$$\tilde{E}_n = \left(1 - \frac{\pi^2}{30}(1+v)(5-4v)\Omega\right)E \tag{1}$$

where Ω is the scalar volumetric crack density ($\Omega = \frac{N}{V}l^3$), E is the undamaged isotropic modulus, and v is Poisson's ratio. This change in stiffness is equated with the stiffness change from the damage ISV to find:

$$D = \frac{\pi^2}{30}(1+v)(5-4v)\Omega. \tag{2}$$

By differentiating Eq. 2 with respect to time, the temporal evolution of D is determined:

$$\dot{\mathrm{D}} = \frac{\pi^2}{10}(1+v)(5-4v)\frac{N}{V}l^2\dot{l}, \tag{3}$$

where l is the characteristic crack length, and N is the number of cracks in volume V. An expression for $\dot{l}$ can be obtained using crack growth kinetics as in Paliwal et al. [20].

This definition of the damage ISV is applied to obtain a transversely isotropic damaged compliance tensor in the plane of the crack, $\tilde{\boldsymbol{S}}$. In matrix form:

$$\tilde{\mathbf{S}} = \begin{bmatrix} 1/E_t & -v/E_t & -v/E_n & 0 & 0 & 0 \\ -v/E_t & 1/E_t & -v/E_n & 0 & 0 & 0 \\ -v/E_n & -v/E_n & 1/E_n & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/G_{tn} & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/G_{tn} & 0 \\ 0 & 0 & 0 & 0 & 0 & 2(1+v)/E_t \end{bmatrix}, \quad (4)$$

where E_t is the transverse modulus ($E_t = E$), and G_{tn} is the cracked shear modulus, which is assumed to follow the form $G_{tn} = \frac{E_n}{2(1+v)}$. Poisson's ratio in a cracked body is expected to slightly increase [21], but some researchers have observed no significant change [22] or even a decrease in Poisson's ratio [16] after onset of cracking in a brittle material. Due to a lack of experimental data for this material system and the conflicting results in the literature, Poisson's ratio is kept constant in this model. The compliance in global axes is obtained by rotating the damaged compliance tensor from principal axes to global axes as follows (in Einstein notation):

$$S'_{ijkl} = R_{ip} R_{jq} \tilde{S}_{pqrs} R_{kr} R_{ls}, \quad (5)$$

where $\boldsymbol{R}$ is the rotation matrix whose rows are the unit vectors associated with the principal stresses and are the basis vectors for the principal frame, and the indices $i, j \ldots r, s$ range from 1 to 3. As a result of the rotation from principal axes, the resulting compliance tensor, $\tilde{\boldsymbol{S}}'$, and the corresponding stiffness tensor, $\tilde{\boldsymbol{C}}'$, are fully anisotropic in the global frame where loads are applied.

Multiscale Modeling Framework

The improved fracture mechanics-informed damage model is implemented in the MSGMC framework [9] to link material constitutive behavior and capture effects of damage initiation and evolution at each relevant length scale. This model is applied to 5HS woven C/SiC CMCs in this work, but the model has application to additional 2D weave architectures and material systems, including SiC/SiC CMCs. The MSGMC framework takes advantage of material periodicity at each length scale, and homogenization and localization algorithms are used to traverse up and down length scales. The response of each length scale is obtained by analyzing a RUC at that length scale using GMC. Each RUC can consist of monolithic material subcells or subcells which are themselves modeled using an RUC for a lower length scale. The recursive localization and analysis of unit cells at progressively lower and lower length scales are repeated until all unit cells contain only monolithic material consisting of the base constituents, where the elastic constitutive and damage models are applied. This methodology can accurately reproduce actual CMC thermomechanical behavior because the behavior at each relevant length scale is obtained and linked to the global composite response.

In the case of a 2D woven architecture, the weave can be represented by a macroscale RUC which is triply periodic and is discretized into $N_\alpha x N_\beta x N_\gamma$ subcells, where N_α, N_β, and N_γ correspond to the number of subcells in the 1, 2, and 3 directions, respectively (see Fig. 1). The subcells in the macroscale RUC are in turn modeled as GMC unit cells, each consisting of various combinations of weft, warp, overlapping, and matrix subcell stacks. By varying the arrangement of these stacks, a wide range of woven composite architectures can be simulated. The matrix subcell stacks consist of monolithic matrix material, so the elastic constitutive and damage models are directly applied. The tow subcells are modeled using a doubly periodic mesoscale (tow-level) RUC which is further discretized into $N_\beta x N_\gamma$ subcells consisting of matrix and matrix/fiber subcells. The constitutive and damage models are again applied directly to the monolithic matrix subcells and the matrix/fiber subcells are represented using a doubly periodic microscale RUC discretized into $N_\beta x N_\gamma$ fiber, matrix, and interphase constituent subcells. The response of the microscale RUC is obtained by homogenization after applying the constitutive and damage models to the constituents. This homogenized microscale response is passed up through the next length scale as the response of the matrix/fiber subcells in the tow-level RUC. The tow-level response is obtained by homogenization and is passed up through the next length scale to the weave level RUC where additional homogenization is performed to obtain the global composite response. These localization/homogenization algorithms allow for an accurate semi-analytical solution that can include the effects of damage, inelasticity, and temperature at each length scale. For a detailed derivation of the GMC and MSGMC theories, the reader is directed to Refs. [8, 9].

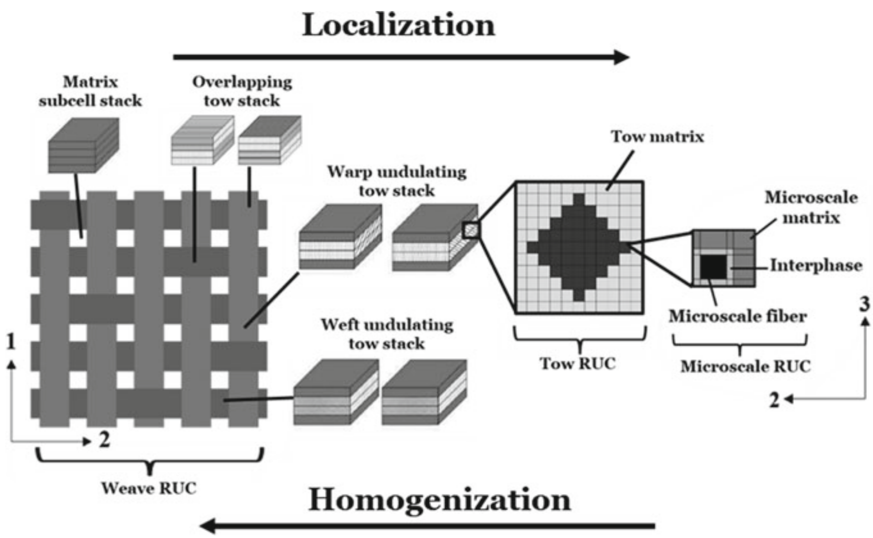

Fig. 1 Schematic of repeating MSGMC unit cell for 5HS woven CMC

Results and Discussion

Monolithic SiC Response

To demonstrate the improved damage model, the stress/strain response of bulk SiC matrix material is simulated and compared to the linear elastic and isotropic damage cases. Table 1 presents relevant material properties as well as the initial values for crack density and characteristic crack length used in the simulation. The model captures the quasi-brittle behavior of the bulk SiC matrix as shown in the simulated stress/strain curves in Fig. 2. In both the isotropic and anisotropic damage cases, stress increases linearly with strain until the stress intensity factor exceeds the fracture toughness and cracking is activated. The crack grows rapidly, causing material property degradation until a critical crack length is reached and failure occurs. The maximum stress increases when the cracked matrix is modeled as an anisotropic material and occurs at a slightly higher value of strain compared to the isotropic damage case. Additionally, as shown in Fig. 3b, the effective stiffness of the bulk matrix material is higher when anisotropy due to damage is considered. This is as expected, since cracking initiates and propagates in the principal plane, which is aligned at an angle relative to the global (loading) axes. When crack direction and transverse isotropy are accounted for, the maximum stiffness degradation occurs normal to the crack surface, and no degradation occurs transverse to the crack. It is interesting to note that the stiffness of the anisotropic damaged matrix is higher than that of the isotropic case even though damage initiates earlier and evolves more

Table 1 Material properties and model parameters used to simulate monolithic SiC

K_{IC} $(MPa\sqrt{m})$	E (GPa)	ν	Ω_0	l_0
4.9	415	0.17	0.001	0.005

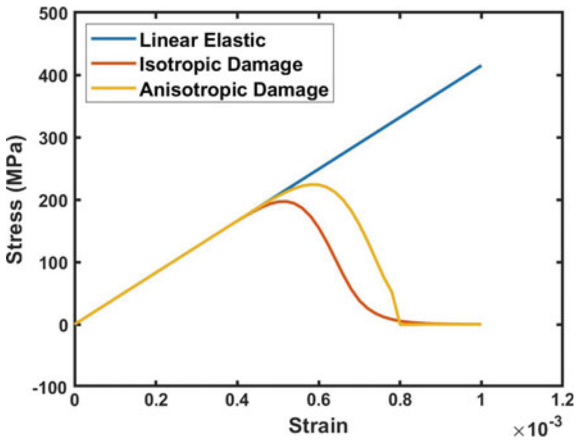

Fig. 2 Simulated stress/strain response of monolithic SiC with isotropic and anisotropic damage

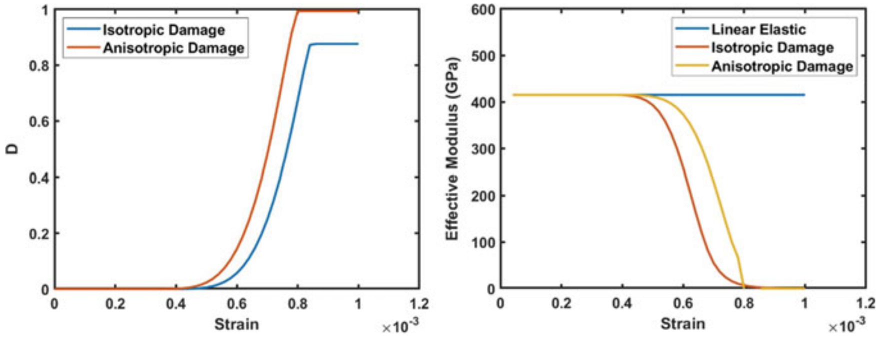

Fig. 3 Evolution of damage and effective modulus in monolithic SiC. **a** Isotropic and anisotropic damage parameters versus strain; **b** effective SiC modulus versus strain

rapidly in the anisotropic case than the isotropic case. This is because as the damaged stiffness tensor in the plane of the crack is rotated from principal axes to global axes, the reduction in stiffness for each direction will be less than that observed normal to the crack face, and a significantly longer crack is required to release energy and have a similar effect on global stiffness. The damage variable computed in the principal plane in the isotropic case releases additional energy and degrades the entire stiffness tensor equally without considering the effects of crack orientation or transverse isotropy.

The damage parameter and effective damaged stiffness of the bulk SiC material for both isotropic and anisotropic damage cases are shown in Fig. 3. After crack activation, the crack length increases rapidly, causing a rapid increase in the damage ISV until material failure occurs when $D \approx 0.9$ for the isotropic damage case, and when $D \approx 1$ for the anisotropic case.

Woven Composite Response

The stress/strain simulation results for a 5HS woven C/SiC CMC are shown in Fig. 4, and effects of damage using isotropic and anisotropic damage are compared. Additionally, localized concentrations of manufacturing induced cavities were modeled as explained in Ref. [14] to capture realistic CMC behavior. The simulation results show trends that match those seen in literature. The fracture mechanics-informed matrix microcracking damage model effectively captures first matrix cracking, which results in deviation from linear elastic material behavior. The anisotropic damage case predicts first matrix cracking at slightly higher stress than the isotropic damage case and remains slightly stiffer after first matrix cracking due to the stiffer behavior of the damaged matrix when cracks are modeled as transversely isotropic. The effective woven composite modulus is presented in Fig. 5 and key matrix damage mechanisms are indicated, illustrating the model's ability to capture the multiscale

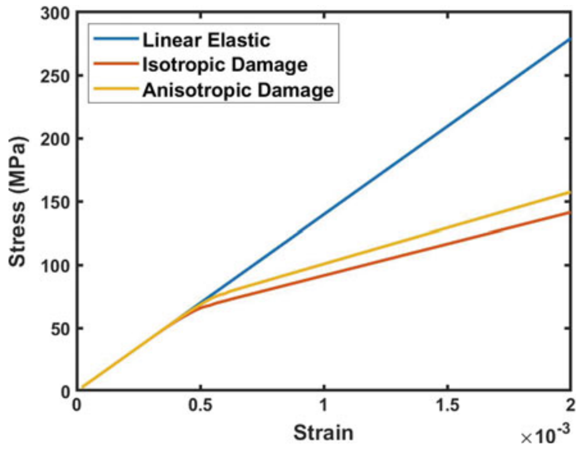

Fig. 4 Simulated response of 2D woven C/SiC CMC with isotropic and anisotropic damage

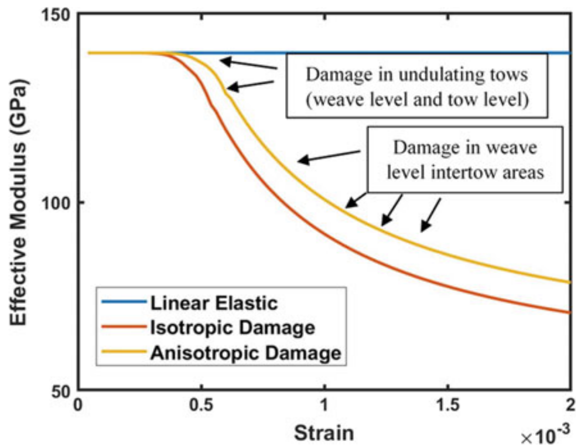

Fig. 5 Simulated stress/strain response of 2D woven C/SiC CMC with isotropic and anisotropic damage

physics of matrix damage in woven CMCs. The woven composite has undulating tows, which cause local stress concentrations that accelerate crack activation and significantly decrease effective modulus. Damage initiates in the undulating tows, and the local tow-level damage contributes to the overall composite degradation. As strain increases, cracks initiate and propagate in the matrix-rich interweave regions between tows and the overall composite modulus is further degraded.

Conclusions

An improved fracture mechanics-informed thermomechanical damage model was implemented using internal state variable theory within a thermodynamic framework. The stress/strain constitutive behavior of damaged ceramic matrix material was derived using damage variables which capture the effects of cracking on the stiffness tensor of the SiC matrix. The matrix cracking damage variable, which is a function of the crack density in the matrix and is determined using fracture mechanics and the self-consistent scheme, reduces the stiffness of the cracked matrix. Matrix cracks, which initiate and grow from manufacturing induced cavities, are activated when stress intensity factors exceed the fracture toughness of the material, and crack growth kinetics govern the growth of cracks and the progression of cracking in the matrix. Matrix cracks are assumed to be transversely isotropic in the plane of the crack, and matrix anisotropy occurs when the damaged stiffness tensor is rotated from the crack plane to the global axes. The model was implemented within the MSGMC multiscale modeling framework and the nonlinear predictive capabilities of the improved model were demonstrated for monolithic silicon carbide and a 5HS 2D woven C/SiC CMC. The improved model more accurately reflects the physics of brittle matrix cracking, and the model predictions match trends found in experimental results from literature.

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