Strain Rate Dependent Modeling of Polymer Matrix Composites

Robert K. Goldberg
Glenn Research Center, Cleveland, Ohio

Donald C. Stouffer
University of Cincinnati, Cincinnati, Ohio

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Robert K. Goldberg
National Aeronautics and Space Administration
Glenn Research Center
Cleveland, Ohio 44135

and

Donald C. Stouffer
University of Cincinnati
Cincinnati, Ohio 45221

Summary

A research program is in progress to develop strain rate dependent deformation and failure models for the analysis of polymer matrix composites subject to high strain rate impact loads. Strain rate dependent inelastic constitutive equations have been developed to model the polymer matrix, and have been incorporated into a micromechanics approach to analyze polymer matrix composites. The Hashin failure criterion has been implemented within the micromechanics results to predict ply failure strengths. The deformation model has been implemented within LS-DYNA, a commercially available transient dynamic finite element code. The deformation response and ply failure stresses for the representative polymer matrix composite AS4/PEEK have been predicted for a variety of fiber orientations and strain rates. The predicted results compare favorably to experimentally obtained values.

Introduction

NASA Glenn Research Center has an ongoing research program to investigate the feasibility of developing jet engine fan containment systems composed of polymer matrix composite materials. To design a composite containment system, the ability to correctly predict the deformation and failure behavior of the composite under high rate loading conditions is required. Furthermore, composites composed of relatively ductile matrix materials are more likely to be used for containment applications. As a result, an analytical model must have the capability to account for nonlinearities and rate dependence in the material response.

Previous work conducted by researchers such as Daniel, et al. (ref. 1) have determined that the material properties of a graphite fiber reinforced polymer matrix composite are strain rate dependent in matrix dominated deformation modes, and strain rate independent in fiber dominated deformation modes. These results indicate that the matrix drives any rate dependence of the composite. An example of efforts to model the rate dependent, inelastic response of polymer matrix composites is given by Weeks and Sun (ref. 2). In this work, the deformation response of the composite was modeled on the macroscopic level using a fiber orientation dependent plastic potential function.

This paper describes strain rate dependent, inelastic constitutive equations for a ductile polymer and the incorporation of these equations into a mechanics of materials based micromechanics approach. The implementation of the Hashin failure criterion into the micromechanics model is discussed, and efforts to implement the deformation model into the LS-DYNA transient dynamic finite element code are described. Verification studies for the deformation and ply strength models are presented for a representative composite system composed of AS-4 fibers in a PEEK thermoplastic matrix.

Polymer Matrix Constitutive Model

The Ramaswamy-Stouffer viscoplastic state variable model (ref. 3), which was originally developed for metals, was modified to simulate the rate dependent inelastic deformation of a ductile polymer. As discussed in (refs. 4 and 5), there are sufficient similarities between the deformation response of metals and the deformation response of ductile polymers to permit the use of equations developed for metals to analyze ductile
crystalline polymers. An important point to note is that small strain conditions are currently assumed in order to limit the complexity of the formulation.

In the modified Ramaswamy-Stouffer model, the inelastic strain rate, \( \dot{\varepsilon}_{ij}^I \), is defined as a function of the deviatoric stress, \( S_{ij} \), and back stress state variable \( \Omega_{ij} \) in the form:

\[
\dot{\varepsilon}_{ij}^I = D_o \exp \left[ -\frac{1}{2} \left( \frac{Z_o^2}{3K_2} \right)^n \right] \cdot \frac{S_{ij} - \Omega_{ij}}{\sqrt{K_2}}
\]

(1)

where \( D_o \), \( Z_o \), and \( n \) are material constants and \( K_2 \) is defined as follows:

\[
K_2 = \frac{1}{2} \left( S_{ij} - \Omega_{ij} \right) \left( S_{ij} - \Omega_{ij} \right)
\]

(2)

The elastic components of strain are added to the inelastic strain to obtain the total strain. The following relation defines the back stress variable rate:

\[
\dot{\Omega}_{ij} = \frac{2}{3} q \Omega_m \dot{e}_{ij}^I - q \Omega_{ij} \dot{e}_{ij}^E
\]

(3)

where \( q \) is a material constant, \( \Omega_m \) is a material constant that represents the maximum value of the back stress, and \( \dot{e}_{ij}^I \) is the effective inelastic strain. The material constants are determined in the manner discussed in references 3 and 5.

The hydrostatic stress state has been found to have a significant effect on the yield behavior of a polymer (refs. 4 and 6). Bordonaro (ref. 7) indicated that the proper way to account for such effects in a state variable constitutive model is to modify the effective stress terms. In this work, pressure dependence was included by multiplying the shear terms in the \( K_2 \) invariant in equation (2) by the following correction factor:

\[
\alpha = \left( \frac{\sigma_m}{\sqrt{J_2}} \right)^\beta
\]

(4)

In this term, \( \sigma_m \) is the mean stress, \( J_2 \) is the second invariant of the deviatoric stress tensor, and \( \beta \) is a rate independent material constant. Since only uniaxial data was available for the polymer under consideration in this study, the value of the parameter \( \beta \) was determined empirically by fitting data from uniaxial composites with shear dominated fiber orientation angles, such as [15°].

To correlate the equations, the PEEK thermoplastic matrix was characterized and modeled based on uniaxial tensile data found in reference 7 for strain rates ranging from \( 1 \times 10^{-6} \)/sec to \( 1 \times 10^{-3} \)/sec. While the ultimate goal of this research is to model high strain-rate (up to several hundred per second) impact problems, at the current time high strain-rate data is not available, so all of the analyses presented in this study will be at relatively low strain rates. The analysis methods described in this report can be extrapolated to high strain-rate applications once appropriate data becomes available. The elastic modulus of the material is 4000 MPa and the Poisson's ratio is 0.40. The inelastic material constants were determined to be as follows (refs. 5 and 6): \( D_o = 1 \times 10^4 \)/sec, \( n = 0.70 \), \( Z_o = 630 \) MPa, \( q = 310 \), \( \Omega_m = 52 \) MPa, \( \beta = 0.45 \). Experimental (ref. 7) and computed results for strain rates of \( 1 \times 10^{-6} \)/sec and \( 1 \times 10^{-3} \)/sec are shown in figure 1. As can be seen in the figure, there is an excellent correlation between the experimental and predicted results. Note that while the tensile data was used to obtain the material constants, the constants were not explicitly modified in order to improve the fit of the computed results to the experimental data.

**Composite Micromechanics Model**

To compute the effective properties of the composite material considered in this study, a micromechanics technique was utilized. In micromechanics, the effective properties and response of a composite material are computed based on the properties of the individual constituents. The common procedure is to analyze a unit cell of the composite, the smallest material unit for which the response can be considered as representative of
the response of the composite. For this study, the unit cell will be defined as a single fiber and its surrounding matrix. Furthermore, only unidirectional laminated composites at various fiber orientation angles will be examined.

A mechanics of materials based micromechanics method was utilized, based on an approach developed by Sun and Chen (ref. 8). In this approach, the composite unit cell is divided into four subregions (fig. 2). Assumptions of uniform stress or uniform strain are then made within the unit cell. Along the fiber direction (1 direction in fig. 2), strains in each subregion are assumed to be uniform, and the subregion stresses are combined using volume and local stiffness averaging. The transverse normal stresses (2 direction in fig. 2) and the in-plane shear stresses (1-2 direction) in subregions A_f and A_m are equal, while the equivalent strains are combined using volume averaging. The same is true for subregions B_1 and B_2. The total transverse (2 direction) and in-plane shear (1-2 direction) strains in Row 1 and Row 2 (fig. 2) are assumed to be equal, and the equivalent stresses are combined using volume averaging. These assumptions, when combined with the constitutive equations for the fiber and matrix, can then be used to set up systems of equations that can be solved for the stresses in each subregion. The subregion stresses are then used in the polymer constitutive equations to compute the inelastic strain rates in the matrix subregions. More details and the full equations can be found in reference 9.

To verify the micromechanics equations, a composite composed of AS-4 carbon fibers embedded in a PEEK matrix was analyzed. The fiber volume fraction is 0.62, the longitudinal elastic modulus of the fiber is 214 GPa, the transverse and in-plane shear moduli of the fiber are 14 GPa, and the longitudinal Poisson's ratio is 0.2. The matrix properties are as defined above. In figure 3, the experimental (ref. 2) and predicted results for a [30°] unidirectional laminate are shown for strain rates of 1x10^-2/sec and 0.1/sec. As can be seen in the figure, for both strain rates the micromechanics model predicts the rate dependence and nonlinearity of the composite response reasonably well. Note that there is some discrepancy between the experimental and computed results in the elastic range. As this discrepancy was not seen for [0°] or [90°] laminates, these results indicate that the shear moduli or transverse Poisson’s ratio used for the fiber may not be correct.

### Ply Strength Predictions

A variety of failure criteria exist to predict the ply level ultimate strength in polymer matrix composites. Several “classic” criteria are in use, which are often discussed in composite texts (e.g. (ref. 10)). Simple criteria such as Maximum Stress or Maximum Strain simply compare macroscopic (ply level) stresses (or strains) in each coordinate direction to maximum values. More sophisticated criteria, such as Tsai-Hill and Tsai-Wu, utilize quadratic (and tensor in the case of Tsai-Wu) combinations of the stresses to account for stress interaction. However, none of these criteria account for specific local failure mechanisms.

Hashin (ref. 11) developed failure criteria that utilize quadratic combinations of the macroscopic stresses to approximate local failure mechanisms, such as fiber failure or matrix cracking. One advantage of utilizing this type of failure criteria is that by identifying specific local failure mechanisms, eventually property degradation models can be developed which allow for reductions in specific material properties and stresses as loading takes place. For this work, the Hashin failure criteria were utilized. Even though constituent level stresses are computed in the micromechanics, ply level strength data were more readily available and considered to be more reliable than constituent level strength data. Since only in-plane loads were considered in this study and the out-of-plane stresses were reasonably small, the plane stress versions of the criteria were employed. However, in the future study of impact problems, where out-of-plane stresses will be significant, the full three-dimensional version of the failure criteria will be used. Since only tensile loads were significant, only the tensile fiber failure and tensile matrix failure criteria will be presented here. For the purposes of this study, once either of the failure criteria was violated, property degradation was neglected, and total composite failure was considered to have occurred.

Failure criteria for each of the failure modes are as follows. In each of the expressions, \( \sigma_{ij} \) is the stress component, \( X_T \) is the ply tensile strength in the longitudinal (fiber) direction, \( Y_T \) is the tensile strength in the transverse direction, and \( X_S \) is the ply shear strength. Failure is considered to occur when the value of the expression becomes greater than or equal to one (1). The stresses and strengths are assumed to be in the local material axis system, so the stresses must be transformed from the structural axis system to the material axis system for off-axis composites. Tensile fiber failure is predicted by using the following expression:

\[
\sigma_{ij} \leq X_T
\]
Tensile matrix failure is predicted using the following expression:

\[
\left(\frac{\sigma_{11}}{X_T}\right)^2 + \left(\frac{\sigma_{12}}{X_S}\right)^2 = 1
\]  (5)

For the AS4/PEEK material, the longitudinal tensile strength was set to 2070 MPa, and the transverse tensile strength was set to 83 MPa (ref. 12). These values were determined to be strain rate independent for this material. The longitudinal tensile strength of carbon fiber reinforced composites has been found to be rate independent by a variety of researchers (e.g., (ref. 1)). For this material, the transverse modulus was found to be rate independent (ref. 2), leading to the assumption that the transverse tensile strength was most likely also rate independent. The in-plane shear strength was considered to be rate dependent, and was correlated based on data from [15°] off-axis laminates found in (ref. 2). This orientation was chosen since it is a shear dominated fiber orientation angle. From this data, the shear strength for a strain rate of 1\(\times\)10^{-5}/sec was determined to be 63 MPa, and the shear strength for a strain rate of 0.1/sec was determined to be 88 MPa. The strength values and the experimental values for the failure stresses shown below likely have some scatter, but the statistical data was not available.

Using the given strength values, failure stresses were predicted for [30°] and [45°] laminates for both strain rates. The predicted and experimental (ref. 2) results for a strain rate of 1\(\times\)10^{-5}/sec are shown in table I, and the results for a strain rate of 0.1/sec are shown in table II. In all cases, failure was predicted to be due to tensile matrix failure.

For both strain rates and fiber orientations considered, the comparison between the predicted and experimental values is quite good. In particular, the predicted results most likely fall within the scatter of the experimental data. The results indicate that the failure criteria are able to predict ply failure for a variety of fiber orientations and strain rates. The results for this material also indicate that even when some approximations are required in determining the ply failure stresses, reasonable results can still be obtained.

**Finite Element Implementation**

In order to simulate the impact response of a composite structure, finite element methods are required. With that goal in mind, the matrix constitutive equations and micromechanics model described above have been implemented into LS-DYNA (ref. 13), a commercially available transient dynamic finite element code. The implementation was accomplished through the use of the user defined subroutine option. LS-DYNA uses explicit central difference integration methods to integrate the rate equations. In the user defined material subroutine, strain increments are passed into the routine, and the total stresses at the end of the time increment must be computed.

Rocca and Sherwood (ref. 14) implemented a version of the Ramaswamy-Stouffer state variable equations into LS-DYNA for analysis of polycarbonate. Following their formulation, equations (1) to (4) were converted into an incremental form. The back stress rate equation (eq. (3)) was modified as follows:

\[
\Delta \Omega_{ij} = \frac{2}{3} q \Omega_{ij} \Delta \epsilon_{ij}^l - q \Omega_{ij} \Delta \epsilon_c^l
\]  (7)

where the variables are as defined earlier and the \(\Delta\) symbol before a term indicates an increment of the variable. The back stress term \(\Omega_{ij}\) is the total value of the back stress at the end of the previous time increment. The increment in inelastic strain \(\Delta \epsilon_{ij}^l\) is computed for the current time increment by taking the inelastic strain rate computed in the previous time increment (eq. (1)) and multiplying it by the value of the current time increment, which is a forward Euler type of approximation (ref. 15). The new value of the back stress for the current time increment is computed by adding the back stress increment to the previous value of the back stress. The stress and deviatoric stress increments are computed using the strain increments and the inelastic strain increments. The stress increments are then added to the total stresses from the previous time step to determine the new values of the total stresses. The inelastic strain rate for the current time step is then computed using equation (1).
To test the implementation of the matrix constitutive equations, the tensile response of the PEEK material was computed using a finite element analysis at a strain rate of 1.0/sec. The results were compared to those computed using the stand-alone computer code that was used to generate the results shown in figure 1. Note, however, that the stresses at a strain rate of 1.0/sec are higher than those shown in figure 1. Four noded shell elements were used in a square mesh, ten elements on a side. One side of the model was clamped, and the other side had an enforced displacement to simulate a strain controlled load application. The finite element model was designed to simulate the behavior of the polymer at an infinitesimal material point. A mesh convergence study showed that this mesh was adequate.

The analytical and finite element results are shown in figure 4. As can be seen in the figure, the finite element results compare reasonably well to those computed using the stand alone computer code. The discrepancy between the finite element and analytical results is most likely due to the nature of the integrator used on the rate equations. A fourth order Runge-Kutta integrator (ref. 15) was used in the stand alone computer code used to compute the analytical results. As mentioned earlier, a central difference explicit integrator is used within LS-DYNA. Furthermore, forward Euler types of approximations were used in converting the rate equations into an incremental form. The forward Euler method is less accurate than the Runge-Kutta method (ref. 15). Since the matrix constitutive equations are stiff differential equations (ref. 3), the nature of the integrator used can significantly affect the results. Future efforts may concentrate on improving the nature of the integration used within the user defined material subroutine. Currently, efforts are also underway to combine the matrix constitutive equations with the micromechanics method described above to be able to compute the rate-dependent nonlinear response of polymer matrix composites using the LS-DYNA finite element code.

Conclusions

In this study, rate-dependent inelastic constitutive equations have been developed to simulate the deformation response of ductile polymers. The constitutive equations were implemented within a mechanics of materials based micromechanics technique. The Hashin failure criteria were utilized to predict the ply ultimate strengths. Preliminary efforts to implement the deformation model into the LS-DYNA finite element code were also discussed. Predictions made using the analytical model for an AS4/PEEK composite system compared well to experimental values.

Future efforts will include completing the implementation of the deformation model into the LS-DYNA finite element code. Furthermore, full implementation of failure and strength models (including property degradation) into LS-DYNA will be completed. High strain rate experiments will be conducted on a representative polymer matrix composite, and the deformation model will be characterized and validated for high strain rate conditions. Furthermore, the deformation model will be extended into the large deformation regime, and the developed techniques will be extended to the analysis of woven composites.

References


| TABLE I.—FAILURE STRESS PREDICTIONS FOR AS4/PEEK: STRAIN RATE = 1 x 10^-5/sec |
|---------------------------------------------|-----------------|
| Predicted failure stress, MPa | Experimental failure stress, MPa |
| [30°] Laminate | 130 | 140 |
| [45°] Laminate | 98 | 104 |

| TABLE II.—FAILURE STRESS PREDICTIONS FOR AS4/PEEK: STRAIN RATE = 0.1/sec |
|---------------------------------------------|-----------------|
| Predicted failure stress, MPa | Experimental failure stress, MPa |
| [30°] Laminate | 165 | 170 |
| [45°] Laminate | 114 | 112 |
Figure 1: Model Correlations of PEEK Thermoplastic at Strain Rates of $1\times10^{-6}$/sec (1E-06) and $1\times10^{-3}$/sec (1E-03).

Figure 2: Geometry and Layout of Unit Cell Model.

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<td>(1-$\sqrt{k_f}$)</td>
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<td>$\sqrt{k_f}$</td>
<td>Af</td>
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<td>sqrt($k_f$)</td>
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$k_f$=Fiber Volume Fraction
Af=Fiber Subregion
Am,B1,B2=Matrix Subregions
Figure 3: Model Predictions for AS4/PEEK [30°] Laminate at Strain Rates of $1 \times 10^{-5}$/sec (1E-05) and 0.1 sec.

Figure 4: Comparison of Predictions by Stand-Alone Computer Code (Analytical) and LS-DYNA Finite Element Analysis (FEM) for PEEK Thermoplastic at Strain Rate of 1.0/sec.
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Robert K. Goldberg and Donald C. Stouffer

National Aeronautics and Space Administration
John H. Glenn Research Center at Lewis Field
Cleveland, Ohio 44135-3191

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