

Thermomicromechanical Damage in Composites

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A thermomicromechanical model of failure is presented based on thermodynamic principles, that is, using the balancing laws: the conservation of momentum and the first and second laws of thermodynamics. The model is oriented toward damage initiation and damage progression in a composite structure under an intense pressure shock wave. A micromechanical damage approach is considered where three damage modes are modeled: tensile damage, shear damage, and interphase or material mismatch discontinuity between the composite's matrix and fiber. A homogenization technique is incorporated in the development to simplify the representation of the nonhomogeneous material. A summary of the equations for the thermomicromechanical model of failure is presented where a damage parameter D is defined to characterize the lamina's damage based on energy dissipation. Numerical analyses are presented to demonstrate the model characterization to damage.

Nomenclature

c_ϵ	=	specific heat at a constant strain
D	=	damage parameter
d	=	power of dissipation
H	=	Heavyside unit step function
K	=	bulk modulus
q_i	=	component of the heat flux vector
t	=	time
u_v	=	internal energy
v_i	=	component of the velocity
\dot{v}_i	=	component of the acceleration
α_v	=	coefficient of thermal expansion
Γ	=	inelastic proportionality constant
Δ	=	difference between the fiber and matrix residual strains
δ_{ij}	=	Kronecker delta
ϵ_{ij}	=	total Cauchy strain tensor
ϵ_{ij}^e	=	elastic portion of the Cauchy strain tensor
$\epsilon_{ij}^{\text{in}}$	=	inelastic portion of the Cauchy strain tensor
$\tilde{\epsilon}_{ij}$	=	difference between the fiber and matrix residual strains
η	=	entropy
θ	=	thermodynamic absolute temperature
μ, λ	=	Lame's constants
ρ	=	mass density
σ_{ij}	=	Cauchy symmetric stress tensor
ψ_v	=	free energy
ω	=	tensile damage parameter
ω_Δ	=	interfacial damage parameter
ϖ	=	shear damage parameter

I. Introduction

THE life expectancy and survivability of structures have been the focus of many studies where safety as well as economical factors are major concerns. Damage plays a significant role, and the understanding of its characteristics can advance the material designs. There are many established failure criteria in the literature. Some failure criteria are based on strength of the materials for composite and isotropic materials alike. For example, models of maximum strain,¹ maximum stress,¹ Tsai-Hill (see Ref. 1), Tsai-Wu (see Ref. 1), Lee,² and Hashin³ (among others) are used to investigate fiber failure, matrix failure, and delamination. These failure criteria and others are widely used to predict damage based on a macromechanics isothermal approach. Other models investigate mi-

cro-mechanical damage and are based on matrix failures, for example, those of Averill,⁴ Bakukas et al.,⁵ and Joshi and Goode.⁶ The density of microcracks and microcavities in a material to characterize the phenomena of damage for an isotropic material through an energy representation was first introduced by Kachanov⁷ where a scalar damage parameter was used. Since then, the concept was generalized within the framework of irreversible thermodynamics for isotropic material under multiaxial loads by Lemaitre,⁸ Lemaitre and Chaboche,⁹ Hult,¹⁰ Leckie,¹¹ Murakami,¹² Krajcinovic,¹³ and others.

The damage process is greatly influenced by loading conditions as well as the complexity of the multiphase decomposition of the material. The motivation behind the present work is to investigate the survivability of a composite structure under an intense pressure shock wave where such loading conditions could raise the need for an equation of state, for example, Hugoniot (see Zukas¹⁴ and Schwer et al.¹⁵). For example, a thin-walled fluid-filled tank impacted by a solid steel sphere at high velocity results in a hemispherical shock wave that eventually impacts the tanks walls at high intensity.¹⁶ Under such severe loading conditions, the effect of the loading rate, inelastic strain rate, and thermomechanical coupling on the material response becomes significant and must be considered.¹⁷ The problems considered herein, however, have been simplified, that is, the equation of state is not considered, to carry out parametric evaluations within the established criterion. Thus, the focus of the present work is to introduce a micromechanical damage model applicable to composite structures under loading that is developed by an impact of ~ 100 m/s (Refs. 14, 15, 17, and 18) and to evaluate certain damage characteristics within the model.

II. Theory

The mathematical derivation of the thermodynamic model of failure is based on the conservation laws, the first and second law of thermodynamics, and the state laws or the constitutive laws of the continuum. The governing equations are formulated using Lagrangian representation. The conservation of mass, the conservation of linear momentum, the conservation of angular momentum, the first law and second law of thermodynamics assuming no heat source in the continuum and no body forces, can be stated as¹⁹

$$\frac{\partial \rho}{\partial t} + \rho \frac{\partial v_i}{\partial x_j} = 0, \quad \sigma_{ij,j} = \rho \dot{v}_i, \quad \sigma_{ij} = \sigma_{ji} \quad (1)$$

$$\dot{u}_v = \sigma_{ij} \dot{\epsilon}_{ij} - q_{i,i} \quad (2)$$

$$\dot{\eta} \geq -q_{i,i}/\theta + q_i \theta_{,i} / \theta^2 \quad (3)$$

where the dot indicates the time t derivative, that is, $\dot{x} = \partial x / \partial t$, and θ is measured from an initial absolute temperature θ_0 , that is, the absolute zero Kelvin temperature is -273.3°C . Furthermore, the following assumptions will be used in the formulation of the

Received 26 June 1999; revision received 5 January 2000; accepted for publication 9 June 2000. This material is declared a work of the U.S. Government and is not subject to copyright protection in the United States.

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damage model. First, the strain tensor is written in two parts: the elastic strain ε_{ij}^e and the inelastic strain $\varepsilon_{ij}^{\text{in}}$,

$$\varepsilon_{ij} = \varepsilon_{ij}^e + \varepsilon_{ij}^{\text{in}} \quad (4)$$

Second, the elastic strain ε_{ij}^e is a linear elastic strain, that is, infinitesimal strain $\varepsilon_{ij}^e, \varepsilon_{ij}^{\text{in}} \ll 1.0$, where the strain used is the Cauchy strain tensor ε_{ij}^e and the corresponding stress is the Cauchy stress tensor σ_{ij} . Note that the governing equations are not restricted to any loading range and that they are applicable to either phase.

An irreversible thermodynamics approach is used, where damage is introduced as an internal variable. To be acceptable, these damage internal variables must be identifiable and related to dominant modes of irreversible rearrangement of the material microstructure. Traditionally there are two types of damage models to constitute these micromechanisms: isotropic damage (damage scalar)²⁰ and anisotropic damage (a fourth-order damage tensor).^{21–26} In the present model, which is geared toward capturing damage in structures exposed to high-intensity loading, special isotropic internal damage variables are assumed, where the micromechanisms are considered either transgranular or intergranular mechanisms, in addition to the interphase damage and the residuals in the composite material. The assumed special isotropic internal damage variables are a simplified form of an anisotropic damage. Hence, two internal damage variables are considered to model the large number of microdefects, such as microcracks, dislocations, pores, and decohesions within a microstructure of a typical engineering material. They are the tensile damage parameter ω (transgranular) and the shear damage parameter ϖ (intergranular). These two internal damage variables in some averaging sense represent existing micropore and microslip development, respectively. They are based on reasonable assumptions. Experiments show that the mechanism of dynamic fracture and the damage of a material is a process of nucleation, growth, and coalescence of microvoids as well as microslip.^{27–29} In addition, the exposure of a material to an intense pressure shock wave enhances the dynamic expansion of cavities.^{17,30,31} To develop a damage model for a two-phase composite, the residual state and interfacial damage between the composite's phases must be included in the model based on experimental observations. The magnitudes of the residual state vary, for example, thermal strain, moisture absorption strains, inelastic deformation, etc., but may be quite substantial, often exceeding those induced by allowable mechanical loading. Therefore, residual fields may cause internal damage of the physical properties of the composite materials.^{18,32,33} Furthermore, interfaces between constituents within the composite material may influence damage development,^{18,33} and interfacial damage can lead to a significant effect on the composite's global response. Thus, it is modeled in an averaged sense using the damage parameter ω_Δ in addition to the difference between the two-phase strains Δ , that is, initially defined as the difference between the fiber and matrix residual strains $\bar{\varepsilon}$, which is $\Delta = \bar{\varepsilon}_{11}^{(1)} - \bar{\varepsilon}_{11}^{(2)}$, where the 11-direction is along the fibers and its rate $\dot{\Delta}$ will be defined subsequently.

Hence, the independent state variables of the total free energy per unit volume ψ_v for the damage model become the temperature θ ; the elastic strain ε_{ij}^e ; the inelastic strain $\varepsilon_{ij}^{\text{in}}$; the difference between the two-phase strains in the uniaxial loading direction at the initial state Δ , that is, prestrained state, which allow the inclusion of the residual state effects on damage; the tensile damage parameter ω related to micropore development; the shear damage parameter ϖ related to microslip development; and interphase discontinuity between the matrix and fiber of the composite ω_Δ . Thus, the free energy $\psi_v(\theta, \varepsilon_{ij}^e, \varepsilon_{ij}^{\text{in}}, \omega, \varpi, \Delta, \omega_\Delta)$ time derivative is equal to

$$\begin{aligned} \dot{\psi}_v = & \frac{\partial \psi_v}{\partial \varepsilon_{ij}^e} \dot{\varepsilon}_{ij}^e + \frac{\partial \psi_v}{\partial \varepsilon_{ij}^{\text{in}}} \dot{\varepsilon}_{ij}^{\text{in}} + \frac{\partial \psi_v}{\partial \theta} \dot{\theta} + \frac{\partial \psi_v}{\partial \Delta} \dot{\Delta} + \frac{\partial \psi_v}{\partial \omega} \dot{\omega} \\ & + \frac{\partial \psi_v}{\partial \varpi} \dot{\varpi} + \frac{\partial \psi_v}{\partial \omega_\Delta} \dot{\omega}_\Delta \end{aligned} \quad (5)$$

Manipulating the second law of thermodynamics [Eq. (3)], one can deduce (see Appendix A)

$$\begin{aligned} \sigma_{ij} \dot{\varepsilon}_{ij}^{\text{in}} - \frac{\partial \psi_v}{\partial \varepsilon_{ij}^{\text{in}}} \dot{\varepsilon}_{ij}^{\text{in}} - \frac{\partial \psi_v}{\partial \Delta} \dot{\Delta} - \frac{\partial \psi_v}{\partial \omega} \dot{\omega} - \frac{\partial \psi_v}{\partial \varpi} \dot{\varpi} \\ - \frac{\partial \psi_v}{\partial \omega_\Delta} \dot{\omega}_\Delta - \frac{q_i \theta_{,i}}{\theta} \geq 0 \end{aligned} \quad (6)$$

Hence, the power of dissipation d is defined as

$$\begin{aligned} d = & \left(\sigma_{ij} - \frac{\partial \psi_v}{\partial \varepsilon_{ij}^{\text{in}}} \right) \dot{\varepsilon}_{ij}^{\text{in}} - \frac{\partial \psi_v}{\partial \Delta} \dot{\Delta} - \frac{\partial \psi_v}{\partial \omega} \dot{\omega} - \frac{\partial \psi_v}{\partial \varpi} \dot{\varpi} \\ & - \frac{\partial \psi_v}{\partial \omega_\Delta} \dot{\omega}_\Delta - \frac{q_i \theta_{,i}}{\theta} \end{aligned} \quad (7)$$

and Eq. (6) can be written as

$$d \geq 0 \quad (8)$$

which states that the energy dissipated due to damage is not recoverable. Note that the three terms in the dissipation function d are the mechanical dissipation d_m , the dissipation of continual failure d_f , and the thermal dissipation d_θ , respectively, and they are defined as

$$\begin{aligned} d_m = & \left(\sigma_{ij} - \frac{\partial \psi_v}{\partial \varepsilon_{ij}^{\text{in}}} \right) \dot{\varepsilon}_{ij}^{\text{in}} \\ d_f = & - \frac{\partial \psi_v}{\partial \Delta} \dot{\Delta} - \frac{\partial \psi_v}{\partial \omega} \dot{\omega} - \frac{\partial \psi_v}{\partial \varpi} \dot{\varpi} - \frac{\partial \psi_v}{\partial \omega_\Delta} \dot{\omega}_\Delta, \quad d_\theta = - \frac{q_i \theta_{,i}}{\theta} \end{aligned} \quad (9)$$

The mechanical dissipation d_m represents the dissipation due to the inelastic flow, which is defined using constitutive relations; the dissipation of continual failure d_f represents the dissipation due to the continuum damage mechanism, which is an accumulative process in time; and the thermal dissipation d_θ represents the heat energy dissipation flowing from hotter temperature to a colder temperature.

For a composite material, its heterogeneity adds to the complexity of developing a damage model, and the following approach will be adopted. First, one develops the governing equations for each of the composite two-phase materials, for example, Eqs. (1–3). Second, the two-phase composite's governing equations are developed by a homogenization technique, and in the present model it is an averaged form of the two phases based on the rule of mixture. Note that there are many approaches to incorporate the anisotropy of the composite. The ultimate approach is to develop the three-dimensional governing equation for the two-phase materials and solve them numerically, for example, Aboudi's³⁴ cell model and Pagano's³⁵ model based on the Reissner's variational theorem. Averaging the two phases based on the rule of mixture is a simple form of homogenization in comparison. Hence, the homogenization technique included in the present formulation is based on the rule of mixture because of its simplicity and computational efficiency and its wide use in obtaining the averaged properties of a composite material, for example, the composite's effective longitudinal modulus and the composite's effective Poisson's ratio (see Ref. 1). Therefore, the averaged macroscopic quantity X is obtained by averaging the two-phase quantities $X^{(1)}$ and $X^{(2)}$ using the rule of mixture defined as

$$\langle X \rangle = cX^{(1)} + (1 - c)X^{(2)} \quad (10)$$

and the rule of mixture fractional's reversed form, which results from a subsequent algebraic manipulation, is defined as

$$\tilde{X} = (1 - c)X^{(1)} + cX^{(2)} = X^{(1)}X^{(2)}\langle X^{-1} \rangle \quad (11)$$

where c is the volume fraction or the volumetric concentration of the fiber, that is, $c = \text{fibers volume}/\text{total volume}$ and $1 - c = \text{matrix volume}/\text{total volume}$. By the considering of the damage as a nonconservative process, which is characterized by irreversible energy dissipation, the free energy $\psi_v(\theta, \varepsilon_{ij}^e, \varepsilon_{ij}^{\text{in}}, \omega, \varpi, \Delta, \omega_\Delta)$ is decomposed

into a thermoelastic free energy $\psi_v^e(\theta, \varepsilon_{ij}^e)$, which is conservative, and inelastic specific free energy $\psi_v^{\text{in}}(\varepsilon_{ij}^{\text{in}}, \omega, \overline{\omega}, \Delta, \omega_\Delta)$, which is nonconservative:

$$\psi_v(\theta, \varepsilon_{ij}, \omega, \overline{\omega}, \Delta, \omega_\Delta) = \psi_v^e(\theta, \varepsilon_{ij}^e) + \psi_v^{\text{in}}(\theta, \varepsilon_{ij}^{\text{in}}, \omega, \overline{\omega}, \Delta, \omega_\Delta) \quad (12)$$

The homogenization is developed based on a thermoelastic law (no inelastic response or damage), which will subsequently be used in the thermomicromechanical model. Considering a two-phase lamina (see Fig. 1) under a uniaxial condition where the two-phase quantities are measured from a reference state (e.g., $\theta = \bar{\theta} - \theta_0$, where θ is measured from the temperature of a reference state θ_0 and $\bar{\theta}$ is measured from a zero state), the homogenized macroscopic quantities are obtained based on the following conditions. The total strains are continuous in the uniaxial direction, and the total strains in the transverse direction are averaged using the rule of mixture Eqs. (11). The stresses at the interface of the two phases are continuous, the temperature is continuous at the interface under an adiabatic assumption, and the macroscopic entropy is averaged using the rule of mixture Eqs. (11). To eliminate the two-phase stresses and entropy from these conditions in terms of the two-phase strains and temperatures, the thermoelastic equations for the two-phase entropies and stresses are incorporated (because no damage or inelastic behavior is considered in the homogenization). Therefore, the following thermoelastic equations will be used (see Appendix A):

$$\eta^{(\alpha)} = (c_\varepsilon^{(\alpha)} | \theta_0^{(\alpha)}) (\theta^{(\alpha)} - \theta_0^{(\alpha)}) + K^{(\alpha)} \alpha_v^{(\alpha)} \varepsilon_{kk}^{(\alpha)} \quad (13)$$

$$\sigma_{ij}^{(\alpha)} = 2\mu^{(\alpha)} \varepsilon_{ij}^{(\alpha)} + [\lambda^{(\alpha)} \varepsilon_{kk}^{(\alpha)} - (K^{(\alpha)} \alpha_v^{(\alpha)} \theta_0^{(\alpha)} | c_\varepsilon^{(\alpha)}) \eta^{(\alpha)}] \delta_{ij} \quad (14)$$

where α indicates the material phase, that is, $\alpha = 1$ for the fiber phase and $\alpha = 2$ for the matrix phase, $\theta_0^{(\alpha)}$ is the phase temperature at the initial state, and $\varepsilon_{ij}^{(\alpha)}$ is the phase elastic strain tensor. Equations (13) and (14) are then used to rewrite the stress, strain, temperature, and entropy conditions in terms of the two-phase strains and entropies. These relationships are then substituted into the two-phase thermoelastic free energy per unit volume (see Appendix A),

$$\begin{aligned} \psi_v^{e(\alpha)} &= (\lambda^{(\alpha)} | 2) (\varepsilon_{kk}^{(\alpha)})^2 + \mu^{(\alpha)} (\varepsilon_{ij}^{(\alpha)})^2 - K^{(\alpha)} \alpha_v^{(\alpha)} \varepsilon_{kk}^{(\alpha)} \theta^{(\alpha)} \\ &\quad - (2c_\varepsilon^{(\alpha)} | 2\theta_0^{(\alpha)}) (\theta^{(\alpha)})^2 \end{aligned} \quad (15)$$

to obtain the macroscopic thermoelastic free energy per unit volume $\psi_v^e(\eta, \varepsilon_{ij}^e)$, which is

$$\begin{aligned} \psi_v^e &= \frac{1}{2} C_{11} (\varepsilon_{11}^e)^2 + \frac{1}{2} C_{22} (\varepsilon_{22}^e)^2 + \frac{1}{2} C_{22} (\varepsilon_{33}^e)^2 \\ &\quad + C_{12} \varepsilon_{11}^e (\varepsilon_{22}^e + \varepsilon_{33}^e) + C_{23} \varepsilon_{22}^e \varepsilon_{33}^e + C_{66} (\varepsilon_{12}^e \varepsilon_{21}^e + \varepsilon_{23}^e \varepsilon_{32}^e \\ &\quad + \varepsilon_{31}^e \varepsilon_{13}^e) + \frac{1}{2} B \Delta^2 + \frac{1}{2} P \left\{ \frac{\langle c_\varepsilon \rangle}{1 - \kappa \theta_0} \theta + \left(\frac{c(1-c)\hat{B}}{\langle \hat{E} \rangle} \right. \right. \\ &\quad \left. \left. + (2\kappa - 1)AB \right) \frac{\Delta}{1 - \tilde{\kappa}} + \tilde{\kappa} (\varepsilon_{22}^e + \varepsilon_{33}^e) + \hat{\kappa} \varepsilon_{11}^e \right\}^2 \\ &\quad - [d_1 \varepsilon_{11}^e - d_2 (\varepsilon_{22}^e + \varepsilon_{33}^e)] \left\{ \frac{\langle c_\varepsilon \rangle}{1 - \kappa \theta_0} \theta + \left(\frac{c(1-c)\hat{B}}{\langle \hat{E} \rangle} \right. \right. \\ &\quad \left. \left. + (2\kappa - 1)AB \right) \frac{\Delta}{1 - \tilde{\kappa}} + \tilde{\kappa} (\varepsilon_{22}^e + \varepsilon_{33}^e) + \hat{\kappa} \varepsilon_{11}^e \right\} \\ &\quad + \theta_0 \left\{ \frac{\langle c_\varepsilon \rangle}{1 - \kappa \theta_0} \theta + \left(\frac{c(1-c)\hat{B}}{\langle \hat{E} \rangle} + \tilde{\kappa} AB \right) \frac{\Delta}{1 - \tilde{\kappa}} \right. \\ &\quad \left. + \tilde{\kappa} (\varepsilon_{22}^e + \varepsilon_{33}^e) + \hat{\kappa} \varepsilon_{11}^e \right\} \end{aligned} \quad (16)$$

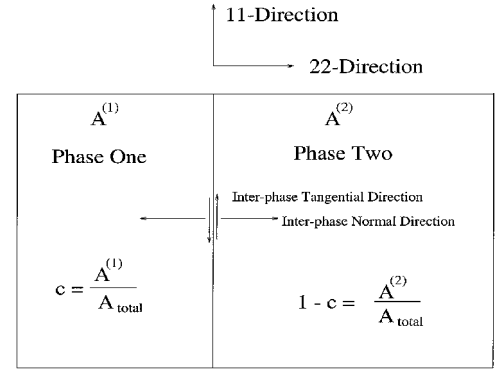


Fig. 1 Two-phase composite.

and the inelastic part of the free energy rate in Eq. (5) is integrated to obtain $\psi_v^{\text{in}}(\varepsilon_{ij}^{\text{in}}, \omega, \overline{\omega}, \Delta, \omega_\Delta)$, which is

$$\begin{aligned} \psi_v^{\text{in}} &= -\frac{1}{2} \mu \Gamma \varepsilon_{ij}^{\text{in}} \varepsilon_{ij}^{\text{in}} - K Y_\sigma \int_0^\omega \dot{\omega} d\omega \\ &\quad - 2\mu Y_\tau \int_0^{\overline{\omega}} \overline{\omega} d\overline{\omega} - \mu Y_\Delta \int_0^{\omega_\Delta} \dot{\omega}_\Delta d\omega_\Delta \end{aligned} \quad (17)$$

Hence, the free energy $\psi_v(\eta, \varepsilon_{ij}^e, \varepsilon_{ij}^{\text{in}}, \omega, \overline{\omega}, \Delta, \omega_\Delta)$ is

$$\begin{aligned} \psi_v &= \frac{1}{2} C_{11} (\varepsilon_{11}^e)^2 + \frac{1}{2} C_{22} (\varepsilon_{22}^e)^2 + \frac{1}{2} C_{22} (\varepsilon_{33}^e)^2 \\ &\quad + C_{12} \varepsilon_{11}^e (\varepsilon_{22}^e + \varepsilon_{33}^e) + C_{23} \varepsilon_{22}^e \varepsilon_{33}^e + C_{66} (\varepsilon_{12}^e \varepsilon_{21}^e + \varepsilon_{23}^e \varepsilon_{32}^e \\ &\quad + \varepsilon_{31}^e \varepsilon_{13}^e) + \frac{1}{2} B \Delta^2 + \frac{1}{2} P \left\{ \frac{\langle c_\varepsilon \rangle}{1 - \kappa \theta_0} \theta + \left(\frac{c(1-c)\hat{B}}{\langle \hat{E} \rangle} \right. \right. \\ &\quad \left. \left. + (2\kappa - 1)AB \right) \frac{\Delta}{1 - \tilde{\kappa}} + \tilde{\kappa} (\varepsilon_{22}^e + \varepsilon_{33}^e) + \hat{\kappa} \varepsilon_{11}^e \right\}^2 \\ &\quad - [d_1 \varepsilon_{11}^e - d_2 (\varepsilon_{22}^e + \varepsilon_{33}^e)] \left\{ \frac{\langle c_\varepsilon \rangle}{1 - \kappa \theta_0} \theta + \left(\frac{c(1-c)\hat{B}}{\langle \hat{E} \rangle} \right. \right. \\ &\quad \left. \left. + (2\kappa - 1)AB \right) \frac{\Delta}{1 - \tilde{\kappa}} + \tilde{\kappa} (\varepsilon_{22}^e + \varepsilon_{33}^e) + \hat{\kappa} \varepsilon_{11}^e \right\} \\ &\quad + \theta_0 \left\{ \frac{\langle c_\varepsilon \rangle}{1 - \kappa \theta_0} \theta + \left(\frac{c(1-c)\hat{B}}{\langle \hat{E} \rangle} + \tilde{\kappa} AB \right) \frac{\Delta}{1 - \tilde{\kappa}} \right. \\ &\quad \left. + \tilde{\kappa} (\varepsilon_{22}^e + \varepsilon_{33}^e) + \hat{\kappa} \varepsilon_{11}^e \right\} - \frac{1}{2} \mu \Gamma \varepsilon_{ij}^{\text{in}} \varepsilon_{ij}^{\text{in}} - K Y_\sigma \int_0^\omega \dot{\omega} d\omega \\ &\quad - 2\mu Y_\tau \int_0^{\overline{\omega}} \overline{\omega} d\overline{\omega} - \mu Y_\Delta \int_0^{\omega_\Delta} \dot{\omega}_\Delta d\omega_\Delta \end{aligned} \quad (18)$$

where Δ is predicated on the prestate conditions, that is, $\Delta = \varepsilon_{11}^{(1)} - \varepsilon_{11}^{(2)} = \bar{\varepsilon}_{11}^{(1)} - \bar{\varepsilon}_{11}^{(2)}$ (see Appendix B for details), and will be used subsequently to model the interphase damage, \hat{B} is equal to

$$\begin{aligned} \hat{B} &= \hat{E}^{(1)} K^{(1)} \alpha_v^{(1)} [1 - \hat{\lambda}^{(1)} | (\hat{\lambda}^{(1)} + \mu^{(1)})] \\ &\quad - \hat{E}^{(2)} K^{(2)} \alpha_v^{(2)} [1 - \hat{\lambda}^{(2)} | (\hat{\lambda}^{(2)} + \mu^{(2)})] \end{aligned} \quad (19)$$

$$\lambda^{(\alpha)} = \lambda^{(\alpha)} - (K^{(\alpha)} \alpha_v^{(\alpha)})^2 \theta_0 | c_\varepsilon^{(\alpha)} \quad (20)$$

A and B are obtained from the prestate condition, that is, the residual state (see Appendix B), and are defined as

$$A = \frac{1}{3}(\alpha_v^{(1)} - \alpha_v^{(2)}), \quad B = \frac{c(1-c)\hat{E}^{(1)}\hat{E}^{(2)}}{\langle \hat{E} \rangle}$$

$$\hat{E}^{(\alpha)} = \frac{\mu^{(\alpha)}(3\hat{\lambda}^{(\alpha)} + 2\mu^{(\alpha)})}{\hat{\lambda}^{(\alpha)} + \mu^{(\alpha)}} \quad (21)$$

and C , d , and P are homogenized material constants that characterize the macroscopic response of the material based on the rule of mixture approach using thermoelasticity principles. For example, in unabridged form C_{11} is

$$C_{11} = c(\hat{\lambda}^{(1)} + 2\mu^{(1)}) + (1-c)(\hat{\lambda}^{(2)} + 2\mu^{(2)})$$

$$- c(1-c) \frac{(\hat{\lambda}^{(2)} - \hat{\lambda}^{(1)})^2}{\tilde{\lambda} + \tilde{\mu}} + \frac{\tilde{\pi}}{\tilde{p}} \left\{ 1 / \left(\frac{c}{\pi^{(1)}} + \frac{(1-c)}{\pi^{(2)}} \right) \right\} \quad (22)$$

and they are defined in abridged form as

$$C_{11} = \langle \hat{\lambda} + 2\mu \rangle - c(1-c) \frac{(\hat{\lambda}^{(2)} - \hat{\lambda}^{(1)})^2}{\tilde{\lambda} + \tilde{\mu}} + \frac{\tilde{\pi}}{\tilde{p}} \langle \pi^{-1} \rangle^{-1}$$

$$C_{12} = \left\langle \frac{\hat{\lambda}}{\hat{\lambda} + \mu} \right\rangle \left\langle \frac{1}{\hat{\lambda} + \mu} \right\rangle^{-1} + \frac{\tilde{\pi}}{\tilde{p}} \langle \pi^{-1} \rangle^{-1}$$

$$C_{22} = \left\langle \frac{1}{\hat{\lambda} + \mu} \right\rangle^{-1} + \left\langle \frac{1}{\mu} \right\rangle^{-1} + \frac{\tilde{\pi}}{\tilde{p}} \langle \pi^{-1} \rangle^{-1}$$

$$C_{23} = \left\langle \frac{1}{\hat{\lambda} + \mu} \right\rangle^{-1} - \left\langle \frac{1}{\mu} \right\rangle^{-1} + \frac{\tilde{\pi}}{\tilde{p}} \langle \pi^{-1} \rangle^{-1}$$

$$C_{66} = \frac{1}{2}(C_{22} - C_{23}) = \left\langle \frac{1}{\mu} \right\rangle^{-1}$$

$$d_1 = \left\langle \frac{\pi}{p} \right\rangle \langle p^{-1} \rangle^{-1} - c(1-c) \frac{(\hat{\lambda}^{(2)} - \hat{\lambda}^{(1)})(\hat{\pi}^{(2)} - \hat{\pi}^{(1)})}{\tilde{\lambda} + \tilde{\mu}}$$

$$d_2 = \left\langle \frac{\pi}{p} \right\rangle \langle p^{-1} \rangle^{-1}$$

$$- c(1-c) \frac{(\hat{\lambda}^{(2)} - \hat{\lambda}^{(1)} + \mu^{(2)} - \mu^{(1)})(\hat{\pi}^{(2)} - \hat{\pi}^{(1)})}{\tilde{\lambda} + \tilde{\mu}}$$

$$P = \langle p^{-1} \rangle - c(1-c) \frac{(\hat{\pi}^{(2)} - \hat{\pi}^{(1)})^2}{\tilde{\lambda} + \tilde{\mu}}, \quad p^{(\alpha)} = \frac{\theta_0}{c_\varepsilon^{(\alpha)}}$$

$$\hat{\pi}^{(\alpha)} = \pi^{(\alpha)} - \frac{\tilde{\pi}}{\tilde{p}} p^{(\alpha)}, \quad \pi^{(\alpha)} = \frac{K^{(\alpha)} \alpha_v^{(\alpha)} \theta_0}{c_\varepsilon^{(\alpha)}}$$

$$\hat{\lambda}^{(\alpha)} = \lambda^{(\alpha)} - \frac{\tilde{\pi}}{\tilde{p}} \pi^{(\alpha)}$$

$$\tilde{\kappa} = d_2 (1-c) \hat{\pi}^{(1)} K^{(1)} \alpha_v^{(1)} + c \hat{\pi}^{(2)} K^{(2)} \alpha_v^{(2)}$$

$$\tilde{\lambda} + \tilde{\mu}$$

$$\bar{\kappa} = \frac{(1-c) K^{(1)} \alpha_v^{(1)} (\lambda^{(1)} + \mu^{(1)}) + c K^{(2)} \alpha_v^{(2)} (\lambda^{(2)} + \mu^{(2)})}{\tilde{\lambda} + \tilde{\mu}}$$

$$\hat{\kappa} = \langle K \alpha_v \rangle + c(1-c) (K^{(1)} \alpha_v^{(1)} + K^{(2)} \alpha_v^{(2)}) \frac{\hat{\lambda}^{(2)} - \hat{\lambda}^{(1)}}{\tilde{\lambda} + \tilde{\mu}} \quad (23)$$

The last four terms in Eq. (18) are nonconservative terms due to inelastic response and three modes of damage. Here ε_{ij}^e is the elastic macroscopic strain tensor measured from an initial state (see

Appendix A), and θ is the absolute temperature measured from an initial state (see Appendix A). Y_σ , Y_τ , and Y_Δ are weight function constants that result from the implementation of the Onsager principle for the nonconservative terms (i.e., in irreversible thermodynamics the constitutive relations are linear with symmetric coefficients³⁶), which leads to

$$\int_0^t \frac{\partial u_v}{\partial \omega} \dot{\omega} dt = -K Y_\sigma \int_0^\omega \dot{\omega} d\omega$$

$$\int_0^t \frac{\partial u_v}{\partial \varpi} \dot{\varpi} dt = -2\mu Y_\tau \int_0^\varpi \dot{\varpi} d\varpi$$

$$\int_0^t \frac{\partial u_v}{\partial \Delta} \dot{\Delta} dt = -\mu Y_\Delta \int_0^{\omega_\Delta} \dot{\omega}_\Delta d\omega_\Delta$$

$$\int_0^t \frac{\partial u_v}{\partial \varepsilon_{ij}^{\text{in}}} \dot{\varepsilon}_{ij}^{\text{in}} dt = -\mu \Gamma \int_0^{\varepsilon_{ij}^{\text{in}}} \dot{\varepsilon}_{ij}^{\text{in}} d\varepsilon_{ij}^{\text{in}} = -\frac{1}{2} \mu \Gamma \varepsilon_{ij}^{\text{in}} \varepsilon_{ij}^{\text{in}} \quad (24)$$

Y_σ , Y_τ , and Y_Δ are weight function constants introduced to capture, in a simple way, the probability function of the damage mode density in composites, that is, tensile, shear, and interphase damage modes. (Note that the modes of failure are predicated on a statistical relationship considering many tests, and for simplicity an assumed weighted characteristic is made.) They range in values between zero and one ($0 \leq Y_\sigma, Y_\tau, Y_\Delta \leq 1$), where zero indicates no probability for the damage mode to exist and one is the highest damage mode probability possible. Γ is an inelastic proportionality material constant that indicates the material's ability to deform inelastically. Also $\dot{\omega}(\omega, \varepsilon_{kk}^e)$, $\dot{\varpi}(\omega, \varpi, \varepsilon^e)$, and $\dot{\omega}_\Delta(\omega, \Delta)$ are phenomenological coefficients of damage that represent the rate of damage. They are determined from damage constitutive relations. These relations are based on the kinetic equation of the Tuler-Butcher type,³⁷ which are

$$\dot{\omega}(\omega, \varepsilon_{kk}^e) = \Omega_\omega \{ [\varepsilon_{kk}^e / (1 - \omega)] - \varepsilon^* \} H \{ [\varepsilon_{kk}^e / (1 - \omega)] - \varepsilon^* \}$$

$$\dot{\varpi}(\omega, \varepsilon^e) = \Omega_\varpi \{ [\varepsilon^e / (1 - \omega)] - \varepsilon_\tau^* \} H \{ [\varepsilon^e / (1 - \omega)] - \varepsilon_\tau^* \}$$

$$\dot{\omega}_\Delta(\omega, \Delta) = \Omega_\Delta \{ [\Delta / (1 - \omega)] - \Delta^* \} H \{ [\Delta / (1 - \omega)] - \Delta^* \} \quad (25)$$

where the second invariant of the deviatoric strain ε^e and the deviatoric strain ε_{ij}^e are defined as

$$\varepsilon^e = \sqrt{\varepsilon_{ij}^e \varepsilon_{ij}^e}, \quad \varepsilon_{ij}^e = \varepsilon_{ij}^e - \frac{1}{3} \varepsilon_{kk}^e \delta_{ij} \quad (26)$$

The damage constitutive relations are based on the following. The tensile damage characterizes cavities and voids initiates, and it is assumed to be a function of the elastic volumetric strain ε_{kk}^e . Tensile damage initiates when the volumetric strain reaches a threshold value ε^* . The shear damage characterizes shear slip, and it is assumed to be a function of the second invariance of the deviatoric elastic strain ε^e , which is analogous to the plasticity theory. The shear mode initiates as the deviatoric elastic strain reaches a threshold value ε_τ^* . The interphase damage is assumed to be a function of the difference between the two-phase strains Δ , and it initiates when Δ reaches a threshold value Δ^* . Ω_ω , Ω_ϖ , and Ω_Δ are macroscopic material constants that characterize the homogenized rate of damage for the two-phase material, that is, $\Omega_\omega^{(\alpha)}$, $\Omega_\varpi^{(\alpha)}$, and $\Omega_\Delta^{(\alpha)}$. Before damage (i.e., $\omega = \varpi = \omega_\Delta = 0$), $\dot{\omega}(\omega, \varepsilon_{kk}^e)$, $\dot{\varpi}(\omega, \varpi, \varepsilon^e)$, and $\dot{\omega}_\Delta(\omega, \Delta)$ are assumed to be a linear functions, where Ω_ω , Ω_ϖ , and Ω_Δ are the initial slopes. Furthermore, the degradation of the two-phase material due to damage is captured by assuming the bulk modulus and Lamé's constants, that is, K , μ and λ , respectively, are linear functions of the tensile damage ω . Thus, $K(\omega)$, $\mu(\omega)$, and $\lambda(\omega)$ are defined as

$$K = K_0(1 - \omega), \quad \mu = \mu_0(1 - \omega), \quad \lambda = \lambda_0(1 - \omega) \quad (27)$$

where K_0 is the bulk modulus and μ_0 and λ_0 are Lamé's constants for an undamaged structure.

Now that the internal energy for the homogenized lamina is established, the internal energy [Eq. (18)] is used to obtain the stresses, that is, $\sigma_{ij} = \partial \psi_v / \partial \varepsilon_{ij}^e$ (see Appendix A), which are

$$\begin{aligned}\sigma_{12} &= 2C_{66}\varepsilon_{12}^e - 2\mu Y_\tau \int_0^\omega \frac{\partial \bar{\omega}}{\partial \varepsilon_{12}^e} d\bar{\omega} \\ \sigma_{23} &= 2C_{66}\varepsilon_{23}^e - 2\mu Y_\tau \int_0^\omega \frac{\partial \bar{\omega}}{\partial \varepsilon_{23}^e} d\bar{\omega} \\ \sigma_{31} &= 2C_{66}\varepsilon_{31}^e - 2\mu Y_\tau \int_0^\omega \frac{\partial \bar{\omega}}{\partial \varepsilon_{31}^e} d\bar{\omega} \\ \sigma_{11} &= C_{11}\varepsilon_{11}^e + C_{12}\varepsilon_{22}^e + C_{12}\varepsilon_{33}^e - d_1(\eta - \bar{\eta}) \\ &\quad - K Y_\sigma \int_0^\omega \frac{\partial \bar{\omega}}{\partial \varepsilon_{11}^e} d\bar{\omega} - 2\mu Y_\tau \int_0^\omega \frac{\partial \bar{\omega}}{\partial \varepsilon_{11}^e} d\bar{\omega} \\ \sigma_{22} &= C_{11}\varepsilon_{11}^e + C_{12}\varepsilon_{22}^e + C_{23}\varepsilon_{33}^e - d_2(\eta - \bar{\eta}) \\ &\quad - K Y_\sigma \int_0^\omega \frac{\partial \bar{\omega}}{\partial \varepsilon_{22}^e} d\bar{\omega} - 2\mu Y_\tau \int_0^\omega \frac{\partial \bar{\omega}}{\partial \varepsilon_{22}^e} d\bar{\omega} \\ \sigma_{33} &= C_{11}\varepsilon_{11}^e + C_{12}\varepsilon_{22}^e + C_{22}\varepsilon_{33}^e - d_2(\eta - \bar{\eta}) \\ &\quad - K Y_\sigma \int_0^\omega \frac{\partial \bar{\omega}}{\partial \varepsilon_{33}^e} d\bar{\omega} - 2\mu Y_\tau \int_0^\omega \frac{\partial \bar{\omega}}{\partial \varepsilon_{33}^e} d\bar{\omega}\end{aligned}\quad (28)$$

Note that Eq. (28) differs from the thermoelastic stress-strain relation [e.g., the thermoelastic stress-strain relation in Eqs. (14) for homogeneous material], such that the damage affects the stress-strain response.

Finally, using an energy balance approach and characterizing the damage in the composite structure as an unrecoverable process equivalent to the dissipation of energy, that is, unrecoverable energy, a criterion for the development of microscopic cracks is introduced. By the use of the second law of thermodynamics, a damage parameter D_v per unit volume that computes the energy dissipation for the system is defined as

$$\begin{aligned}D_v &= \int_0^t \left((\sigma_{ij} + \mu \Gamma \varepsilon_{ij}^{\text{in}}) \dot{\varepsilon}_{ij}^{\text{in}} + K Y_\sigma \dot{\omega}^2 + 2\mu Y_\tau \dot{\bar{\omega}}^2 + \mu Y_\Delta \dot{\omega}_\Delta^2 \right. \\ &\quad \left. - \frac{\partial \psi_v}{\partial \Delta} \dot{\Delta} - \frac{q_i \theta_{,i}}{\theta} \right) dt\end{aligned}\quad (29)$$

where t is the time such that the time integral represents the accumulative process of damage. Note that the damage parameter D_v in Eq. (29) defines the microdamage in the material as a dissipation of energy due to the inelastic behavior of the material, tensile damage, shear damage, interphase discontinuity damage, incompatibility of the deformation between the fiber and matrix (i.e., strain difference between the two phases), and the thermal dissipation. As the microcracks coalesce and the damage parameter reaches a critical value $D_v = D^*$, a macrocrack initiates. The critical damage parameter D^* is a material constant that is determined experimentally, and it indicates when microcracks coalesce into a macrocrack.

The damage model has 10 material constants, Y_σ , Y_τ , Y_Δ , Ω_ω , Ω_Δ , ε^* , ε_τ^* , Δ^* , and D^* , which characterize the macroscopic damage. These are determined through experiments, which can be time consuming and cumbersome, especially for composites. To minimize the effort to obtain all 10 constants, the following technique has been adopted to obtain the damage weight functions or proportionality constants Y_σ and Y_τ based on the theoretical strength of a material's perfect crystal. First, note that even though neither of the two-phase materials exhibit perfect crystal strength, the theory is used as a simplifying means to obtain the proportionality constants. Second, the weight function constants are assumed inversely proportional to the theoretical strength of the material's perfect crystal (see Appendix C) because the weight function constants reflect the tendency of the material to display damage. That is, the higher the strength is, the smaller the damage and vice versa.

Furthermore, because the weight function constants Y_σ and Y_τ are nondimensional, a normalization factor n_f will be used to nondimensionalize the theoretical strength of the crystal. This normalizing factor n_f is assumed to be

$$n_f = (1/\pi)[F_\sigma F_\tau / (F_\sigma + F_\tau)] \quad (30)$$

Hence, the damage weight function constants Y_σ and Y_τ for the tensile and shear damage of a material phase are assumed based on the theoretical strength of the material's perfect crystal (see Appendix C) to be

$$Y_\sigma^{(\alpha)} = \pi n_f |E^{(\alpha)}| \quad (31)$$

$$Y_\tau^{(\alpha)} = \frac{\pi n_f}{\sqrt[3]{8} G^{(\alpha)}} \quad (32)$$

Furthermore, considering a two-phase composite, homogenized damage weight function constants based on the rule of mixture Eq. (10) are assumed, and they are equal to

$$Y_\sigma = c Y_\sigma^{(1)} + (1 - c) Y_\sigma^{(2)} = c(\pi n_f |E^{(1)}|) + (1 - c)(\pi n_f |E^{(2)}|) \quad (33)$$

$$Y_\tau = c Y_\tau^{(1)} + (1 - c) Y_\tau^{(2)} = c \frac{\pi n_f}{\sqrt[3]{8} G^{(1)}} + (1 - c) \frac{\pi n_f}{\sqrt[3]{8} G^{(2)}} \quad (34)$$

Note that the weight function constants are assumed inversely proportional to the strength, where the strength of a two-phase composite is more difficult to predict using the rule of mixture. However, the homogenized weight function constants provide a lower bound estimate using the rule of mixture, which is assumed sufficient for the type of approximation required for this technique. This form of the weight function constants Y_σ and Y_τ also reflects the load and the fiber orientation because the strength of a composite is direction dependent as well as tension and compression dependent.

III. Results

The model is first compared with experimental data available in the literature. Hayakawa and Murakami³⁸ performed a uniaxial tension test on tabular specimens of spheroidized graphite cast iron FCD400. The wall thickness of the specimen is 1 mm, which is sufficient to ensure the continuum assumption, that is, one phase, because the average diameter of the spheroidized graphite particles is about 30×10^{-3} mm. The fracture mechanism of the spheroidized graphite cast iron is decohesion at the interfaces between the graphite particles and the ferrite matrix. In addition, the ductile failure of the ferrite matrix is induced by the development of microcracks. The material properties are the Young's modulus $E = 169$ GPa and the shear modulus $G = 65.76$ GPa. The numerical analysis for the present model is based on the following assumptions. The applied heat flux is assumed negligible, that is, the thermal-mechanical coupling for the problem is assumed insignificant. Tensile and shear damage modes are only considered in this analysis where the residual stresses are assumed insignificant, that is, $Y_\sigma \neq 0$, $Y_\tau \neq 0$, and $Y_\Delta = \Delta \approx 0$. The inelastic proportionality constant Γ is assumed negligible. Furthermore, a uniaxial bar is assumed (see Fig. 2), and for a uniaxial loaded two-phase bar, Eqs. (18–29) reduce to

$$\begin{aligned}\sigma_{ij} &= 0, \quad \text{for } ij \neq 11 \\ \sigma_{11} &= \langle E \rangle \varepsilon_{11}^e + (1 - 2\langle \nu \rangle) \left\{ K Y_\sigma \Omega_\omega \ln(1 - \omega) - \frac{2\sqrt{6} \mu Y_\tau \Omega_\omega \bar{\omega}}{3(1 - \omega)} \right\} \\ \varepsilon_{22}^e &= \varepsilon_{33}^e = -\langle \nu \rangle \varepsilon_{11}^e - \langle \nu \rangle \left\{ K Y_\sigma \Omega_\omega \ln(1 - \omega) - \frac{2\sqrt{6} \mu Y_\tau \Omega_\omega \bar{\omega}}{3(1 - \omega)} \right\} \\ D_v &= \int_0^t [K Y_\sigma \dot{\omega}^2 + 2\mu Y_\tau \dot{\bar{\omega}}^2] dt\end{aligned}\quad (35)$$

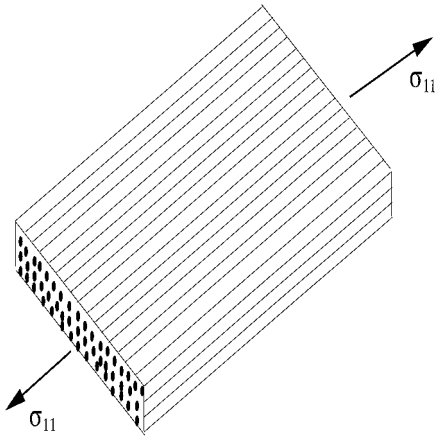


Fig. 2 Uniaxial loaded composite.

where

$$\langle E \rangle = \left\langle \frac{\mu(3\lambda + 2\mu)}{\lambda + \mu} \right\rangle, \quad \langle \nu \rangle = \left\langle \frac{\lambda}{2(\lambda + \mu)} \right\rangle \quad (36)$$

For one-phase material, the volume fraction c is set equal to zero, and the quantities for the two-phase materials are equal and reduce to one phase. These stress-strain relations in Eqs. (35) are obtained by substituting the uniaxial stress conditions (i.e., $\sigma_{12} = \sigma_{13} = \sigma_{23} = \sigma_{22} = \sigma_{33} = 0$, and $\sigma_{11}(t) \neq 0$ is a nonzero known value function of time) into Eq. (28). This leads to three equations with three unknowns, ε_{11} , ε_{22} , and ε_{33} . Furthermore, a transversely isotropic condition will be enforced, that is, the transverse strain are equal $\varepsilon_{22} = \varepsilon_{33}$. Also, for the uniaxial bar, the damage terms simplify to

$$\int_0^\omega \frac{\partial \dot{\omega}}{\partial \varepsilon_{ij}^e} d\omega = -\Omega_\omega \int_0^\omega \frac{1}{(1-\omega)} d\omega = \Omega_\omega \ln(1-\omega) \quad (37)$$

$$\int_0^\omega \frac{\partial \dot{\omega}}{\partial \varepsilon_{ij}^e} d\omega = -\frac{\sqrt{6}}{3} \frac{\Omega_\omega}{(1-\omega)} \int_0^\omega d\omega = -\frac{\sqrt{6}}{3} \frac{\Omega_\omega}{(1-\omega)} \omega \quad (38)$$

These equations are solved using numerical integration.

The damage parameters are selected such that the computed results present a best fit to the experimental data similar to the Hayakawa and Murakami³⁸ approach to determine the damage constants. They are for the present model as follows: $\Omega_\omega = 0.01$, $\Omega_\omega = 2.29$, $\Omega_\Delta = 0$, $Y_\sigma = 1$, $Y_\tau = 1$, and $Y_\Delta = 0$. The comparison between the stress-strain response of the experimental data³⁸ and the present model numerical analysis is shown in Fig. 3. The results show good agreement with the experiments. Also, the degradation of the Young's modulus due to damage is measured experimentally by Hayakawa and Murakami.³⁸ The results are given in Fig. 4. A comparison of the Young's modulus degradation as a function of strain between the experimental data and the present model's results show good agreement. Note that, for the numerical form of Hayakawa and Murakami,³⁸ they assumed an anisotropic form of damage. However, in the present model a special isotropic form of damage is assumed using three damage modes: tensile, shear, and interphase damage. In addition, the damage parameter D_v , which measures the microcrack density, is computed (no experimental data available). The damage parameter D_v vs strain is shown in Fig. 5. The result shows that the microcrack density initiates at a strain level where the stress-strain response becomes nonlinear. It also shows that the microcrack density becomes unbounded at strain level equal to 0.23 where the stress approximately reaches its ultimate value (see Fig. 3). The unbound value of the damage parameter D_v is attributed to the microcracks suddenly coalescing into a macrocrack, which occurs at a deformation that is consistent with the ultimate stress. Note that the sudden discontinuous unboundness of the damage parameter D_v is due to the singularity in Eq. (38) because the tensile damage ω is equal to one.

The effect of the rate of loading on damage in composite material is investigated. A uniaxially loaded two-phase bar loaded by linear

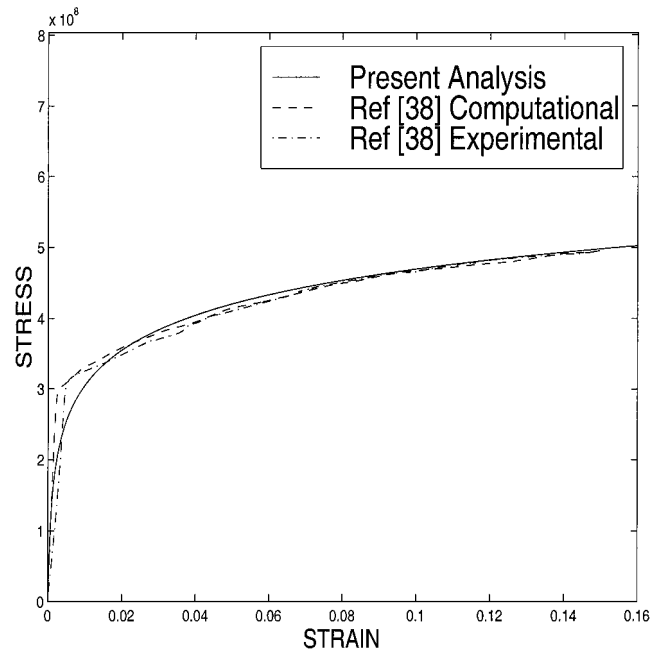


Fig. 3 Comparison between the present analysis's stress-strain response and experimental data.

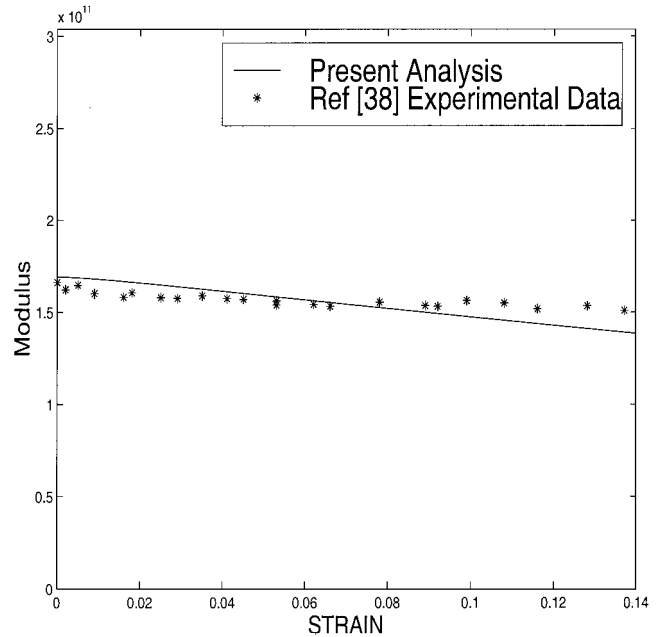


Fig. 4 Comparison between the present analysis's Young's modulus as a function of strain and experimental data.

and half-sine functions, as shown in Fig. 6, is examined. The maximum amplitude of the loading function is set equal to 2.17 GPa, which is in the range of the fiber fracture. The first two-phase material considered is graphite/epoxy, and its material properties are in Table 1. The fiber volume fraction c is set equal to 0.3. Here ε^* and ε_τ^* , which determine the initiation of the tensile and shear damage in the material, respectively, are taken equal to 0.002. Ω_ω and Ω_ω are the rate of damage evolution constants, which are taken as the initial slope to the tensile and shear damage curve, that is, initially $\omega = 0$ and the rates of tensile and shear damage are $\dot{\omega} \propto \Omega_\omega \varepsilon_{kk}^e$ and $\dot{\omega} \propto \Omega_\omega \varepsilon^e$. They are set equal to 0.578 and 4.7, respectively, based on an iterative procedure, that is, they are calibrated for a bar fully failed in 3 s at a maximum loading amplitude of 2.17 GPa or 0.7233-GPa/s load rate. Also, the tensile damage is assumed dominant, that is, $Y_\sigma = 1$ and $Y_\tau = Y_\Delta = 0$. Various load rates slower and faster than 0.7233 GPa/s are considered. Figure 7 shows the stress-strain

Table 1 Two-phase Lamé’s constants for four types of composite materials

Composite material	Lamé’s constant, Pa			
	$\lambda^{(1)}$	$\lambda^{(2)}$	$\mu^{(1)}$	$\mu^{(2)}$
Boron/epoxy	6.8799×10^{10}	7.4275×10^9	1.1920×10^{10}	2.9663×10^9
Aramid/epoxy	1.1138×10^{11}	6.9770×10^9	3.5200×10^9	1.408×10^9
Graphite/epoxy	1.2336×10^{11}	2.1702×10^8	4.9000×10^9	2.9859×10^9
E-glass/epoxy	2.8174×10^{10}	6.2126×10^9	5.7200×10^9	2.5274×10^9

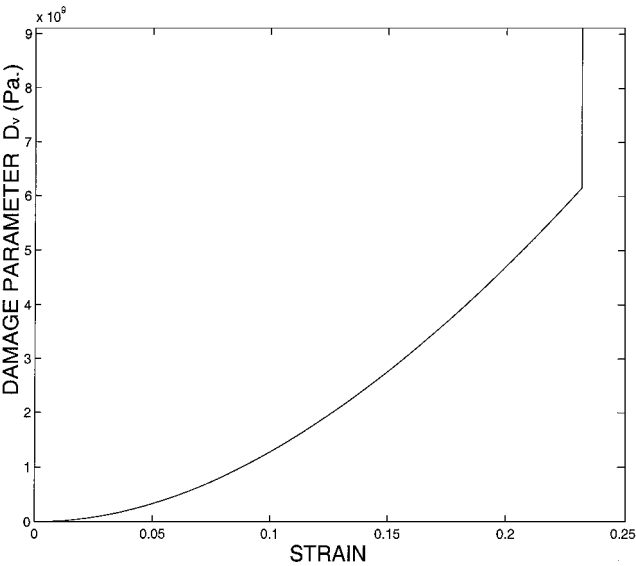


Fig. 5 Damage parameter D_v vs strain.

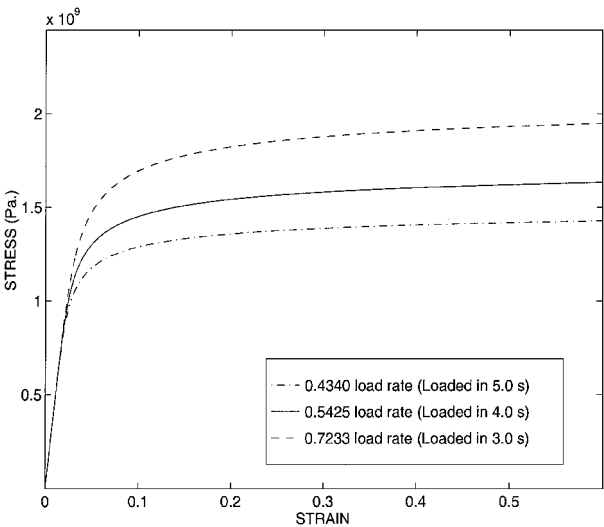


Fig. 7 Stress–strain response for linearly loaded uniaxial two-phase bar with stress rates equal and less than 0.7233 GPa/s.

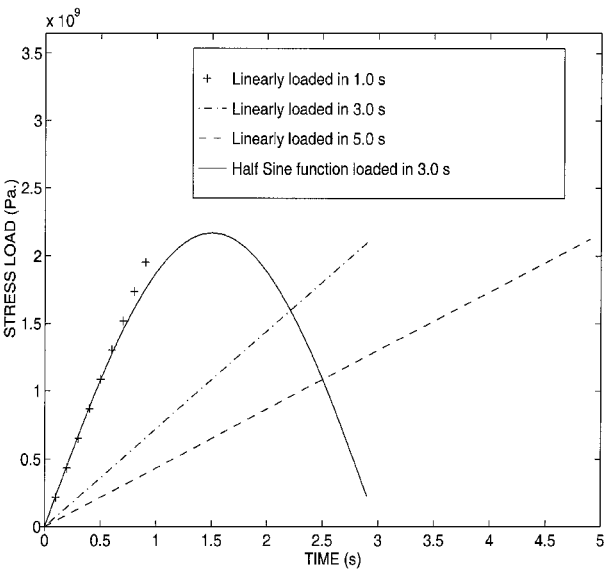


Fig. 6 Type of uniaxial loading used for the bar where the maximum amplitude is $\sigma_0 = 2.17$ GPa.

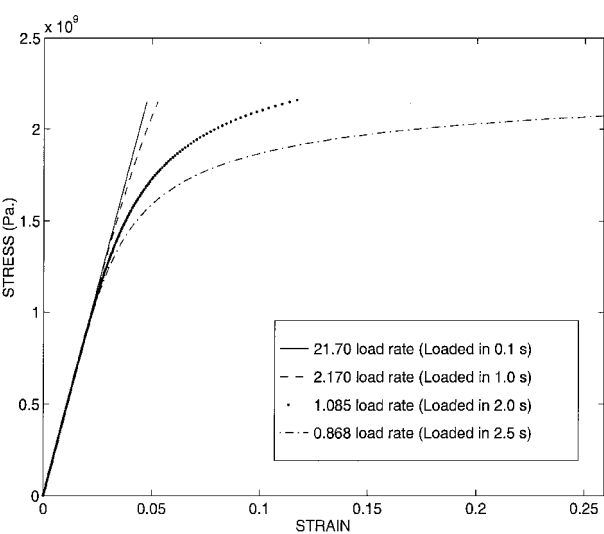


Fig. 8 Stress–strain response for linearly loaded uniaxial two-phase bar with stress rates greater than 0.7233 GPa/s.

response of two-phase bar for a load rate less than 0.7233 GPa/s. The results show that at slower loading rates the bar becomes fully damaged quicker and that the material ability to carry load diminishes. For example, the maximum stress the bar could sustain for a load rate of 0.434 GPa/s is approximately 1.5 GPa compared to approximately 2.0 GPa for a load rate of 0.7233 GPa/s. Furthermore, the stress–strain response of the bar loaded at higher rates than 0.7233 GPa/s are shown in Fig. 8. The results show that at high loading rates the bar response is almost linear elastic and that more strength is exhibited by the material, which is consistent with Ref. 39. Furthermore, one can show that damage is a function of the loading path. For example, considering a linear and a sine loading function with a maximum amplitude of 2.17 GPa, the sine loading

function has a cosine loading rate function (i.e., starts faster than the linear load functions then slows down) compared to a constant loading rate for the linear function. The tensile damage vs time is shown in Fig. 9 for the two loading functions. The results show that the damage progress is higher for the sine loading function compared with the linear loading function, which is attributed to the sine function’s faster loading rate. In addition, one can investigate the effect of stiffness degradation due to damage on the unloading using the sine function. A comparison is shown in Fig. 10.

Damage analyses of graphite/epoxy, boron/epoxy, aramid/epoxy, and E-glass/epoxy uniaxial bar are also investigated using the microscopic features of the model. The weight function constants or proportionality constants Y_σ and Y_τ are determined using the theoretical strength of a material with perfect lattice or crystal

Table 2 Material’s properties for four types of composite materials⁴⁰

Property, Pa	Composite material			
	Graphite/epoxy	Aramid/epoxy	Boron/epoxy	E-glass/epoxy
E_1 (longitudinal)	214.0×10^9	87.8×10^9	201.0×10^9	39.0×10^9
E_2 (transverse)	6.4×10^9	5.5×10^9	21.7×10^9	8.6×10^9
G_{12}	3.9×10^9	2.2×10^9	5.4×10^9	3.8×10^9
μ_{12}	0.23	0.34	0.17	0.28
F_σ (ultimate longitudinal tensile strength)	0.789×10^9	1.28×10^9	1.38×10^9	1.08×10^9
F_σ (ultimate transverse tensile strength)	0.029×10^9	0.030×10^9	0.056×10^9	0.039×10^9
F_τ (ultimate shear strength)	0.0391×10^9	0.049×10^9	0.062×10^9	0.089×10^9

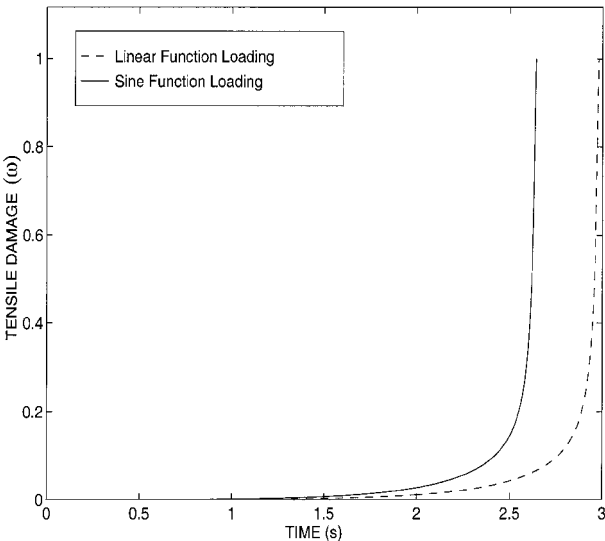


Fig. 9 Tensile damage ω vs time for two different type of loading (sine and linear function) where the maximum amplitude 2.17 GPa is loaded in 3.0 s and $\omega = 1.0$ indicates total damage of the bar.

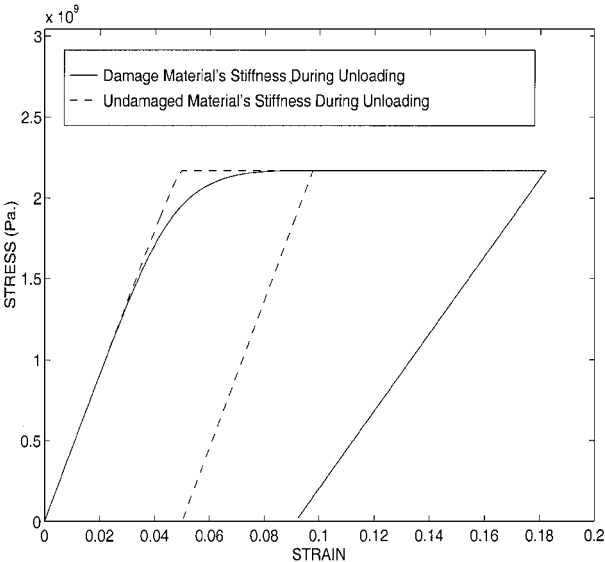


Fig. 10 Stress-strain response of uniaxial two-phase bar loaded with half-sine function with damaged and undamaged material’s stiffness during unloading.

structure (see Appendix C). Lamé’s constants for the four material (graphite/epoxy, boron/epoxy, aramid/epoxy, and E-glass/epoxy) are given in Tables 1 and 2 (see Ref. 40), and the fiber volume fraction c is set equal to 0.6. Using Eqs. (34), the weight function constants for the four composite materials are computed based on longitudinal strength (Table 3). The stress-strain responses are shown in Fig. 11. The results show that the damage accumulates at a rate faster in the graphite/epoxy than in the E-glass/epoxy,

Table 3 Nondimensional weight function constants for four types of composite materials considering longitudinal response

Composite material	Damage weight function constants	
	Y_σ	Y_τ
Boron/epoxy	8.1738×10^{-4}	1.1620×10^{-2}
Aramid/epoxy	2.3469×10^{-3}	2.8808×10^{-2}
Graphite/epoxy	3.4384×10^{-3}	2.8490×10^{-2}
E-glass/epoxy	3.5025×10^{-3}	3.0221×10^{-2}

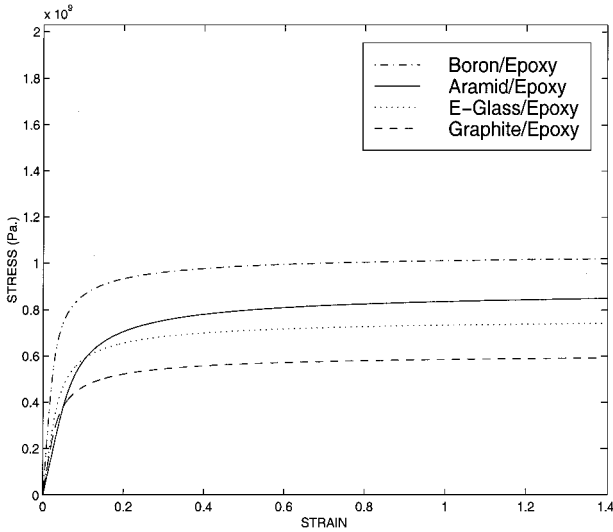
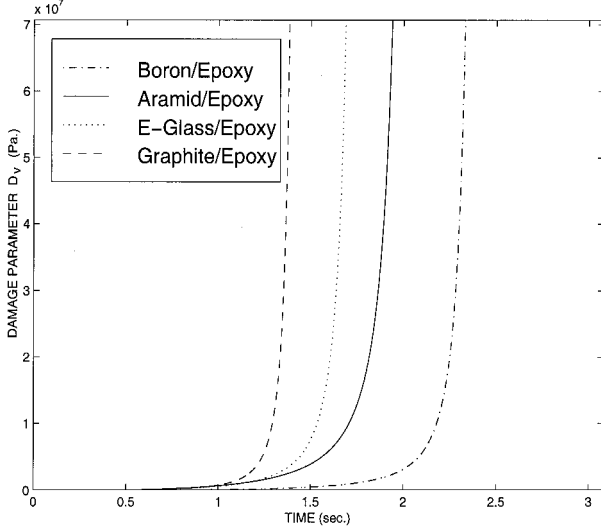


Fig. 11 Stress-strain response for various composite types.

aramid/epoxy, and boron/epoxy, respectively. Note that these results are consistent with the strength of the composite where the ultimate longitudinal tensile strength is lowest for graphite/epoxy, then E-glass/epoxy, aramid/epoxy, and boron/epoxy, respectively (see Table 2). Furthermore, the damage parameters D_v are computed vs time, and they are shown in Fig. 12. The results indicate that the values of the damage parameter D , which represent the density of microcracks in the composite, become unbounded with time. This is attributed to the initiation of macrocracks due to the coalescing of microcracks. Furthermore, one could obtain a numerical value for D^* based on the results in Fig. 12 by setting its value equal to the value of D_v as it becomes unbounded. That is, D^* for the graphite/epoxy, E-glass/epoxy, aramid/epoxy, and boron/epoxy based on the results in Fig. 12 are approximately 1.0×10^7 , 2.0×10^7 , 3.0×10^7 , and 4.0×10^7 Pa at 1.25, 1.55, 1.85, and 2.25 s, respectively. Furthermore, because the composite’s properties are direction dependent, for example, longitudinal strength is different from transverse strength, the weight function constants for the four composite materials are also computed based on the composite’s transverse properties (Table 4). The analysis results using transverse strength to compute the weight function constants show similar trends to the one computed based on the longitudinal strength but have lower damage accumulation.

Table 4 Nondimensional weight function constants for the four types of composite materials considering transverse response

Composite material	Damage weight function constants	
	Y_σ	Y_τ
Boron/epoxy	1.7943×10^{-2}	7.5711×10^{-3}
Aramid/epoxy	3.7466×10^{-2}	3.5030×10^{-2}
Graphite/epoxy	1.0423×10^{-1}	2.8490×10^{-2}
E-glass/epoxy	1.5884×10^{-2}	3.5335×10^{-2}


Fig. 12 Damage parameter D_v vs time for various composite types.

IV. Conclusions

A thermomicromechanical model of failure is presented, which is based on thermodynamic principles, that is, using the balancing laws: the conservation of momentum and the first and second law of thermodynamics. A homogenization technique is incorporated in the development to simplify the representation of the nonhomogeneous material and to allow the inclusion of thermomicromechanical phenomenon in a composite lamina. A summary of the equations for the thermomicromechanical model of failure is shown, and a damage parameter D that characterizes the damage in the lamina based on energy dissipation is introduced. The following conclusions can be stated. First, the model is compared with experimental and theoretical data for a one-phase material that are available in the literature, and it showed reasonably good agreement. Second, a parametric study of the homogenized material was carried out. To obtain the weight function constants, experiments are required. However, in this investigation they were chosen based on the theoretical strength assumption of the material's perfect crystal as a simplifying approach. The results demonstrated the following:

1) For dynamic tests, the material deformation and failure process are greatly influenced by the loading condition, for example, loading rate, and for high-intensity loading, the rate of loading has significant effects on the composite response where an increase in the loading rate causes an increase in the material strength.

2) The damage progress for a composite lamina is a function of the rate of loading.

3) The choice of the weight function constants Y_σ , Y_τ , and Y_Δ for tensile damage and shear damage influence the damage progress.

4) The damage parameter D_v shows singular behavior, which suggests that microcrack nucleation and density reaches a critical value sufficient to coalesce and initiate a macrocrack ($D = D^*$).

Appendix A: Thermoelastic Energy

The power of dissipation can be obtained as follows. Starting with the time derivative of the thermodynamic relation between the internal and the free energy

$$u_v = \psi_v + \eta\theta \quad (A1)$$

and rearranging, one deduces

$$\dot{\eta} = (\dot{u}_v - \dot{\psi}_v - \eta\dot{\theta})/\theta \quad (A2)$$

Using the first law of thermodynamics [Eq. (2)] and time derivative of the free energy [Eq. (5)], one can rewrite (Eq. (A2)) as

$$\begin{aligned} \dot{\eta} &= \frac{1}{\theta} \left(\sigma_{ij} \dot{\epsilon}_{ij} - q_{i,i} - \frac{\partial \psi_v}{\partial \epsilon_{ij}^e} \dot{\epsilon}_{ij}^e - \frac{\partial \psi_v}{\partial \epsilon_{ij}^{in}} \dot{\epsilon}_{ij}^{in} - \frac{\partial \psi_v}{\partial \theta} \dot{\theta} - \frac{\partial \psi_v}{\partial \Delta} \dot{\Delta} \right. \\ &\quad \left. - \frac{\partial \psi_v}{\partial \omega} \dot{\omega} - \frac{\partial \psi_v}{\partial \varpi} \dot{\varpi} - \frac{\partial \psi_v}{\partial \omega_\Delta} \dot{\omega}_\Delta - \eta\dot{\theta} \right) \\ &= \frac{1}{\theta} \left[\left(\sigma_{ij} - \frac{\partial \psi_v}{\partial \epsilon_{ij}^e} \right) \dot{\epsilon}_{ij}^e + \left(\sigma_{ij} - \frac{\partial \psi_v}{\partial \epsilon_{ij}^{in}} \right) \dot{\epsilon}_{ij}^{in} - q_{i,i} \right. \\ &\quad \left. - \left(\frac{\partial \psi_v}{\partial \theta} + \eta \right) \dot{\theta} - \frac{\partial \psi_v}{\partial \Delta} \dot{\Delta} - \frac{\partial \psi_v}{\partial \omega} \dot{\omega} - \frac{\partial \psi_v}{\partial \varpi} \dot{\varpi} - \frac{\partial \psi_v}{\partial \omega_\Delta} \dot{\omega}_\Delta \right] \end{aligned} \quad (A3)$$

Using the thermodynamic relations ($\eta = -\partial \psi_v / \partial \theta$) and ($\sigma_{ij} = \partial \psi_v / \partial \epsilon_{ij}^e$), we have

$$\begin{aligned} &\left(\sigma_{ij} - \frac{\partial \psi_v}{\partial \epsilon_{ij}^{in}} \right) \dot{\epsilon}_{ij}^{in} - \frac{\partial \psi_v}{\partial \Delta} \dot{\Delta} - \frac{\partial \psi_v}{\partial \omega} \dot{\omega} - \frac{\partial \psi_v}{\partial \varpi} \dot{\varpi} \\ &\quad - \frac{\partial \psi_v}{\partial \omega_\Delta} \dot{\omega}_\Delta - \frac{q_i \theta_{,i}}{\theta} \geq 0 \end{aligned} \quad (A4)$$

Furthermore, one can obtain the thermoelastic free energy $\psi_v^e(\epsilon_{ij}, \bar{\theta})$ as follows. The thermoelastic free energy $\psi_v^e(\epsilon_{ij}, \bar{\theta})$ is assumed to be a function of the elastic strain ϵ_{ij} and temperature $\bar{\theta}$. The free energy expression is obtained by expanding the free energy $\psi_v^e(\epsilon_{ij}, \bar{\theta})$ per unit volume into the Taylor series in the vicinity of the initial state, that is, $\epsilon_{ij} = \epsilon_{ij}^0$ and $\bar{\theta} = \bar{\theta}_0$ where ϵ_{ij}^0 and $\bar{\theta}_0$ are the strain and temperature at the initial state, respectively. Thus,

$$\begin{aligned} \psi_v^e(\epsilon_{ij}, \bar{\theta}) &= \psi_{v0} + \frac{\partial \psi_{v0}}{\partial \epsilon_{ij}} (\epsilon_{ij} - \epsilon_{ij}^0) + \frac{\partial \psi_{v0}}{\partial \bar{\theta}} (\bar{\theta} - \bar{\theta}_0) \\ &\quad + \frac{1}{2} \left(\frac{\partial^2 \psi_{v0}}{\partial \epsilon_{ij} \partial \epsilon_{kl}} (\epsilon_{ij} - \epsilon_{ij}^0) (\epsilon_{kl} - \epsilon_{kl}^0) \right. \\ &\quad \left. + 2 \frac{\partial^2 \psi_{v0}}{\partial \epsilon_{ij} \partial \bar{\theta}} (\epsilon_{ij} - \epsilon_{ij}^0) (\bar{\theta} - \bar{\theta}_0) + \frac{\partial^2 \psi_{v0}}{\partial \bar{\theta}^2} (\bar{\theta} - \bar{\theta}_0)^2 \right) \\ &\quad + \dots \text{higher-order terms} \end{aligned} \quad (A5)$$

where ψ_{v0} is the free energy per unit volume at the initial state [i.e., $\psi_{v0} = \psi_v(\epsilon_{ij}^0, \bar{\theta}_0)$], $\partial \psi_{v0} / \partial \epsilon_{ij}$ is the stress tensor at the initial state, and $\partial \psi_{v0} / \partial \bar{\theta}$ is the entropy at the initial state. Also, consider the strain and temperature are measured from the initial state and one can write

$$\epsilon_{ij} = \epsilon_{ij} - \epsilon_{ij}^0, \quad \theta = \bar{\theta} - \bar{\theta}_0 \quad (A6)$$

Thus, to develop the thermoelastic material properties, one assumes that the free energy per unit volume, stresses, and entropy at the initial state are zero for convenience, and retaining only the quadratic terms in the series (i.e., quadratic strain terms, quadratic temperature term, and a coupled quadratic term consisting of strain and temperature terms), one can express the material constants as

$$c_{ijkl} = \frac{\partial^2 \psi_{v0}}{\partial \epsilon_{ij} \partial \epsilon_{kl}}, \quad \beta_{ij} = \frac{\partial^2 \psi_{v0}}{\partial \epsilon_{ij} \partial \bar{\theta}}, \quad m = \frac{\partial^2 \psi_{v0}}{\partial \bar{\theta}^2} \quad (A7)$$

and the free energy per unit volume becomes

$$\psi_v^e(\epsilon_{ij}, \theta) = \frac{1}{2} c_{ijkl} \epsilon_{ij} \epsilon_{kl} - \beta_{ij} \epsilon_{ij} \theta - \frac{1}{2} m \theta^2 \quad (A8)$$

where c_{ijkl} are the elastic constants for anisotropic material, which is related to the initial state, that is, isothermal; β_{ij} are the elastic-thermal property constants for anisotropic material, which is also related to the initial state, that is, isothermal; and m is the thermal property constant. Assume that the material is isotropic; the elastic constants c_{ijkl} and the elastic-thermal property constants β_{ij} can be written as

$$c_{ijkl} = \mu(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) + \lambda\delta_{ij}\delta_{kl}, \quad \beta_{ij} = \gamma\delta_{ij} \quad (\text{A9})$$

where the elastic-thermal property constants for isotropic material are assumed independent of the volumetric directions only. The elastic-thermal property constant γ for isotropic material is obtained by first computing the stresses, that is, the Duhamel-Neumann relation computed from the initial state:

$$\sigma_{ij} = (\tilde{\sigma}_{ij} - \sigma_{ij}^0) = \frac{\partial \psi_v}{\partial \varepsilon_{ij}} = 2\mu\varepsilon_{ij} + (\lambda\varepsilon_{kk} - \gamma\theta)\delta_{ij} \quad (\text{A10})$$

where σ_{ij}^0 is the stress tensor at the initial state, σ_{ij} is measured from the initial state, that is, $\tilde{\sigma}_{ij}$ is the total stress tensor, and the strain tensor ε_{ij} is measured also from initial state. From Eq. (A10), the bulk stress is

$$\sigma_{kk} = 3(K\varepsilon_{kk} - \gamma\theta) \quad (\text{A11})$$

or

$$\varepsilon_{kk} = \sigma_{kk}/3K + (\gamma/K)\theta \quad (\text{A12})$$

Note that in Eqs. (A11) and (A12) it is evident that a change of volume is proportional to temperature θ , that is, $\varepsilon_{kk}^{\text{thermal}} = \alpha_v\theta$, where α_v is the coefficient of thermal expansion. Thus, by comparison, the elastic-thermal property constant γ for isotropic material is equal to

$$\gamma = K\alpha_v \quad (\text{A13})$$

The thermal property constant m is obtained by computing the entropy as

$$\eta = -\frac{\partial \psi_v}{\partial \theta} = \gamma\varepsilon_{kk} - m\theta = \gamma\varepsilon_{kk} - \frac{\partial C(\theta)}{\partial \theta} \quad (\text{A14})$$

where $C(\theta) = -\frac{1}{2}m\theta^2$ is defined for convenience. The specific heat at a constant strain c_ε is defined as

$$c_\varepsilon = \theta \frac{\partial \eta}{\partial \theta} = -\theta \frac{\partial^2 C(\theta)}{\partial \theta^2} \quad (\text{A15})$$

Rearrange Eq. (A15) and integrate once with respect to temperature, which gives

$$\frac{\partial^2 C(\theta)}{\partial \theta^2} = -\frac{c_\varepsilon}{\theta}, \quad \frac{\partial C(\theta)}{\partial \theta} = -\int_{\theta_0}^{\theta} \frac{c_\varepsilon}{\bar{\theta}} d\bar{\theta} = -c_\varepsilon \ln\left(1 + \frac{\theta}{\theta_0}\right) \quad (\text{A16})$$

One can expand the natural log $\ln(\theta/\theta_0)$ into an infinite power series,

$$\ln\left(1 + \frac{\theta}{\theta_0}\right) = \frac{\theta}{\theta_0} - \frac{1}{2}\left(\frac{\theta}{\theta_0}\right)^2 + \frac{1}{3}\left(\frac{\theta}{\theta_0}\right)^3 + \dots \text{higher-order terms} \quad (\text{A17})$$

and then retain the first term only to obtain

$$m = c_\varepsilon/\theta_0 \quad (\text{A18})$$

Hence, the material constants in Eq. (A8) are determined, and the free energy per unit volume [Eq. (A8)] becomes

$$\psi_v^e(\varepsilon_{ij}, \theta) = \mu\varepsilon_{ij}\varepsilon_{ij} + \frac{1}{2}\lambda\varepsilon_{kk}\varepsilon_{kk} - K\alpha_v\varepsilon_{kk}\theta - (c_\varepsilon/2\theta_0)\theta^2 \quad (\text{A19})$$

Furthermore, one can obtain thermodynamic quantities using Eq. (57). For example, the entropy is

$$\eta = -\frac{\partial \psi_v}{\partial \theta} = \frac{c_\varepsilon}{\theta_0}(\theta - \theta_0) + K\alpha_v\varepsilon_{kk} \quad (\text{A20})$$

The internal energy u_v^e is related to the free energy ψ_v , where

$$u_v = \psi_v(\varepsilon_{ij}) + \eta\theta \quad (\text{A21})$$

Hence, using the same procedure, one can write the thermoelastic internal energy per unit volume as

$$u_v^e = (\lambda/2)(\varepsilon_{kk})^2 + \mu(\varepsilon_{ij})^2 - (K\alpha_v\theta_0/c_\varepsilon)\varepsilon_{kk}\eta + \theta_0\eta + (\theta_0/c_\varepsilon)(\eta)^2 \quad (\text{A22})$$

Furthermore, one can obtain thermodynamic quantities using Eq. (A23). For example, the stress tensor is

$$\sigma_{ij} = \frac{\partial \psi_v}{\partial \varepsilon_{ij}} = 2\mu\varepsilon_{ij} + \left(\lambda\varepsilon_{kk} - \frac{K\alpha_v\theta_0}{c_\varepsilon}\eta\right)\delta_{ij} \quad (\text{A23})$$

Appendix B: Prestate Conditions

The prestate or residual state condition affects the failure of the lamina, and it is incorporated into the formulation of the failure model as follows. The residual state is formulated based on a stress-free condition for uniaxial loaded two-phase material, which implies that the mechanical stresses are zero. In other words, the stresses in the two phases along the uniaxial loading direction are in equilibrium with the applied macrostress σ_{11} , which is zero for the prestate, that is,

$$\sigma_{11} = \langle \sigma_{11} \rangle = 0 \quad (\text{B1})$$

and all other stresses for this state are zero for a uniaxial case. The remaining two-phase stresses are zero ($\sigma_{ij}^{(a)} = 0$, for all $ij \neq 11$):

$$\begin{aligned} \sigma_{22}^{(1)} = \sigma_{22}^{(2)} = \sigma_{12}^{(1)} = \sigma_{12}^{(2)} = \sigma_{33}^{(1)} = \sigma_{33}^{(2)} \\ = \sigma_{23}^{(1)} = \sigma_{23}^{(2)} = \sigma_{13}^{(1)} = \sigma_{13}^{(2)} = 0 \end{aligned} \quad (\text{B2})$$

In addition, the prestate strain $\bar{\varepsilon}_{ij}$ in the transverse directions, that is, directions other than the uniaxial loading direction, which are the 22 direction and 33 direction, are symmetric for the two phases, which leads to two constraint equations for a uniaxial loading,

$$\bar{\varepsilon}_{22}^{(1)} = \bar{\varepsilon}_{33}^{(1)}, \quad \bar{\varepsilon}_{22}^{(2)} = \bar{\varepsilon}_{33}^{(2)} \quad (\text{B3})$$

The macrostrain in the uniaxial loading direction is continuous and can be expressed in terms of the two-phase strain as

$$\varepsilon_{11} = \varepsilon_{11}^{(1)} - \bar{\varepsilon}_{11}^{(1)} = \varepsilon_{11}^{(2)} - \bar{\varepsilon}_{11}^{(2)} \quad (\text{B4})$$

Note that the elastic macrostrain components are measured from the residual state. Also, the residual entropy $\bar{\eta}$ is assumed to be equal to the averaged entropy of the two phases, that is, satisfy the rule of mixture, which is

$$\bar{\eta} = \langle \eta \rangle \quad (\text{B5})$$

Also, define the difference between the strain between the two strain phases in the uniaxial as Δ :

$$\Delta = \varepsilon_{11}^{(1)} - \varepsilon_{11}^{(2)} = \bar{\varepsilon}_{11}^{(1)} - \bar{\varepsilon}_{11}^{(2)} \quad (\text{B6})$$

and use the thermoelastic relations for the entropy and stress tensor for the two phase, which are

$$\eta^{(a)} = K^{(a)}\alpha_v^{(a)}\varepsilon_{kk}^{(a)} \quad (\text{B7})$$

$$\sigma_{ij}^{(a)} = \lambda^{(a)}\varepsilon_{kk}^{(a)}\delta_{ij} + 2\mu^{(a)}\varepsilon_{ij}^{(a)} - \left(K^{(a)}\alpha_v^{(a)}\right)^2 \left(\theta_0^{(a)}\right) \frac{c_\varepsilon^{(a)}}{c_\varepsilon} \varepsilon_{kk}^{(a)} \delta_{ij} \quad (\text{B8})$$

The solutions for the residual strains from which the strains are counted off become

$$\bar{\varepsilon}_{11}^{(1)} = [(1 - c)\hat{E}^{(2)} | \langle \hat{E} \rangle] \Delta \quad (B9)$$

$$\bar{\varepsilon}_{11}^{(2)} = (c\hat{E}^{(1)} | \langle \hat{E} \rangle) \Delta \quad (B10)$$

$$\bar{\varepsilon}_{22}^{(1)} = -\bar{\varepsilon}_{33}^{(1)} = [\lambda^{(2)} | 2(\lambda^{(1)} + \mu^{(1)})] \bar{\varepsilon}_{11}^{(1)} \quad (B11)$$

$$\bar{\varepsilon}_{22}^{(2)} = -\bar{\varepsilon}_{33}^{(2)} = [\lambda^{(2)} | 2(\lambda^{(2)} + \mu^{(2)})] \bar{\varepsilon}_{11}^{(2)} \quad (B12)$$

$$\bar{\eta} = \langle \bar{\eta} \rangle = c\bar{\eta}^{(1)} + (1 - c)\bar{\eta}^{(2)} = B A \Delta \quad (B13)$$

where $\lambda^{(\alpha)}$, $\hat{E}^{(\alpha)}$, A , and B are defined in Eqs. (20) and (21).

Appendix C: Theoretical Strength of a Perfect Crystal

The theoretical strengths of a perfect crystal are calculated as follows.

Theoretical tensile strength is where materials break under normal stress and the fracture path is perpendicular to the applied stress. The process involves the separation of the atoms along the direction of the applied stress. Orowan⁴¹ developed a simple method for obtaining the theoretical tensile strength of a crystal at the angstrom level. In this method, no stress concentration at the tip of the microcrack is assumed; instead, it is assumed that all of the atoms separate simultaneously once their separation reaches a critical value. The distance required to separate two planes of atoms varies as a function of distance a between the two planes. In this model, the stress is taken as a sine function over the distance between the two planes a (which will be given subsequently). The total energy for the two surfaces is $2e_s A$, where e_s is the surface energy per unit area and A is the cross-sectional area of the specimen considered. The surface energy and the stress dependency on the plane of separation⁴¹ is given as

$$e_s = (E/a_0)(p_s/\pi)^2, \quad \sigma = \sqrt{Ee_s/a_0} \sin[(\pi/p_s)(a - a_0)] \quad (C1)$$

where E is the Young's modulus, a_0 is the distance between the two planes prior to separation under zero stress value $\sigma = 0$, p_s is the periodicity of the sine function, and π is equal to 3.14159. It is found experimentally that $p_s \approx a_0$; hence, the maximum or theoretical tensile strength is

$$\sigma_{\max} \approx E/\pi \quad (C2)$$

Theoretical shear strength of a crystal is obtained by Frenkel⁴² considering two adjacent and parallel lines of atoms subjected to pure shear. Under the action of the shear stress τ , the top line will move in relation to the bottom line. In this theory, the shear stress is taken as a sine function of the displacement x as

$$\tau = (Gb/2\pi a) \sin(2\pi x/b) \quad (C3)$$

where G is the shear modulus, b is the interatomic distance, and a is the distance between the two planes. The maximum theoretical strength is at $x = b/4$, which is equal to

$$\tau_{\max} = Gb/2\pi a \quad (C4)$$

where the ratio b/a based on crystallography is approximated as $\sqrt[3]{2} = 1.2247$ and the maximum theoretical strength reduces to

$$\tau_{\max} \approx \sqrt[3]{2} G / 2\pi \quad (C5)$$

Acknowledgment

The authors acknowledge the financial support received from the Air Force Office of Scientific Research, in particular Len Seikel, for this work.

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