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An Experimental-Computational Framework for UHMWPE Films Based on Deformation and Failure Mechanisms: General Approach and Application to Off-Axis Shear Loading

**by Stephen L Alexander, Richard Becker, and
Tusit Weerasooriya**

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An Experimental-Computational Framework for UHMWPE Films Based on Deformation and Failure Mechanisms: General Approach and Application to Off-Axis Shear Loading

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14. ABSTRACT Finite element simulation of ultra-high-molecular-weight polyethylene (UHMWPE) composites loaded under Army-relevant conditions remains a challenge. The problem is confounded when attempting to predict the response of novel film-based UHMWPE materials, for which there is a lack of data and fundamental understanding relative to traditional fiber-based systems that have been experimentally characterized extensively. Here, a computational framework for simulating the multiaxial and multirate response of UHMWPE films was developed at the subscale of individual UHMWPE layers. The concept was physics-based, directly modeling the governing deformation and failure mechanisms of the films. Plastic deformation of the layers was described with a crystal plasticity approach based on film mesostructure. Failure by delamination between layers was represented with Mode 2 traction-separation relationships dependent on loading rates. Parameter values for UHMWPE films were determined by simulating a unique set of off-axis shear loading experiments on film-based composites across loading rates from quasi-static to dynamic. As far we know, this is the first time that cohesive laws have been obtained and implemented based on actual experiments at multiple strain rates. In addition, the utility of the present subscale approach was demonstrated by transitioning to a higher-length-scale material model previously developed for fiber-based composites.										
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The authors also acknowledge Dr Alan Goertz for helping us with using LS-DYNA. We had been using other finite element software for many years prior to this present research. However, we encountered limitations in the other software and found ourselves needing to use LS-DYNA, with which we were completely unfamiliar. Dr Goertz generously spent a significant amount of time helping us transition, first by guiding us through setting up, debugging, and analyzing several example simulations in LS-DYNA, and then subsequently being available over the course of several months for the many additional software-related questions and issues we had.

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1. Introduction

1.1 Background on UHMWPE Composites and Finite Element Simulations

Ultra-high-molecular-weight polyethylene (UHMWPE) composites are a multiscale hierarchical material. They are formed by cross-stacking layers and then consolidating this stack under pressure and temperature. The layers have traditionally consisted of stiff UHMWPE fibers embedded in a softer matrix. The long axis of the fibers is oriented in a preferred direction within the layer, and therefore the layers are described as unidirectional (UD). A well-known example of these fiber-based UHMWPE composites are the Dyneema series from DSM Protective Materials (Heerleen, Netherlands). As an example, their HB212 material consists of SK99 fibers embedded in a softer rubber matrix (O'Masta et al. 2016).

Recently, UD layers have also been made without fibers. These novel materials, also called films, are formed through solid-state extrusion, which preferentially orients the UHMPWE within the layer analogously to the fibers. Examples of film-based UHMWPE composites are Tensylon from DuPont (Delaware, USA) and Endumax from Teijin (Arnhem, Netherlands).

Finite element (FE) simulation of UHMWPE composites remains a challenge. Previous authors (e.g., Liu et al. 2019) have divided the existing body of FE models of UHMWPE composites based on length scale. Subscale simulations explicitly model each UD layer, assigning appropriate material properties to each layer. Composite-scale simulations model the bulk response rather than each layer and use effective material properties that have already been homogenized over several UD layers.

One example of a composite-scale UHMWPE model is a US Army Combat Capabilities Development Command Army Research Laboratory model documented by Becker (2019). Each element in the model represented several UD layers and is therefore referred to here as elemental macroscale (EMS). The EMS model accounted for interlaminar slip between UD layers by additively decomposing the velocity gradient into an elastic component, an inelastic component due to general plasticity, and an inelastic component due to slip. Slip was assumed to occur along a single slip system. The slip plane was defined by the plane spanned by the UHMWPE fibers, and the slip direction was the direction of maximum shear traction. Stress was calculated as the summation of contributions from the matrix and the fibers, where the matrix was modeled as isotropic.

The approximations in composite-scale models inherent by only modeling the bulk response limit the ability of these models, in general, to explain deformation mechanisms. On the other hand, subscale models enable additional mechanisms to be incorporated. Recently, Liu et al. (2019) have developed subscale FE simulations of fiber-based UHMWPE composites that model each individual UD layer with a crystal plasticity framework. Plastic deformation of the UD layer was dictated by shearing of the matrix, which was restricted to a discrete set of slip systems defined by the topology of the stiff UHMWPE fibers. Their approach based on physical mechanisms successfully enabled investigation of the interplay between material properties and performance. For example, they mapped the interplay between the tensile strength of the UD layer, the shear strength of the composite, and the critical impact velocity below which the fibers in the composite were predicted to remain intact.

Varun Raj et al. (2022) later applied the concept that Liu et al. had originally developed for fiber-based composites to the newer film-based composites only by reducing the number of active slip systems. They modeled film-based composites with the same material properties that Liu et al. had used for fiber-based composites. Thus, the later study was a computational investigation into the effect of only changing the morphology. It did not attempt to identify material properties for film-based UHMWPE layers and did not compare numerical predictions with any film-based experiments.

An additional limitation of the implementation followed by Liu et al. (2019) was that the integration scheme for the material model was fully explicit. Fully explicit integration schemes generally require small timesteps for accurate solutions (Oliver et al. 2008; Roters et al. 2010). Indeed, Liu et al. used a very small timestep of only 0.01 ns for simulating the impact of UHMWPE composites by blunt projectiles.

1.2 Goal and Overview of Present Study

Our goal was to provide a mechanism-based computational framework for FE simulation of film-based UHMWPE composites, such as Tensylon, under multiaxial loading conditions and valid across loading rates from quasi-static to dynamic. The UHMWPE material model was developed at the sub-mesoscale (SMS), with the motivation that direct representation of physical deformation and failure mechanisms would improve predictive capability.

Simulation parameters were determined for the film-based composites by iteratively simulating a unique set of experiments performed on Tensylon. These experiments were specifically designed to characterize the interply shear response as a function of normal stress (Gunnarsson et al. 2023). Simulation parameters were

optimized by comparing load-displacement response between numerical predictions using the SMS model and the off-axis loaded shear experiments. The applicability of the SMS computational framework to larger-scale simulations was then demonstrated by transitioning the SMS-optimized parameters to the EMS model.

Here, the off-axis loaded shear experiments are briefly overviewed first. Then, the corresponding FE simulations are presented with details of the SMS material model. Next are presented the set of FE parameters that were optimized using the SMS model, and the simulated response using this SMS-optimized set is compared to the experiments. Finally, the transition of these SMS-optimized parameters to the larger-scale EMS is described.

2. Off-Axis Loaded Shear Experiments

Details on the off-axis loaded shear experiments will be provided elsewhere (Gunnarsson et al. 2023). Only a brief overview will be provided here, sufficient to explain the simulations. The UHMWPE investigated in this study was Tensylon HSBD-30A commercially available from DuPont (Delaware, USA) and referred to hereafter as “Tensylon.” This Tensylon material was sold as a precursor sheet wound into a roll. The precursor sheet consisted of two preconsolidated layers. Each of these layers was referred to as UD because the UHMWPE was extruded into a single direction within the layer. Thus, the UD layer had a preferential alignment and was transversely isotropic. Photographs of the UD layer showing this preferential alignment can be found in a previous publication, ARL-TR-9430 (Gunnarsson et al. 2022). The two UD layers were preconsolidated in orthogonal directions, $0^\circ/90^\circ$, in the manufacturer-supplied precursor sheet.

A panel of $[0^\circ/90^\circ]_n$ Tensylon was consolidated by stacking a sufficient number of precursor sheets to fill a custom-built mold. The thickness of each UD layer after consolidation was calculated as $57\text{ }\mu\text{m}$ by dividing the thickness of the panel by the number of stacked UD layers. For the larger experimental program (Gunnarsson et al. 2023), the off-axis loaded shear specimens were extracted from the panel using a water-jet cutter at various angles. The current study focused on the specimens extracted at 15° as shown in Fig. 1.

The specimens were compressed in the z-direction such that the compression direction formed a 15° angle with the plane of each UD ply (Fig. 1). The interface between the loading platens and the specimen was lubricated to minimize friction. Experiments were at three different loading rates: low rate (LR), intermediate rate (IR), and high rate (HR). The current study simulated one specimen at each rate, a

total of three specimens.* Table 1 lists the dimensions of these three specimens, together with the experimental loading rates. LR and IR experiments were conducted on a servo-hydraulic Instron test frame. The HR experiment was conducted using a split-Hopkinson pressure bar (SHPB). Figure 2 plots the loading response for all three experiments.

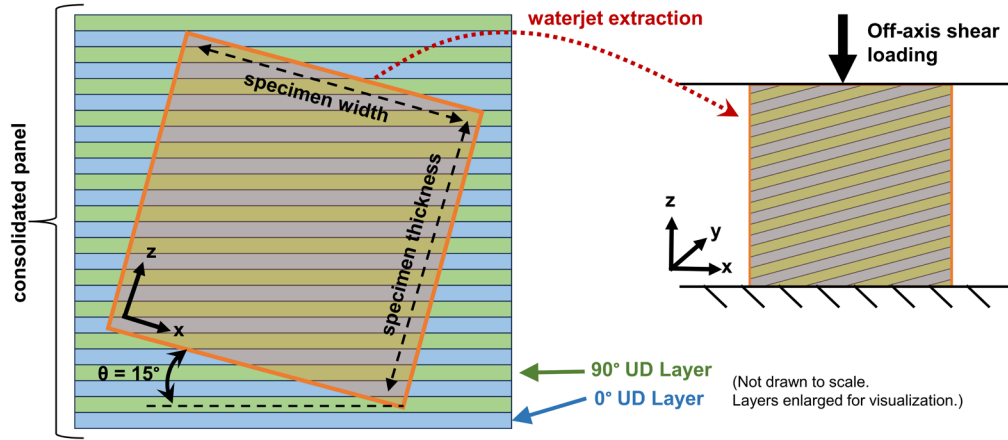


Fig. 1 Representation of an off-axis loaded shear specimen, illustrating relative position within the consolidated panel prior to extraction (left) and loading direction after extraction (right)

Table 1 Tensylon specimens for off-axis loaded shear experiments: dimensions and loading rates

Loading rate	Thickness in z-direction (mm)	Width in x-direction (mm)	Length in y-direction (mm)	Experimental loading rate (m/s)	Experimental strain rate (1/s)
LR	8.92	10.16	10.23	5×10^{-6}	5×10^{-4}
IR	9.985	10.405	10.30	5×10^{-3}	5×10^{-1}
HR	10.33	10.13	10.25	9.785	947

Note: Figure 1 shows x-y-z coordinate system.

* The LR, IR, and HR specimens simulated here are referred to in the experimental documentation (Gunnarsson et al. 2023) as TEN-15DEG-C01, TEN-15DEG-C02, and TEN-15DEG-C04, respectively.

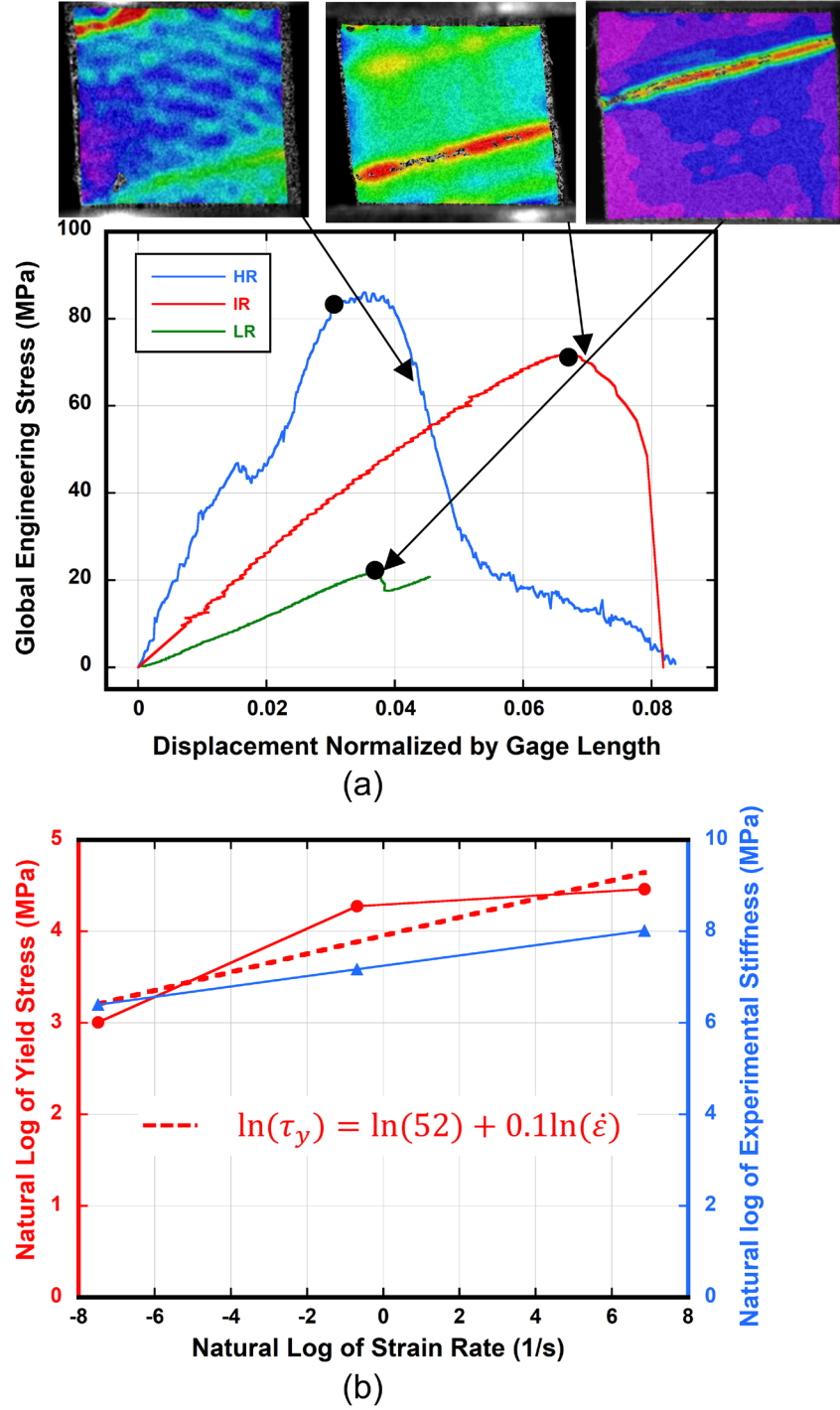


Fig. 2 Experimental response as a function of rate. (a) Normalized load-displacement with maximum shear strain contours at failure initiation provided for each rate. (Details on experimental methods, including how load and shear strain was measured at each rate, will be provided elsewhere [Gunnarsson et al. 2023].) (b) Experimental yield stress and stiffness as a function of loading rate. Linear regression of yield stress is shown as a dashed line with corresponding equation. The approximate yield stress was estimated at a point where the curve deviated substantially from the elastic response, and it is indicated by the black circles in (a).

3. Finite Element Simulations

Explicit FE simulations were executed for each off-axis loaded shear specimen (Table 1) with a developmental version of the commercial code LS-DYNA (Ansys, Inc.) running on DoD High Performance Computing machines. All initial FE mesh geometry, boundary conditions, and material properties were specified in the LS-DYNA input file, known as a keyword file, or k-file.

This section first describes the SMS material model. It next details the FE meshes and boundary conditions. Finally, the method of simulating delamination between UD layers using tiebreak contacts is presented. Parameters in the SMS material model and tiebreak contacts are presented in this section as variables, without values. Parameter value identification is presented in Section 4. Material density for all loading rates was taken from previous Tensylon composite measurements as 927 kg/m^3 (Alexander and Weerasooriya 2021).

3.1 SMS Material Model

3.1.1 Notation

Bold uppercase letters are tensors, and the identity is given by $\mathbf{I}$. Bold lowercase letters represent vectors. Quantities that are not bold are scalars. A bullet between two second-order tensors (e.g., $\mathbf{A} \cdot \mathbf{B}$) indicates the product of the two tensors, and a colon indicates a product of a fourth-order tensor with a second-order tensor (e.g., $\mathcal{L} : \mathbf{C}$) or the contraction of two second-order tensors.

3.1.2 Model Overview

The material model was implemented in LS-DYNA via the custom-written user-defined material subroutine, referred to as the “LS-DYNA umat.” In the user-defined subroutine, for each time increment in the simulation, the FE solver passed to the LS-DYNA umat the incremental strains for each integration point together with additional information regarding the state of the simulation at the end of the previous step. The current time increment, Δt , spanned from the end of the previous step, t_1 , until the end of the current step, t_2 , such that $t_2 = t_1 + \Delta t$. Two key pieces of information provided by LS-DYNA were the size of Δt and the total deformation gradient at the end of the increment, $\mathbf{F}^{t_2}$. The LS-DYNA umat then calculated the Cauchy stress for t_2 , $\boldsymbol{\sigma}^{t_2}$, and the history-dependent state variables for each integration point and passed these back to FE solver.

The SMS material model was at the length-scale of the UD layer (meso) such that each UD layer was assumed to consist of one or more elements. Therefore, all material within an element belonged to a single UD layer. The UD layer was

modeled as transversely isotropic elastic with crystal plasticity slip occurring along designated slip planes. Modeling each UD layer as transversely isotropic required the SMS material model to have more elastic constants than the EMS model. The total deformation gradient, $\mathbf{F}$, was multiplicatively decomposed into an elastic component, $\mathbf{F}_e$, and plastic component, $\mathbf{F}_p$:

$$\mathbf{F} = \mathbf{F}_e \cdot \mathbf{F}_p. \quad (1)$$

The plastic part accommodates inelastic slip and the elastic part accounts for reversible stretching and distortion. The constitutive model is formulated in the intermediate configuration. The elastic deformation and the work conjugate second Piola–Kirchhoff stress, $\mathbf{\Sigma}$, are referenced to this intermediate configuration. This stress is then mapped to the Cauchy stress in the current configuration, $\boldsymbol{\sigma}$.

The integration of the SMS material model was semi-implicit: $\mathbf{\Sigma}$ at the end of the increment was determined implicitly through convergence of a Newton iteration scheme using the fiber state from the beginning of the time step. The material state was then updated explicitly after the stress iteration with no further checks on stress convergence. The semi-implicit integration was developed by adapting the fully implicit crystal plasticity framework set forth by Weerasooriya (1991) and by Kalidindi et al. (1992).

This section overviews the model in a form following the procedural flow of the LS-DYNA umat, as summarized in Fig. 3. A more detailed presentation is provided in Appendix A.

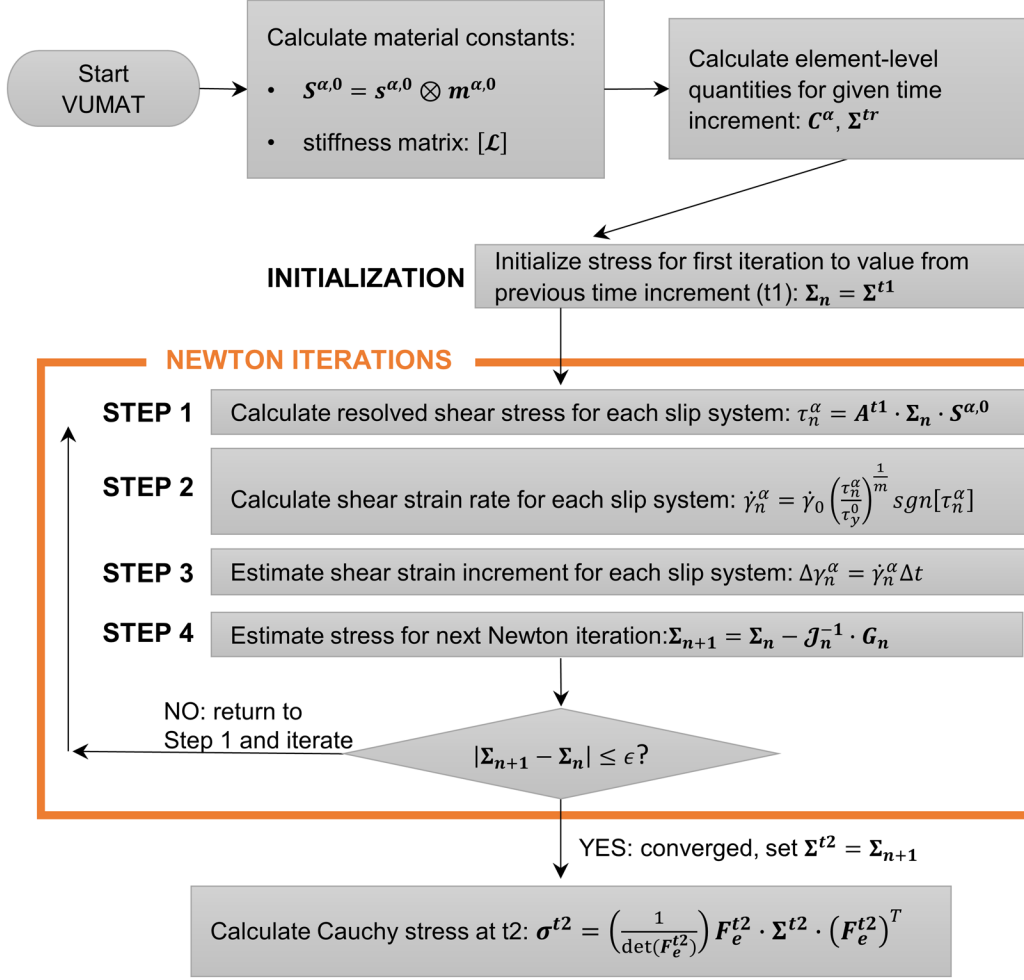


Fig. 3 Overview of procedural flowchart in the LS-DYNA umat for SMS model of UHMWPE composites

3.1.3 Material Constants

The LS-DYNA umat started by calculating material constants that were invariant with time and applicable to all elements within a UD layer. These constants defined the slip systems and the stiffness matrix, as described here.

In the SMS model, plastic deformation of the UD Tensylon layer was assumed to occur along four different slip systems. Figure 4 illustrates the four assumed slip systems. In Fig. 4, the dominant direction (extrusion direction) of the UD layer was defined as X1, the plane of the UD layer was in the X1 and X2 directions, and the X3 direction represented the stacking direction. An ideal film-based UD layer would have strength in the X1 and X2 directions. Inelastic slip would only occur in the plane normal to X3, accommodating only slip modes #2 and #3 from Fig. 4. However, prior work by Gunnarsson et al. (2022), see Fig. 5, has demonstrated that a UD layer of Tensylon has low coherence in the transverse direction. Considering

this data, it is further assumed that inelastic shear deformation can occur in the plane normal to X2, allowing slip modes #1 and #4.

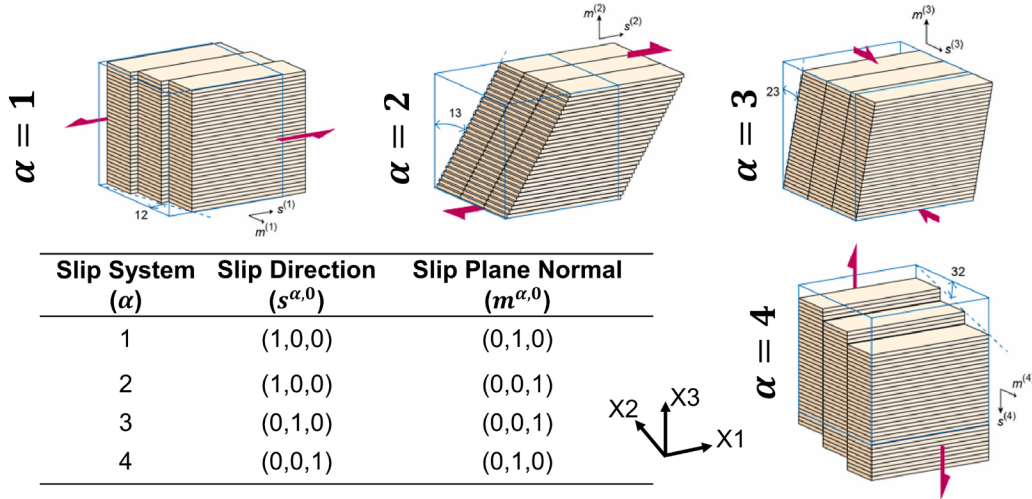


Fig. 4 Illustration of the four slip systems assumed for a Tensylon UD layer (adapted from Varun Raj et al. 2022). Inset chart denotes the direction cosines for the slip direction and slip normal for each slip system.

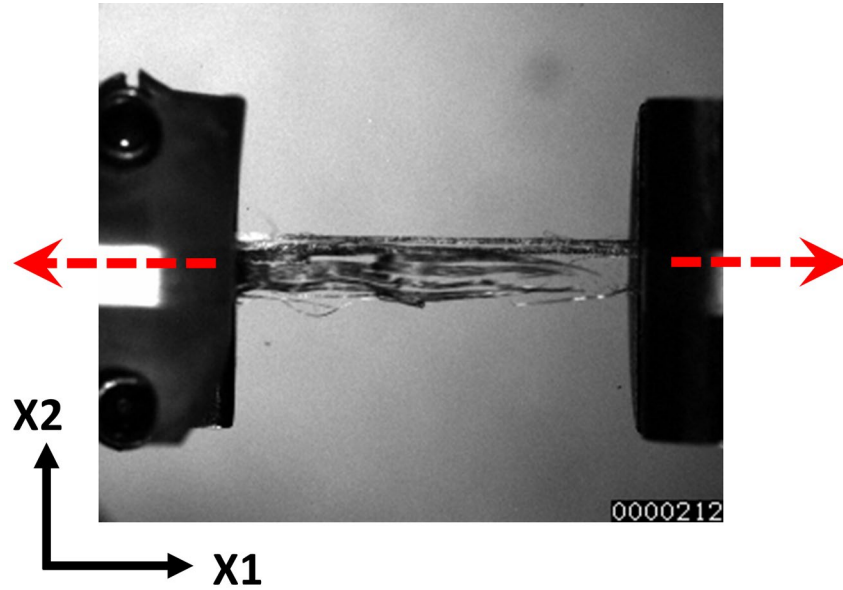


Fig. 5 High-rate tensile loading of a single UD layer of Tensylon showing lack of strength in the orthogonal direction, from the experiments and report of Gunnarsson et al. (2022). Tension was applied along the dominant direction of the UD layer (X1), indicated by the red dashed arrows. The specimen exhibits severe delamination orthogonal to the tensile axis (X2).

Slip systems were referred to by the superscript α . The original configuration at the start of the simulation prior to any deformation was referred to by the superscript 0. The original configuration of each slip system was defined by two orthogonal

unit vectors: the direction of slip, $\mathbf{s}^{\alpha,0}$, and the normal to the plane of the slip, $\mathbf{m}^{\alpha,0}$. The dyadic product of these two vectors was calculated as the tensor $\mathbf{S}^{\alpha,0}$:

$$\mathbf{S}^{\alpha,0} = \mathbf{s}^{\alpha,0} \otimes \mathbf{m}^{\alpha,0}. \quad (2)$$

The stiffness matrix, $\mathcal{L}$, is also commonly referred to as the elasticity tensor. The stiffness matrix was calculated by assuming that the UD layers were transversely isotropic, having a preferred orientation in the direction of UHMWPE extrusion within the film. The preferred orientation was denoted by f . The two transverse directions that were orthogonal to f were denoted as t , and the plane spanned by these two transverse directions was assumed to be isotropic. The reader is referred to previous documentation for further explanation of different classes of material symmetries and their related stiffness and compliance matrices (Alexander and Weerasooriya 2021). As detailed previously, the assumption of transverse isotropy limited the number of independent engineering constants to five denoted here as the Young's modulus in the principal direction of the UD layer (E_f), the Young's modulus in the plane transverse to the principal direction (E_t), the shear modulus in the plane of the UD layer (G_{ft}), and the Poisson's ratios ν_{ft} and ν_{tt} . The stiffness matrices of the 0° and 90° UD layers in the undistorted lattice configuration were calculated from the engineering constants as:

$$[\mathcal{L}] = \begin{bmatrix} \frac{1}{E_f} & -\frac{\nu_{ft}}{E_f} & -\frac{\nu_{ft}}{E_f} & 0 & 0 & 0 \\ -\frac{\nu_{ft}}{E_f} & \frac{1}{E_t} & -\frac{\nu_{tt}}{E_t} & 0 & 0 & 0 \\ -\frac{\nu_{ft}}{E_f} & -\frac{\nu_{tt}}{E_t} & \frac{1}{E_t} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{2(1+\nu_{tt})}{E_t} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{G_{ft}} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{G_{ft}} \end{bmatrix}^{-1} \quad \text{for } 0^\circ \text{ UD Layer} \quad (3)$$

$$[\mathcal{L}] = \begin{bmatrix} \frac{1}{E_t} & -\frac{\nu_{ft}}{E_f} & -\frac{\nu_{tt}}{E_t} & 0 & 0 & 0 \\ -\frac{\nu_{ft}}{E_f} & \frac{1}{E_f} & -\frac{\nu_{ft}}{E_f} & 0 & 0 & 0 \\ -\frac{\nu_{tt}}{E_t} & -\frac{\nu_{ft}}{E_f} & \frac{1}{E_t} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{G_{ft}} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{2(1+\nu_{tt})}{E_t} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{G_{ft}} \end{bmatrix}^{-1} \quad \text{for } 90^\circ \text{ UD Layer} \quad (4)$$

3.1.4 Element-Level Quantities that Remained Constant During Newton Iterations

Next, the LS-DYNA umat calculated quantities that changed from timestep to timestep but were not updated during the Newton iterations that took place within each timestep. These quantities were independently calculated for each element.

The quantity $\mathbf{C}^\alpha$ was calculated for each slip system, α , as

$$\mathbf{C}^\alpha = \mathcal{L} : \frac{\mathbf{B}^\alpha}{2}, \quad (5)$$

where

$$\mathbf{B}^\alpha = \mathbf{A}^{t1} \cdot \mathbf{S}^{\alpha,0} + (\mathbf{S}^{\alpha,0})^T \cdot \mathbf{A}^{t1} \quad (6)$$

and

$$\mathbf{A}^{t1} = (\mathbf{F}_e^{t1})^T \cdot \mathbf{F}_e^{t1}. \quad (7)$$

In Eq. 7, $\mathbf{A}^{t1}$ represented the right Cauchy–Green stretch of the lattice based in the configuration of the undeformed lattice.

In addition, a trial second Piola–Kirchhoff stress, $\boldsymbol{\Sigma}^{tr}$, was calculated for the element. The trial stress assumed that there was no additional plasticity during the current timestep. Therefore, the trial stress was calculated using the plastic component of the deformation gradient at the start of the current increment, $\mathbf{F}_p^{t1}$, as further described in Appendix A. From Eq. A-6:

$$\boldsymbol{\Sigma}^{tr} = \mathcal{L} : \frac{\mathbf{A}^* - \mathbf{I}}{2}, \quad (8)$$

where

$$\mathbf{A}^* = (\mathbf{F}_e^*)^T \cdot \mathbf{F}_e^* \quad (9)$$

given that

$$\mathbf{F}_e^* = \mathbf{F}^{t2} \cdot \mathbf{F}_p^{t1^{-1}}. \quad (10)$$

3.1.5 Implicit Stress Calculation

The LS-DYNA umat then entered the Newton iteration loop to implicitly calculate the second Piola–Kirchhoff stress at the end of the increment, $\boldsymbol{\Sigma}^{t2}$. The current Newton iteration was referred to by subscript n . The first step in the loop calculated the resolved shear stress, τ , for each slip system:

$$\tau_n^\alpha = \mathbf{A}^{t1} \cdot \boldsymbol{\Sigma}_n \cdot \mathbf{S}^{\alpha,0}. \quad (11)$$

For the first Newton iteration ($n = 1$), $\boldsymbol{\Sigma}_n$ was set to the value of the second Piola–Kirchhoff stress at $t1$:

$$\boldsymbol{\Sigma}_{n=1} = \boldsymbol{\Sigma}^{t1}. \quad (12)$$

The second step in the loop calculated the shear strain rate for each slip system:

$$\dot{\gamma}_n^\alpha = \dot{\gamma}_0 \left(\frac{\tau_n^\alpha}{\tau_y^0} \right)^{\frac{1}{m}} \text{sgn}[\tau_n^\alpha], \quad (13)$$

where $\dot{\gamma}_0$ was the reference shear strain rate, m was the rate sensitivity exponent, and τ_y^0 was the shear yield strength of the lamina. These three parameters were material constants specified in the k-file. The value of τ_y^0 was assumed constant during the deformation. This is equivalent to assuming no strain hardening occurs in the slip systems and there is no latent hardening among the slip systems. The same value of τ_y^0 was applied to all slip systems, assuming that the critical resolved shear stress was the same for each system. In addition, the calculation of the resolved shear stress was pressure independent. In their crystal plasticity framework for modeling UHMWPE, Liu et al. (2019) and later Varun Raj et al. (2022) have modified the resolved shear stress by including a pressure term. Future upgrades to the SMS model have been planned to add pressure dependency and strain hardening once those behaviors have been adequately characterized experimentally and to also include strain hardening.

We assume there is very little temperature rise in the whole specimen. Therefore, the model is formulated as isothermal. Plastic work is small until it localizes (see the stress–strain response in Fig. 2) into a band, and the overall temperature rise is assumed not to be consequential. However, the temperature rise within a well-formed band could influence the load.

The third step calculated the shear strain increment for each slip system:

$$\Delta\gamma_n^\alpha = \dot{\gamma}_n^\alpha \Delta t. \quad (14)$$

The fourth step calculated the stress estimate for the next Newton iteration, $\boldsymbol{\Sigma}_{n+1}$. The calculation of $\boldsymbol{\Sigma}_{n+1}$ is derived in Appendix A (Eqs. A-13 through A-16) and is summarized as

$$\boldsymbol{\Sigma}_{n+1} = \boldsymbol{\Sigma}_n - (\mathbf{J}_n)^{-1} : \mathbf{G}_n, \quad (15)$$

where the fourth-order tensor $\mathbf{J}_n$ was given by

$$\mathbf{J}_n = \mathbf{I} + \sum_{\alpha} \frac{\Delta \gamma_n^{\alpha}}{m \tau_n^{\alpha}} \mathbf{C}^{\alpha} \mathbf{S}^{\alpha,0} \quad (16)$$

and the iteration residual was

$$\mathbf{G}_n = \mathbf{\Sigma}_n - (\mathbf{\Sigma}^{tr} - \sum_{\alpha} \Delta \gamma_n^{\alpha} \mathbf{C}^{\alpha}). \quad (17)$$

The last step of the loop tested the convergence of stress:

$$|\mathbf{\Sigma}_{n+1} - \mathbf{\Sigma}_n| \leq \epsilon, \quad (18)$$

where ϵ was a small number taken to be 1×10^{-6} . If Eq. 18 was not satisfied, the code iterated to the first step (Eq. 11), where $\mathbf{\Sigma}_n$ for the new iteration was now set as $\mathbf{\Sigma}_{n+1}$ from the previous iteration. Once Eq. 18 was satisfied, $\mathbf{\Sigma}_{n+1}$ was accepted as the value of the stress at $t2$ and the code exited the loop.

3.1.6 After Stress Convergence

After convergence for $\mathbf{\Sigma}^{t2}$, the approximate inverse of the plastic deformation gradient at $t2$ was calculated as

$$(\mathbf{F}_p^{t2})^{-1} = (\mathbf{F}_p^{t1})^{-1} \cdot (\mathbf{I} - \sum_{\alpha} \Delta \gamma_n^{\alpha} \mathbf{S}^{\alpha,0}), \quad (19)$$

where $\Delta \gamma_n^{\alpha}$ was the shear strain increment for each slip system calculated in Eq. 14 during the last Newton iteration prior to convergence. Then the elastic deformation gradient at $t2$ was calculated as

$$\mathbf{F}_e^{t2} = \mathbf{F}^{t2} \cdot (\mathbf{F}_p^{t2})^{-1}. \quad (20)$$

Finally, the Cauchy stress at $t2$ was calculated as

$$\boldsymbol{\sigma}^{t2} = \left(\frac{1}{\det(\mathbf{F}_e^{t2})} \right) \mathbf{F}_e^{t2} \cdot \mathbf{\Sigma}^{t2} \cdot (\mathbf{F}_e^{t2})^T. \quad (21)$$

3.2 Finite Element Meshes

Each FE mesh was constructed to match the thickness and width of the corresponding experimental specimen, as listed in Table 1. The out-of-plane direction (y-dimension, Fig. 1) of the meshes consisted of only one element. Initial mesh setup was completed in CUBIT (Sandia Corporation) and LS-PrePost (Ansys, Inc.). The initial meshes were then scaled for the specific thickness and width of each specimen by adjusting the x and z coordinates of each node using Python scripts.

Two different length-scale meshes were created for each specimen, shown in Fig. 6 as an example for the HR specimen. A coarse-approximation mesh was generated by dividing the specimen into 15 layers. This “15-layer” mesh consisted of 2,176 hexahedral elements with nominal side length of 200 μm . The perpendicular distance across each layer was approximately 820 μm , spanned by four hexahedral elements on average. A higher-fidelity finer mesh was generated to match the experimental geometry more closely. This “full-scale” mesh consisted of 206 UD layers. The perpendicular distance across each of these layers was nominally 60 μm . This distance was spanned by six hexahedral elements on average, each with a nominal side length of 10 μm , for a total of 587,868 elements. Both meshes used the LS-DYNA default hexahedral element type, which was a constant stress solid element with a single integration point.

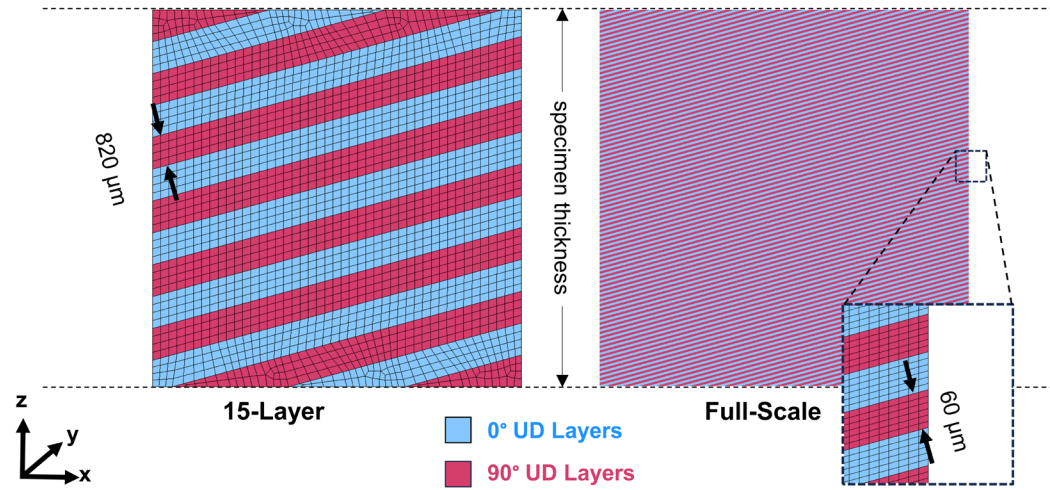


Fig. 6 15-layer and full-scale meshes for the HR specimen. Width in x-dimension was same for both meshes. Each mesh had one element in the out-of-plane (y) dimension. Nominal element side lengths were 200 μm for the 15-layer mesh and 10 μm for the full-scale mesh.

3.3 Boundary Conditions

The FE boundary conditions were analogous for all three loading rates; the only difference was the magnitude of the loading velocity as explained later in this section. Plane strain was applied by constraining the displacement of all nodes in the y-direction. The specimen was positioned between two rigid walls in the x-y plane. The contact between the specimen and the two rigid walls was assumed to be frictionless because lubrication was used between the loading surfaces and the specimen in the experiments. Appendix B demonstrates the effect of the friction parameter, showing that friction stiffens the response and postponed the failure. The rigid wall positioned at the bottom of the specimen was fixed in space. The normal reaction force of this wall was recorded.

A moving rigid wall was positioned at the top of the specimen. This wall moved at a constant velocity in the negative z-direction. Table 2 lists the magnitude of this velocity for each simulation. The velocity matched the experimental loading rate for the HR simulation. The maximum time step in the explicit FE simulation was set by the Courant condition. Because the time steps were limited to be small, the velocities in the LR and IR simulations were artificially increased to complete the simulations in a reasonable amount of computational time.

Table 2 Loading rates

Loading rate	Experimental loading velocity (m/s)	Simulation loading velocity (m/s)	Scaling factor
LR	5×10^{-6}	5×10^{-1}	1×10^5
IR	5×10^{-3}	2.0	4×10^2
HR	9.785	9.785	[none]

For the LR and IR rates, where the inertial effects were negligible, the experimental loading rate was multiplied by a scale factor, SF, listed in Table 2, to decrease the computation time. In addition, the same value of SF was applied to the $\dot{\gamma}_0$ parameter of the SMS model. Setting the scaling of $\dot{\gamma}_0$ equal to the scaling of the loading rate keeps the stress ratio in Eq. 12 invariant with respect to the scaling of the loading rate. This renders the material model insensitive to scaling, but the scaling must still be limited to avoid introduction of inertial effects. Therefore, the value of SF was determined through preliminary iterative simulations in which different SF values were used. Convergence of the load displacement response was examined to ensure inertial effects were not being introduced. In addition, the contribution of inertial effects was confirmed to be negligible to the overall response.

3.4 Delamination between UD Layers of UHMWPE

Delamination between UD layers was modeled using the tiebreak contact capability of LS-DYNA with a mixed-mode (Modes 1 and 2) traction–separation law. The relationship was triangular (bilinear) for each mode. In LS-DYNA, this option (OPTION=9) corresponded to *MAT_COHESIVE_MIXED_MODE, also referred to as *MAT_138. Figure 7 represents the traction–separation law for Mode 2 and illustrates the following relevant parameters: shear failure strength (SFS, units of MPa), initial stiffness (k , units of MPa/mm), and energy release rate (GIIC, units of MPa×mm). The off-axis loading conditions in the experiments induced only a shearing mode of deformation and failure. Therefore, the analogous Mode 1 traction–separation relationship was ignored in these simulations by setting the

corresponding failure strength to a much higher value than SFS. Following Mode 2 failure, the interfaces functioned as frictionless slide surfaces. For all rates, the mode-mixity exponent, called PARAM in LS-DYNA, was set to PARAM=1.

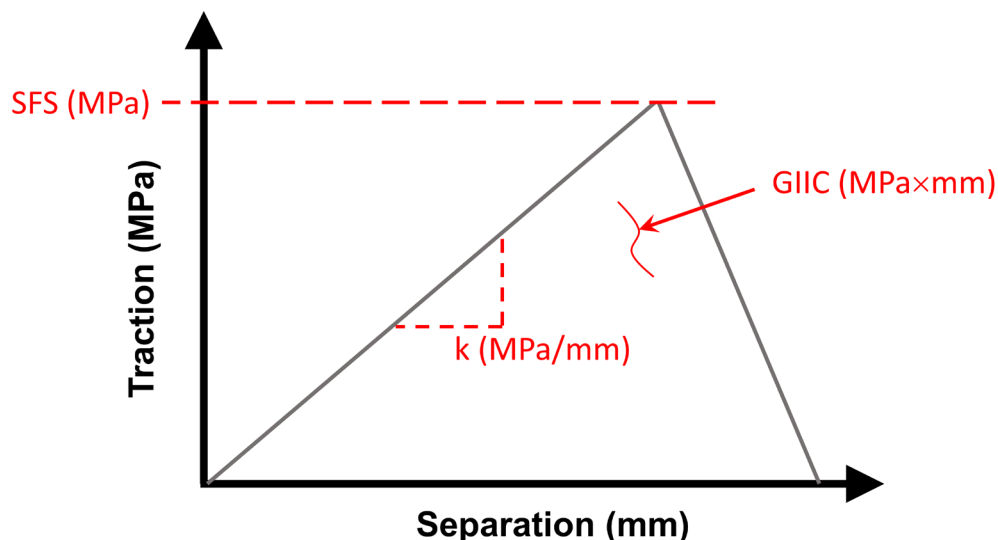


Fig. 7 Schematic of bilinear Mode 2 traction–separation law, illustrating the relevant parameters: shear failure strength (SFS), initial stiffness (k), and energy release rate (GIIC).

The 15-layer ($0^\circ/90^\circ$) mesh had 14 interlayer interfaces. Tiebreak contacts were specified at each of the 14 interfaces allowing for possible delamination at each interface. The full-scale mesh had 205 interlayer interfaces. When using the full-scale mesh, 14 tiebreak contacts were specified at 14 interfaces located at relative positions analogous to the 14 interfaces in the 15-layer mesh. At the remaining 191 interfaces of the full-scale mesh, the nodes were merged, thereby precluding any interlayer delamination at these interfaces.

4. Results

The FE simulations had two groups of parameters: those for the material model and those for the traction–separation law used to model interlayer delamination. This section presents the optimized values for the parameters, compares the load–displacement response between the simulations and their corresponding experiments, and shows the rate dependence of the optimized parameter values.

4.1 Simulation Sets

Four different sets of simulations were run: Sets A, B, C, and D. A set referred to a collection of three simulations, one at each loading rate (LR, IR, and HR), that were run with similar conditions. The specific conditions for Sets A–D are described in

Sections 4.1.1–4.1.4, respectively. Figure 8 compares the load–displacement response between the experiments and the simulation sets.

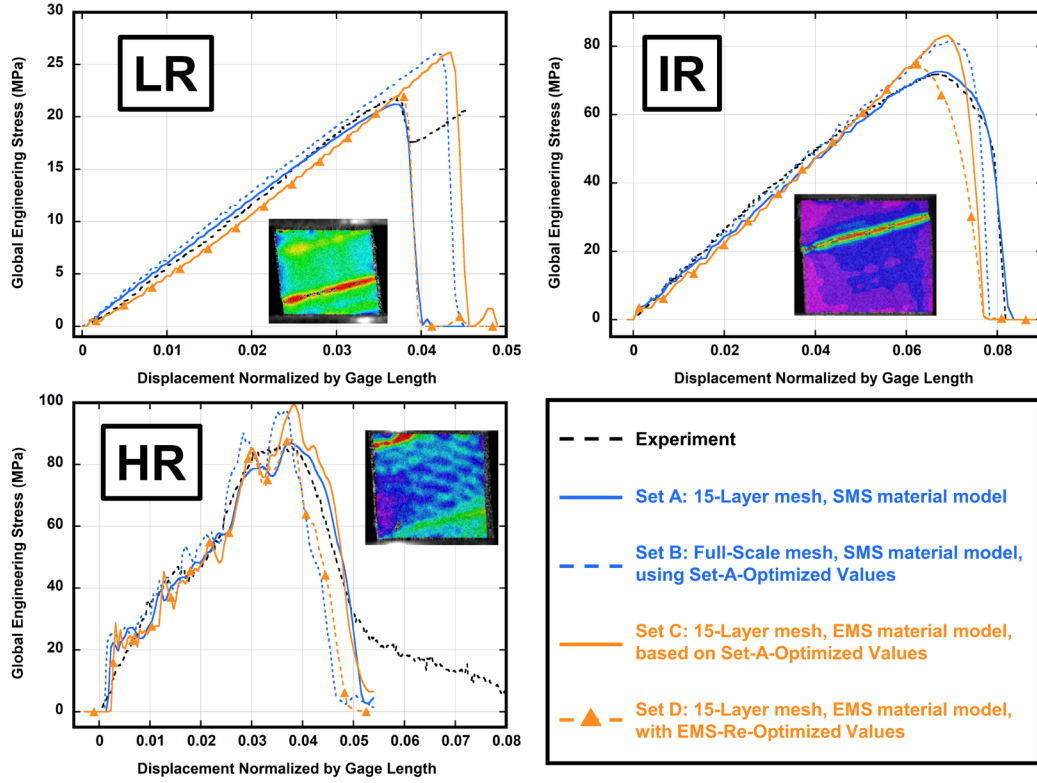


Fig. 8 Load–displacement response from the experiment compared with the Sets A–D simulations at each loading rate. Also included are experimental maximum shear strain contours for each rate.

4.1.1 Set A: Using 15-Layer Mesh and SMS Material Model for Preliminary Parameter Optimization

The parameters for the SMS material model and the parameters for the traction–separation law were identified for each loading rate by iteratively running simulations using the 15-layer mesh and the SMS material model at each rate. Appendix C provides examples from the iterative process showing how changing these parameters affects the simulation response. The plasticity model is rate dependent (Eq. 12), so the plastic response can be represented by a single set of parameters that are applicable across strain rates. However, such functional forms relating to strain rate are not available for the transversely isotropic elastic and the tiebreak de-cohesive behavior, as far as we were aware. Therefore, the elastic and tiebreak parameters were optimized for each loading rate to represent the experimental observation.

Set A referred to the final set of these simulations with the optimized values, with Appendix C providing additional examples from the iterative process used to

identify these values. Table 3 lists these “Set A optimized values.” The apparent stiffness of the Set A simulations was calculated for each rate from the global load–displacement response (Fig. 8) as approximately 600, 1100, and 2800 MPa at LR, IR, and HR, respectively. These apparent stiffnesses are close to the values of E_t used in the SMS material model.

Table 3 Set A optimized values for simulation parameters

Parameter	Description (units)	Values			Source
		LR	IR	HR	
SMS Material Model					
E_f	Young’s modulus in film primary direction (MPa)	102,100	114,900	140,600	Table 1 in Gunnarsson et al. (2022)
E_t	Young’s modulus in transverse direction (MPa)	565	1400	3500	Optimized ^a
ν_{ft}	Poisson’s ratio between primary and transverse directions	0.35	0.35	0.35	Gunnarsson et al. (2022)
ν_{tt}	Poisson’s ratio in the transverse plane	0.50	0.50	0.50	Liu et al. (2019)
G_{ft}	Out-of-plane shear modulus (MPa)	3000	3000	3000	Liu et al. (2019)
$\dot{\gamma}_0$	Reference shear strain rate (s ⁻¹) ^b	1	1	1	Assumed
τ_y^0	Reference shear yield strength of UD layer (MPa)	52.4	52.4	52.4	Experiments (see Fig. 2b)
m	Rate sensitivity exponent	0.1	0.1	0.1	Experiments (see Fig. 2b)
Traction-Separation Law for Tiebreak Contacts ^c					
SFS	Shear failure strength, peak of traction–separation law (MPa)	5.6	19.0	20.0	Optimized ^a
k	Slope of initial part of traction–separation law (MPa/mm)	423	250	423	Interply shear experiments ^d
GIIC	Energy release rate (MPa×mm)	0.5	8.55	4.0	Optimized ^a

^aOptimized by iteratively comparing the numerical output with the corresponding experimental response and adjusting parameters to reduce the error between them. Appendix C provides a summary of optimization process.

^bEven though the reference shear strain rate is 1, we increased it for the LR and IR simulations to speed up the calculation by multiplying the rate by the scaling factor, SF, listed in Table 2.

^cFigure 7 illustrates the parameters of the traction–separation law.

^dFrom preliminary interply shear experiments performed on Tensylon composites in collaboration with University of South Carolina (Frank Thomas and Dr Sockalingam, January 2023).

4.1.2 Set B: Using Full-Scale Mesh and SMS Material Model

Set B was exactly the same as Set A, except using the full-scale mesh rather than the 15-layer mesh. The parameters for the SMS material model and traction–separation law were the Set A optimized values (Table 3).

4.1.3 Set C: Using 15-Layer Mesh and EMS Material Model, Based on Set A Optimized Parameters

Set C used the 15-layer mesh with the EMS material model. The slip model has the form

$$\tau^\alpha = \hat{\tau}_0 \left(1 + \hat{c} \frac{\dot{\gamma}^\alpha}{\dot{\gamma}_0} \right)^{\hat{m}} \quad (22)$$

As with the SMS model, the elasticity and tiebreak models do not incorporate specific functional forms that vary across strain rate, so separate optimized parameters are optimized for each loading rate based on comparison with the experiments. The parameters for the slip model and other relevant material constants (Becker 2019) are listed in Table 4. In Set C, several EMS material model parameters were calculated from the Set A optimized values, as noted in Table 4. For the traction–separation law parameters, Set C directly used the Set A optimized values.

Table 4 EMS material model parameters used in Set C

EMS model parameter	Description	Values			Source ^a
		LR	IR	HR	
ρ	Material density (kg/m ³)	927	927	927	Alexander and Weerasooriya (2021)
μ	Matrix shear modulus (MPa)	188	467	1167	$\frac{E_t}{2(1+\nu_{tt})}$ (23)
κ	Matrix bulk modulus (MPa)	628	1556	3889	$\frac{E_t}{3(1-2\nu_{ft})}$ (24)
κ'	Pressure derivative of κ	8	8	8	~
$\hat{\tau}_0$	Shear yield strength of matrix (MPa)	15.5	15.5	15.5	Derived from τ_y^0
$\hat{c}$	Slip rate constant	2×10^5	2×10^5	2×10^5	~
$\hat{m}$	Strain rate exponent	0.1	0.1	0.1	m
$\hat{\gamma}_0$	Reference slip rate (s ⁻¹) ^b	1	1	1	$\dot{\gamma}_0$
E	Elastic modulus of fiber/film (MPa)	102100	114900	140600	E_f
σ_{ff}	Failure stress for single fiber/film (MPa)	1240	1470	1890	Gunnarsson et al. (2022)

Note: For the parameters in the traction–separation law, Set C used the Set A optimized values (listed in Table 3).

^aParameters in red were from the SMS material model and were described in Table 3. The Set C simulations used the Set A optimized values for these parameters given in Table 3. No source listed (~) indicates that the EMS parameter value either matched what was used in the original publication (Becker 2019) or was obtained by adjusting to match the Tensylon experimental load–displacement response.

^bEven though the reference shear strain rate is 1, we increased it for the LR and IR simulations to speed up the calculation by multiplying the rate by the scaling factor, SF, listed in Table 2.

4.1.4 Set D: 15-Layer Mesh and EMS Material Model, with EMS Re-Optimized Values

As shown in Fig. 8, the EMS model using the Set A optimized values failed at higher peak stresses compared to the experiments. Therefore, additional iterations were run of the LR and IR simulations using the EMS model and 15-layer mesh to bring the EMS model predictions closer to the experimental response by adjusting the SFS and GIIC parameters of the traction–separation law. The final set of parameters after these iterations was referred to as “EMS re-optimized values” and the corresponding simulations as Set D. Table 5 lists the EMS re-optimized values for the EMS material model and traction–separation law used in Set D.

Table 5 EMS re-optimized values used in Set D simulations, showing changes made to the Set A optimized values

Parameter (units)	Values		
	LR	IR	HR
SFS (MPa)	4.7	17.0	18.0
GIIC (MPa×mm)	(unchanged)	12.75	(unchanged)

Note: For the parameters of the EMS material model and traction–separation law not shown here, the Set D simulations used the same values as in the Set C simulations.

4.2 Rate Dependency of FE Simulation Parameters

Figure 9 shows the dependence on strain rate of the Set A optimized values (Table 3) and EMS re-optimized values (Table 5) for the FE simulation parameters. The elastic constants of the SMS material model closely followed a power law relationship with the strain rate. Figure 9 includes these power laws, which could be incorporated in future improvements of the modeling framework. This would be a step toward making the entire framework include rate dependency in order to be readily applicable to FE simulations at any rate.

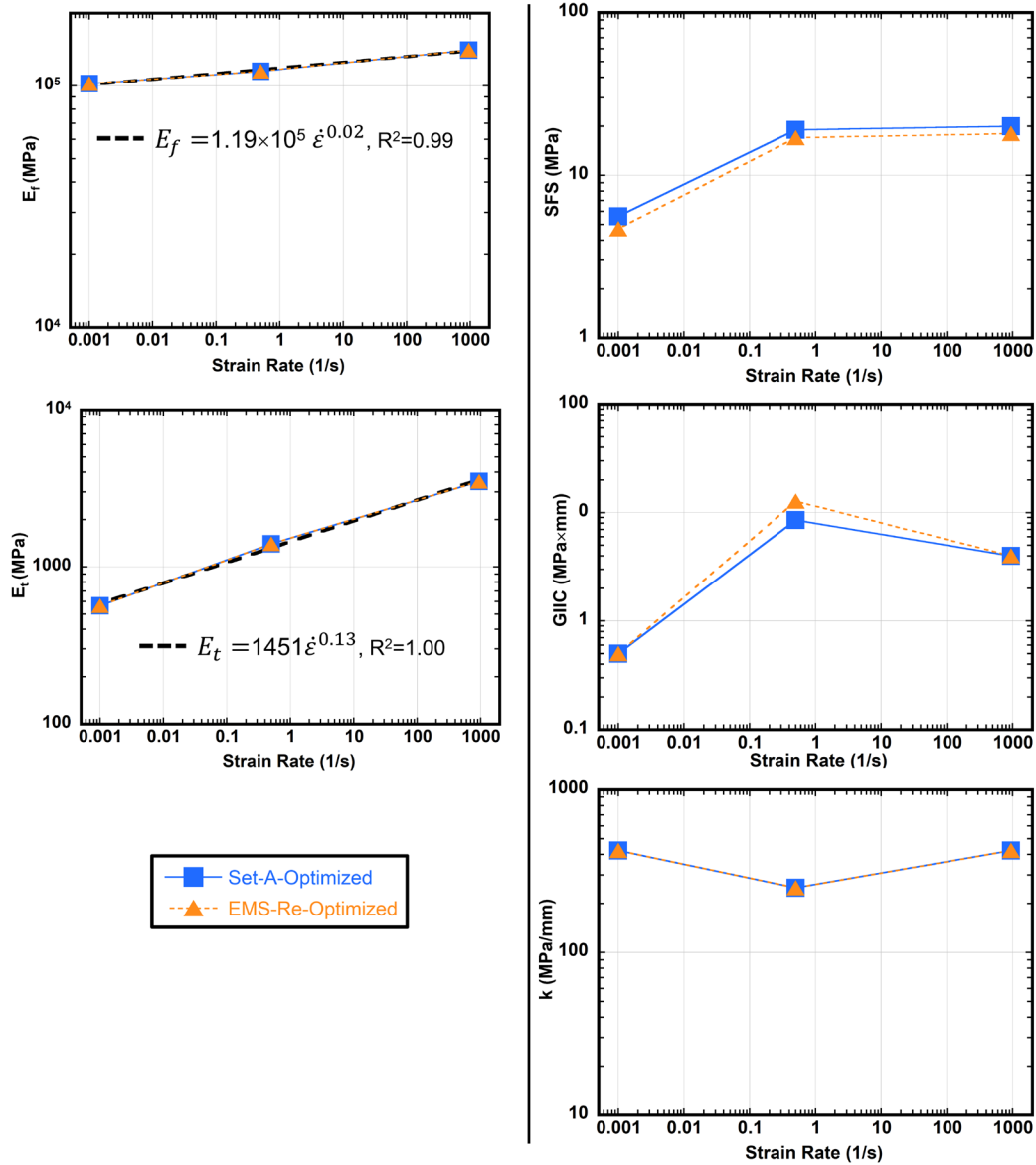


Fig. 9 Log-log plots of the FE simulation parameters against strain rate. Plots in the left column are elastic constants from the SMS material model and include the fitted power law equation. Plots in the right column are from the traction–separation law. Set A optimized values (blue squares, solid line) are compared with the EMS re-optimized values (orange triangles, dashed line).

5. Discussion

5.1 Comparison of Techniques for Simulating UHMWPE Composites

Sets A, B, and C used analogous parameter values but were at three different levels of approximation of the actual Tensylon composite. Set B provided the closest

approximation to the physical geometry since it used the full-scale mesh. The UD layers in the full-scale mesh were nominally 60 μm thick, based on our previously reported measurements of the thickness of UD layers in Tensylon composites after consolidation (Alexander and Weerasooriya 2021). However, complete fidelity would require each UD layer to be able to potentially delaminate from neighboring UD layers. There were 205 interlayer interfaces in the full-scale mesh, but tiebreak contact was only specified at 14 interfaces. The layers at the remaining 191 interfaces shared nodes and were thereby modeled as perfectly bonded. This approximation was employed due to the time-intensive preprocessing involved in establishing tiebreak contacts between the layers. The tiebreak contacts used in the simulations were defined by segment sets, which had to be manually created in the preprocessing graphical user interface.

The computational time needed for the Set B simulations made them suboptimal for iteratively identifying FE parameters. Therefore, the 15-layer mesh was adapted to reduce run time and was used in Set A for identifying the FE parameters by iteratively running simulations, comparing load displacement with the experiments, and adjusting values. In the Set A simulations, the UD layers were approximately 820 μm thick, which was a lower-scale representation of the physical geometry compared to the full-scale mesh. Figure 8 shows that this lower-level approximation was reasonable compared to the full-scale mesh, with the overall stiffness closely matching. One noticeable difference was that using the 15-layer mesh in Set A consistently underpredicted the peak stress compared to the full-scale mesh used in Set B.

The Set C and Set D simulations also used the 15-layer mesh, but with the EMS material model. Figure 8 shows that switching from the SMS material model (Set A) to the EMS material model (Set C) had a similar effect of increasing the peak stress as when using the full-scale mesh relative to the 15-layer mesh.

5.2 Limitations

The goal of the present study was to develop and demonstrate a computational framework for mechanism-based simulation of deformation and failure by each hypothesized dominant mechanisms of UHMWPE composites, including newer SSE films under multiaxial loading conditions. Parameter values were optimized under limited conditions and may not be applicable elsewhere. The large variation of parameters across the range of strain rates suggests that rate dependence is needed in the functional forms for the moduli, flow strength, and tiebreak models. Since simulations can only employ a single set of parameters per simulation, use of the current models requires choosing a set of parameters that are most

representative of the expected loading conditions. As shown in Fig. 8, we found that the rate dependence of the transversely isotropic elastic constants could be represented with a power relationship. In the future, the modeling framework could incorporate these power relationships for the elastic constants. This would be an improvement allowing users to apply the models in FE simulations where, in general, each element is loaded at a different strain rate.

There is also a question of uniqueness. For example, only one experiment at each loading rate was used for optimization and comparison. Statistical variation in the experimental response at each loading rate was not considered. In addition, parameters were optimized for off-axis loaded shear experiments performed at only a single offset angle (15°). The applicability of these values to match experiments performed at other angles was not investigated. Furthermore, mesh convergence was not studied, and the number of elements per UD layer may have a significant effect on global response.

Values for the FE simulation parameters were identified by various methods starting from the measured elastic constants and did not represent a global minimum or a unique set; but, as we are starting from measured values, it could be assumed that we are iteratively optimizing closer to the correct minima at each iteration (the next set of parameters for iteration was selected guided by intuition). One limitation in the identification process was the choice of which parameters to optimize at each loading rate and which parameters to assume a priori. An additional limitation was the optimization method itself. Both the choice of which parameters to optimize and the optimization method were based on subject matter expertise combined with preliminary simulation iterations. For example, preliminary simulations showed that varying G_{ft} did not have a substantial effect on the predicted response, and therefore the experimentally measured values used by Liu et al. (2019) were assumed to be sufficient.

However, the identification process did not yield a unique set of values; a different combination of values could likely give a similar predicted response. We did not have a defined objective function such as, for example, the square root of the sum of errors between predicted and experimentally measured because our goal here was also to demonstrate the concept at this time. As an example of this limitation, both the reference shear yield strength parameter (τ_y^0) in the crystal plasticity framework and the peak shear stress (SFS) of the traction–separation law affected the peak stress in the simulations (examples included in Appendix C). This is further complicated in that the shear yield strength is a parameter in the material constitutive behavior, and the tiebreak strength is intimately coupled to the FE contact model. These are applied in completely different phases of the numerical algorithm. In addition, as shown in Appendix C, the Young’s modulus in the

tangential direction (E_t) used in the elastic stiffness matrix for the UD layers affected the predicted stiffness of the composite at the macroscale; the stiffness (k) of the traction–separation law also affected the predicted stiffness for the response near the peak stress.

6. Conclusion

A computational framework was developed for simulating the deformation and failure (especially the Mode 2 shear delamination failure) response of UHMWPE composites to applied loading across rates. The framework was mechanism based: the physics-based parameters directly described the elastic response of the UD layers, the shearing mechanism of deformation and failure, and interlayer delamination. The capabilities of this technology were demonstrated by successfully simulating a unique collection of offset-shear experiments (uniquely selected to magnify the shear delamination failure, excluding the Mode 1 tensile delamination failure) performed on Tensylon film-based UHMWPE composites at low, intermediate, and high rates of loading. As far as we are aware, this is the first time a procedure (combined hybrid experimental-modeling-computational) was developed to obtain cohesive law parameters that vary with rate, especially Mode 2. We also found that the variation of the transversely isotropic elastic parameters with strain rate could be very well approximated with power law relationships, which could more generalize the framework for rate dependency. In addition, a process was also demonstrated whereby the parameters from the present subscale model could be transferred to larger-scale material models. Therefore, the parameter values identified by these simulations provide a preliminary set of material properties for this novel material at vastly different strain rates, where response (deformation and especially failure) has been thus far insufficiently characterized and understood due to its departure from the traditional paradigm of fiber-based UHMWPE composites.

7. References

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Appendix A. Sub-mesoscale (SMS) Material Model

This appendix presents additional details for the sub-mesoscale (SMS) material model, expanding upon the overview that was presented in Section 3.1.

A.1 Stress and Deformation Kinematics

The constitutive model update was performed on the intermediate configuration of the elastic–plastic decomposition indicated by Eq. 1. The stress in this configuration was determined by

$$\boldsymbol{\Sigma} = \mathcal{L} : \mathbf{E}_e, \quad (\text{A-1})$$

where $\boldsymbol{\Sigma}$ was the second Piola–Kirchhoff stress referred to as the intermediate configuration and $\mathbf{E}_e$ was the elastic Green–Lagrange strain determined from

$$\mathbf{E}_e = \frac{1}{2} (\mathbf{F}_e^T \cdot \mathbf{F}_e - \mathbf{I}). \quad (\text{A-2})$$

In the incremental integration scheme, the stress at the end of the time step (labeled $t2$) was determined by

$$\boldsymbol{\Sigma}^{t2} = \mathcal{L} : \mathbf{E}_e^{t2} = \mathcal{L} : (\mathbf{E}_e^{t1} + \Delta \mathbf{E}_e) = \mathcal{L} : (\mathbf{E}_e^{t1} + \Delta \mathbf{E}) - \mathcal{L} : \Delta \mathbf{E}_p \quad (\text{A-3})$$

where the additive decomposition of the strain increment was used to obtain the rightmost expression.

The quantity in parentheses in the rightmost expression of Eq. A-3 was the elastic strain at the end of the previous time step plus the total increment in strain over the time step. This was the basis for the "trial stress," $\boldsymbol{\Sigma}^{tr}$. This sum was computed from the deformation gradient derived from the following:

$$\mathbf{F}^{t2} = \Delta \mathbf{F} \cdot \mathbf{F}^{t1} = \Delta \mathbf{F} \cdot \mathbf{F}_e^{t1} \cdot \mathbf{F}_p^{t1}. \quad (\text{A-4})$$

Moving the plastic part of the deformation gradient to the left-hand side of the equation provided $\mathbf{F}_e^*$ as

$$\mathbf{F}_e^* = \Delta \mathbf{F} \cdot \mathbf{F}_e^{t1} = \mathbf{F}^{t2} \cdot \mathbf{F}_p^{t1^{-1}}. \quad (\text{A-5})$$

The quantity $\mathbf{F}_e^*$ was the basis for the Green–Lagrange strain used to compute the trial stress. This was computed as

$$\boldsymbol{\Sigma}^{tr} = \mathcal{L} : (\mathbf{E}_e^{t1} + \Delta \mathbf{E}) = \frac{1}{2} \mathcal{L} : [(\mathbf{F}_e^*)^T \cdot \mathbf{F}_e^* - \mathbf{I}] \quad (\text{A-6})$$

The last term in Eq. A-3 was the plastic contribution. This was obtained by mapping the fiber direction and normal of the Schmid tensor to the global reference frame,

symmetrizing, applying plastic slip increments to create the plastic part of the rate of deformation tensor, $\mathbf{d}_p$, and then mapping back to the intermediate configuration to compute the stress. The plastic part of the rate of deformation tensor was

$$\mathbf{d}_p = \frac{1}{2} \sum_{\alpha} \dot{\gamma}^{\alpha} \left(\left(\mathbf{F}_e^{t1} \cdot \mathbf{S}^{\alpha 0} \cdot \mathbf{F}_e^{t1^{-1}} \right) + \left(\mathbf{F}_e^{t1} \cdot \mathbf{S}^{\alpha 0} \cdot \mathbf{F}_e^{t1^{-1}} \right)^T \right). \quad (\text{A-7})$$

Here, $\mathbf{S}^{\alpha 0}$ is the Schmid tensor defined in Eq. 2, and $\dot{\gamma}^{\alpha}$ is the slip rate on slip system α . This was mapped to the Green–Lagrange strain increment:

$$\Delta \mathbf{E}_p = \Delta t \mathbf{F}_e^{t1^T} \cdot \mathbf{d}_p \cdot \mathbf{F}_e^{t1} = \frac{1}{2} \Delta t \sum_{\alpha} \dot{\gamma}^{\alpha} \left(\mathbf{A}^{t1} \cdot \mathbf{S}^{\alpha 0} + \mathbf{S}^{\alpha 0^T} \cdot \mathbf{A}^{t1} \right) \quad (\text{A-8})$$

where the right Cauchy–Green stretch tensor was

$$\mathbf{A}^{t1} = \mathbf{F}_e^{t1^T} \cdot \mathbf{F}_e^{t1}. \quad (\text{A-9})$$

Substituting the expression from Eqs. A-6 and A-8 into A-3, the stress at the end of the time step was expressed as

$$\boldsymbol{\Sigma}^{t2} = \boldsymbol{\Sigma}^{tr} - \sum \Delta t \dot{\gamma}^{\alpha} \mathbf{C}^{\alpha} \quad (\text{A-10})$$

where the second-order tensor

$$\mathbf{C}^{\alpha} = \frac{1}{2} \mathcal{L} : \left(\mathbf{A}^{t1} \cdot \mathbf{S}^{\alpha 0} + \mathbf{S}^{\alpha 0^T} \cdot \mathbf{A}^{t1} \right) \quad (\text{A-11})$$

was a constant during the iteration over the time step.

A.2 Slip System Properties

The model definition is completed with specification of the slip rate in Eq. A-9. The composite was taken to be a power law rate-dependent material with a reference shear strength τ_y^0 and reference slip rate $\dot{\gamma}_0$:

$$\dot{\gamma}^{\alpha} = \gamma_0 \left| \frac{\tau^{\alpha}}{\tau_y^0} \right|^{\frac{1}{m}} \text{sign}(\tau^{\alpha}). \quad (\text{A-12})$$

The resolved shear stress was computed using the current stress through

$$\tau^{\alpha} = (\mathbf{A}^{t1} \cdot \boldsymbol{\Sigma}^{t2}) : \mathbf{S}^{\alpha 0}. \quad (\text{A-13})$$

In evaluating Eq. A-13 the symmetries of both the stress and stretch tensors must be utilized to extract the symmetric part of the Schmid tensor.

A.3 Stress Integration

The stress was integrated using a Newton iteration algorithm based on Eq. A-9. For the n^{th} iteration the error in the stress took the form

$$\mathbf{G}_n = \boldsymbol{\Sigma}_n - (\boldsymbol{\Sigma}^{tr} - \sum_{\alpha} \Delta t \dot{\gamma}_n^{\alpha} \mathbf{C}^{\alpha}). \quad (\text{A-14})$$

The driving equation to reduce the residual was then

$$0 = \mathbf{G}_n + \frac{d \mathbf{G}_n}{d \boldsymbol{\Sigma}_n} : \Delta \mathbf{T}^{t2} = \mathbf{G}_n + \mathbf{J}_n : \delta \mathbf{T}^{t2} \quad (\text{A-15})$$

where $\delta \mathbf{T}^{t2}$ was the iterative stress correction. The fourth-order Jacobian was

$$\mathbf{J}_n = \mathbf{I}^{4\text{th}} + \sum_{\alpha} \frac{\Delta t \dot{\gamma}_n^{\alpha}}{m \tau_n^{\alpha}} \mathbf{C}^{\alpha} \mathbf{S}^{\alpha 0}. \quad (\text{A-16})$$

In taking the derivative of the slip rate, the right Cauchy–Green stretch tensor was neglected as it deviates little from the identity for small elastic strains. Employing this, the next stress iteration was determined from

$$\boldsymbol{\Sigma}_{n+1} = \boldsymbol{\Sigma}_n - \mathbf{J}_n^{-1} : \mathbf{G}_n. \quad (\text{A-17})$$

The iteration through Eqs. A-13, A-15, and A-16 continued until the stress correction drops below a convergence tolerance:

$$|\boldsymbol{\Sigma}_{n+1} - \boldsymbol{\Sigma}_n| \leq \epsilon. \quad (\text{A-18})$$

A.4 Explicit Component of the Constitutive Update

With the stress and slip rate determined from the stress iteration, the fiber configuration was updated explicitly using the slip increment. The deformation gradient at the end of the time step was

$$\mathbf{F}^{t2} = \mathbf{F}_e^{t2} \cdot \mathbf{F}_p^{t2} = \mathbf{F}_e^{t2} \cdot [(\mathbf{I} + \Delta t \sum_{\alpha} \dot{\gamma}^{\alpha} \mathbf{S}^{\alpha 0}) \cdot \mathbf{F}_p^{t1}]. \quad (\text{A-19})$$

Post-multiplying Eq. A-18 by the inverse of the term in the square brackets provided the elastic part of the deformation gradient at the end of the time step:

$$\mathbf{F}_e^{t2} = \mathbf{F}^{t2} \cdot \mathbf{F}_p^{t1-1} \cdot (\mathbf{I} - \Delta t \sum_{\alpha} \dot{\gamma}^{\alpha} \mathbf{S}^{\alpha 0}). \quad (\text{A-20})$$

In Eq. A-19, the inverse of the plastic deformation increment was approximated as the first-order expansion deformation increment indicated in Eq. A-18.

The updated elastic component of the deformation gradient was then used to map the second Piola–Kirchhoff stress to the global frame:

$$\boldsymbol{\sigma}^{t2} = \frac{1}{\det(\mathbf{F}_e^{t2})} \mathbf{F}_e^{t2} \cdot \boldsymbol{\Sigma}^{t2} \cdot \mathbf{F}_e^{t2T}. \quad (\text{A-21})$$

The components of the elastic part of the deformation gradient were saved as history variables for use in the next time step.

Appendix B. Effect of Friction between Loading Platens and Specimen

In the simulations in the report, the ultra-high-molecular-weight polyethylene (UHMWPE) specimen was positioned between two rigid walls. One wall was stationary and the other moved at a velocity corresponding to the low-rate, intermediate-rate (IR), or high-rate experiments. The contact between the specimen and these rigid walls was assumed to be frictionless because the lubricant was applied to the loading surfaces in the corresponding experiments.

This appendix documents the effect of simulating a finite friction at the interface between the specimen and the rigid walls. The IR simulation of Set A was rerun, which used the sub-mesoscale material model and the 15-layer mesh as presented in Section 4.1.1 in the report. Here, only the value of the Coulomb friction coefficient at the two interfaces was increased from 0.0 (as in the report) to 0.1 and 0.2. Figure B-1 shows the effect of this change on the load–displacement response.

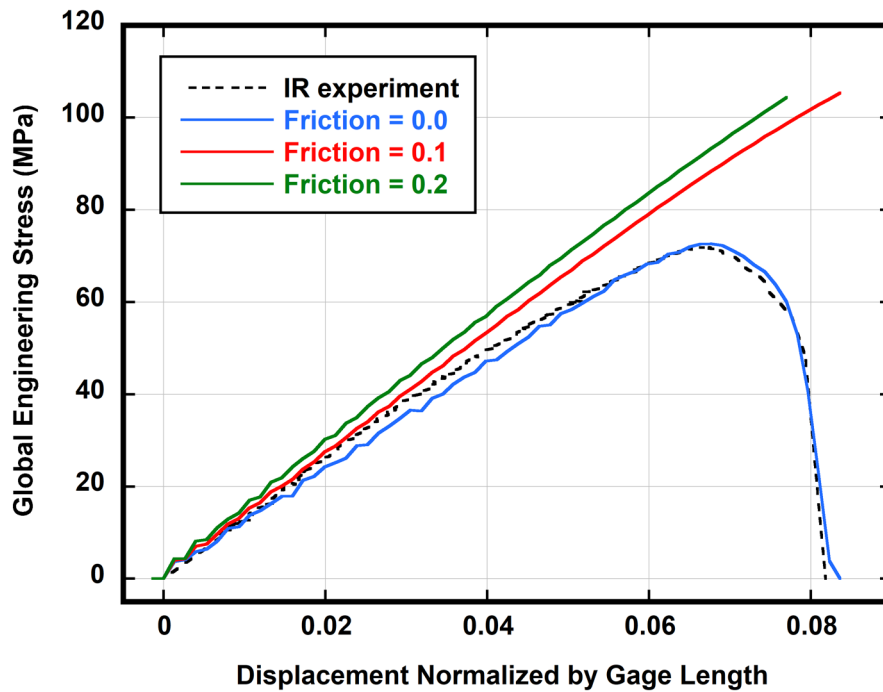


Fig. B-1 Effect of the Coulomb friction coefficient between the rigid walls and the UHMWPE specimen on the IR simulations. All three simulations were run using the Set A optimized values presented in the report. The case of friction = 0.0 corresponds to the simulation from Set A documented in Fig. 8 in the report.

**Appendix C. Effect of the Variation in Model Parameters in the
Sub-mesoscale (SMS) Material Model and the Traction–
Separation Law on the Simulation Response**

This appendix provides examples from the iterative process used to identify the Set A optimized values listed in Table 3 of the report for the sub-mesoscale (SMS) material model and the traction–separation law parameters. The examples in this appendix demonstrate the effect of the different parameters on the simulation response. All of the simulations here were at the intermediate loading rate (IR) using the 15-layer mesh, and the parameters were defined in Table 3 of the report.

The following parameter effects are observed:

- Decreasing τ_y^0 caused the load–displacement response to soften as it reached the peak stress (Fig. C-1).
- Increasing E_t increased the slope of the elastic portion of the response (Fig. C-2), whereas the simulations were comparatively less sensitive to E_f (Fig. C-3).
- Figures C-4 through C-6 show the effect of the parameters GIIC, k , and shear failure strength (SFS) in the traction–separation law.
- Increasing GIIC decreased the slope of the load–displacement response after reaching peak stress (Fig. C-4). Therefore, increasing GIIC caused failure to be more gradual by allowing the specimen to carry additional load after reaching peak stress and before final failure (defined as when stress reached 0).
- Increasing k (Fig. C-5) had a similar effect as E_t in that it increased the slope of the elastic portion of the response.
- Increasing SFS allowed the simulation to have additional elastic deformation and reach higher peak stress prior to delamination failure (Fig. C-6).

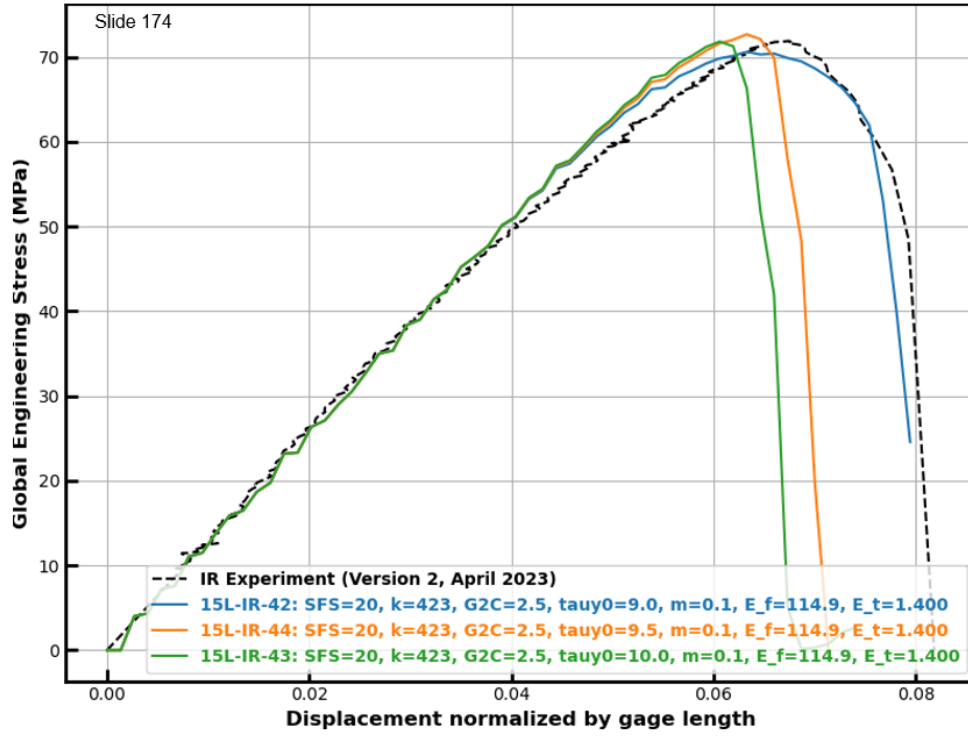


Fig. C-1 Effect of τ_y^0 from 9.0 MPa (blue), 9.5 MPa (orange), and 10.0 (green)

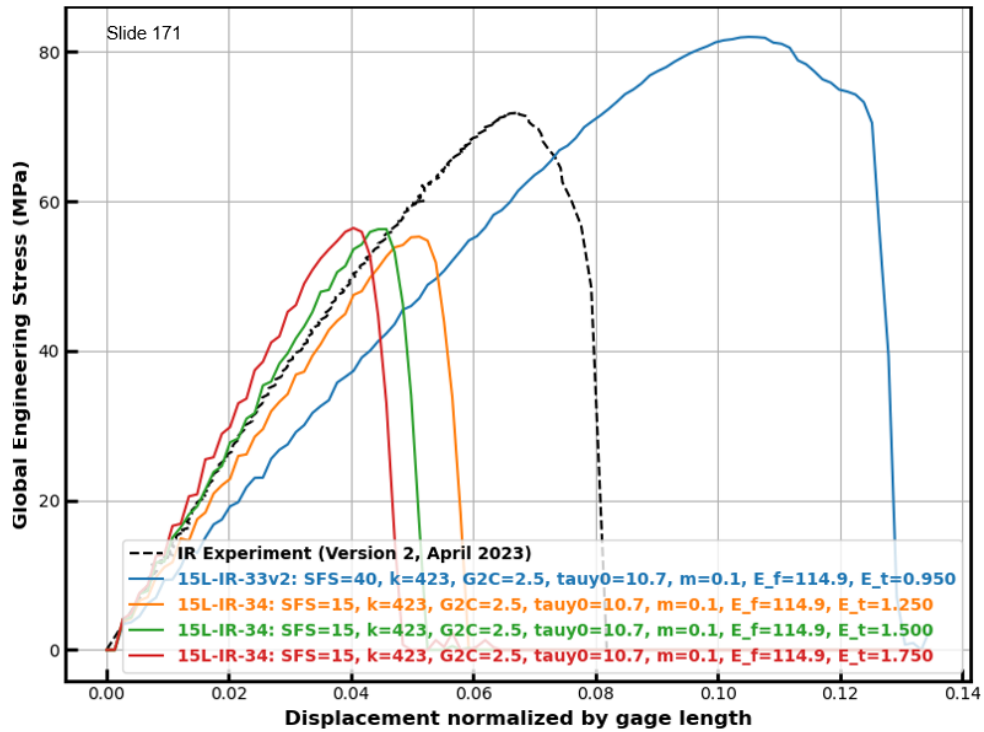


Fig. C-2 Effect of E_t . Only difference between orange, green, and red curves is increasing E_t between 1250 MPa, 1500 MPa, and 1750 MPa, respectively. (Blue curve represents combined effect of both increasing SFS and reducing E_t relative to the other curves.)

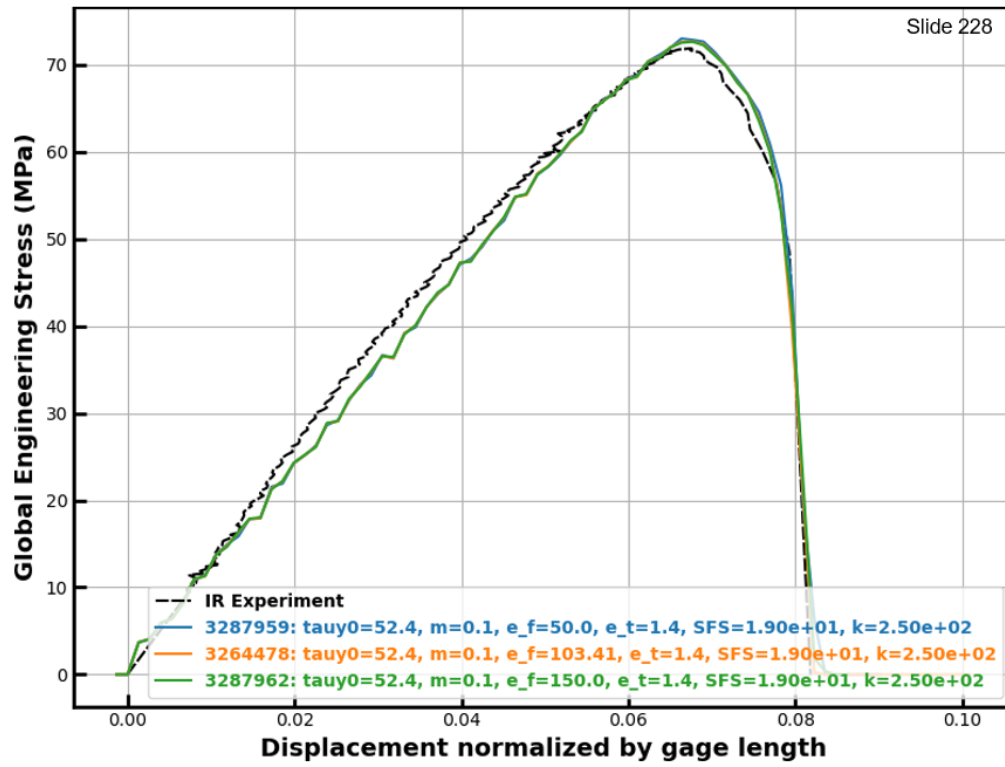
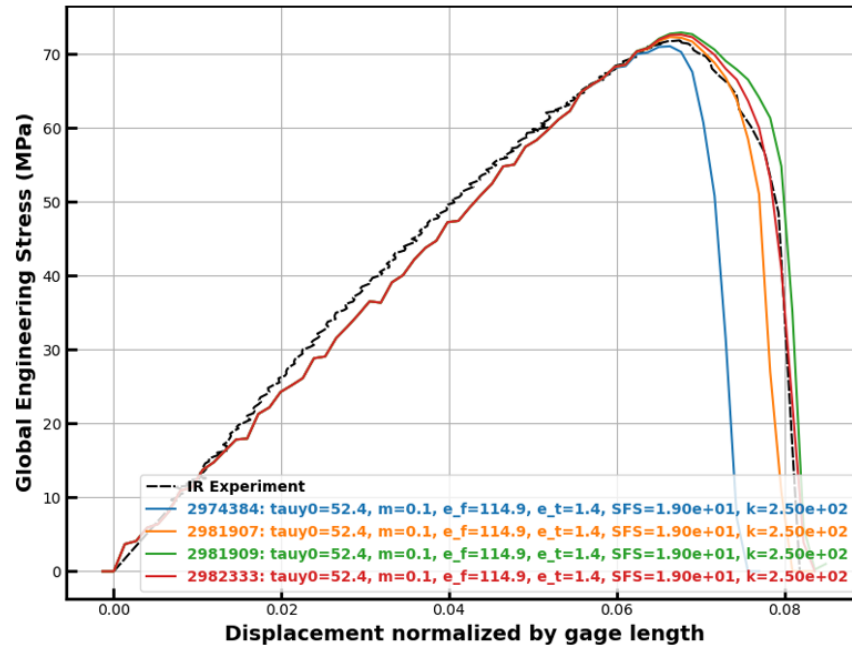
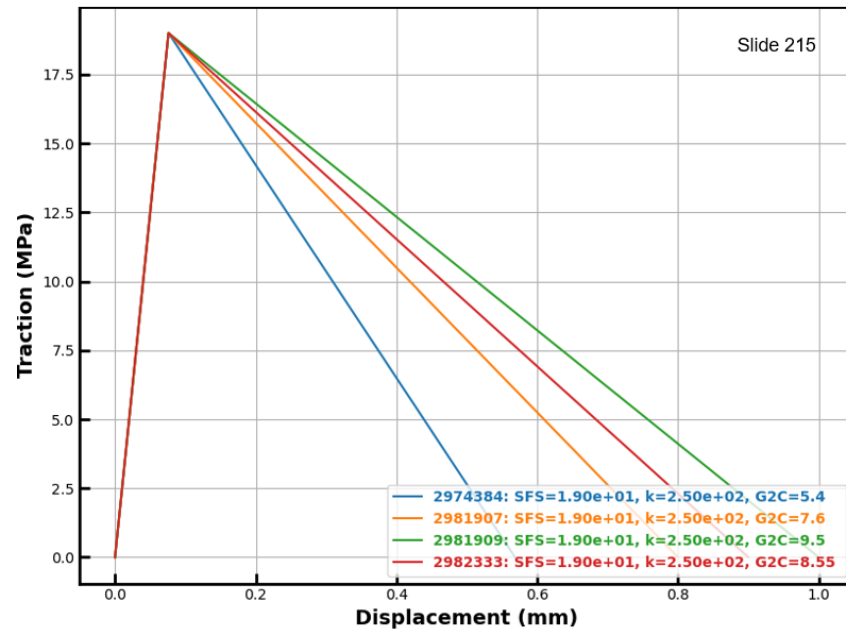


Fig. C-3 Effect of changing E_f between 50 GPa (blue), 103.41 GPa (orange), and 150 GPa (green), with all three curves almost overlapping

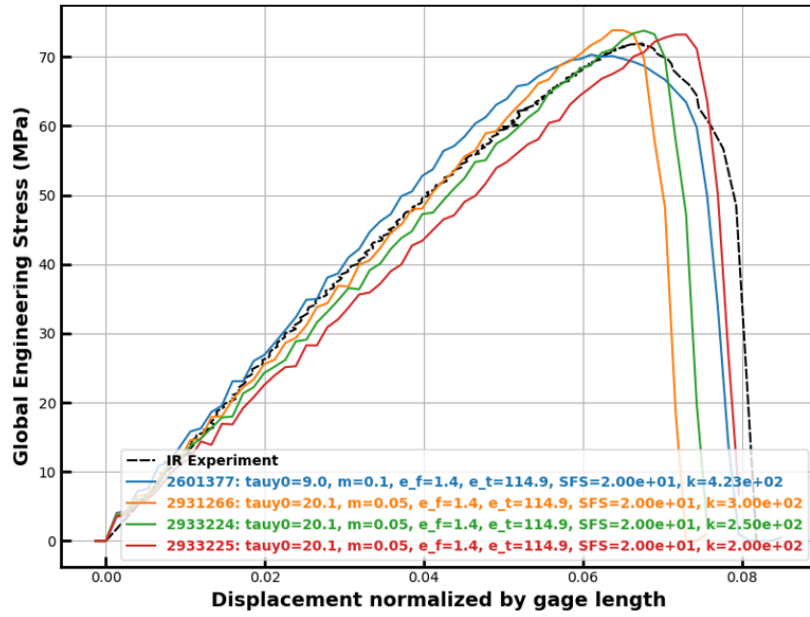


(a)

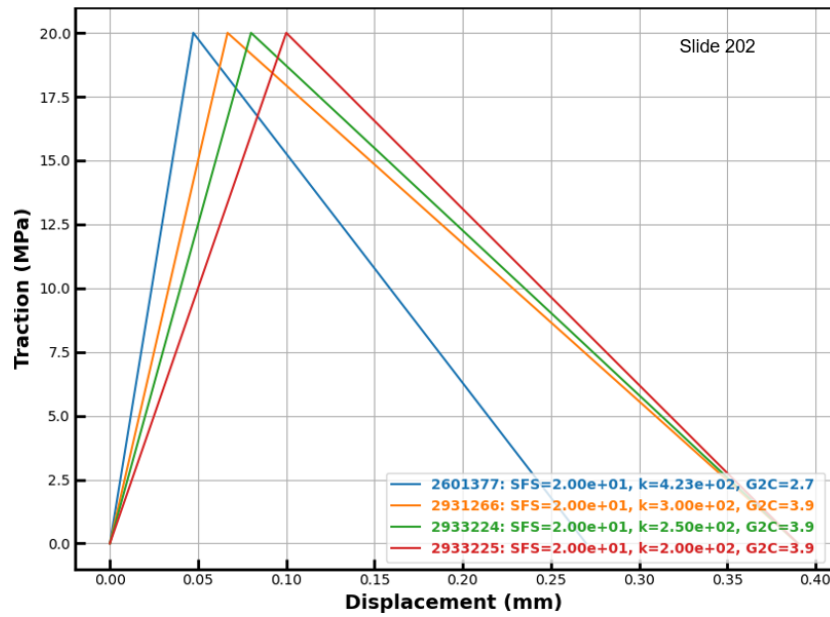


(b)

Fig. C-4 Effect of GIC. (a) Shows load–displacement response for simulations run with the corresponding color-coded traction–separation law shown in (b).



(a)



(b)

Fig. C-5 Effect of k in the traction–separation law. (a) Shows load–displacement response for simulations run with the corresponding color-coded traction–separation law shown in (b). The simulations shown in orange, green, and red were identical apart from the value of k (blue simulation had additional differences relative to the other simulations).

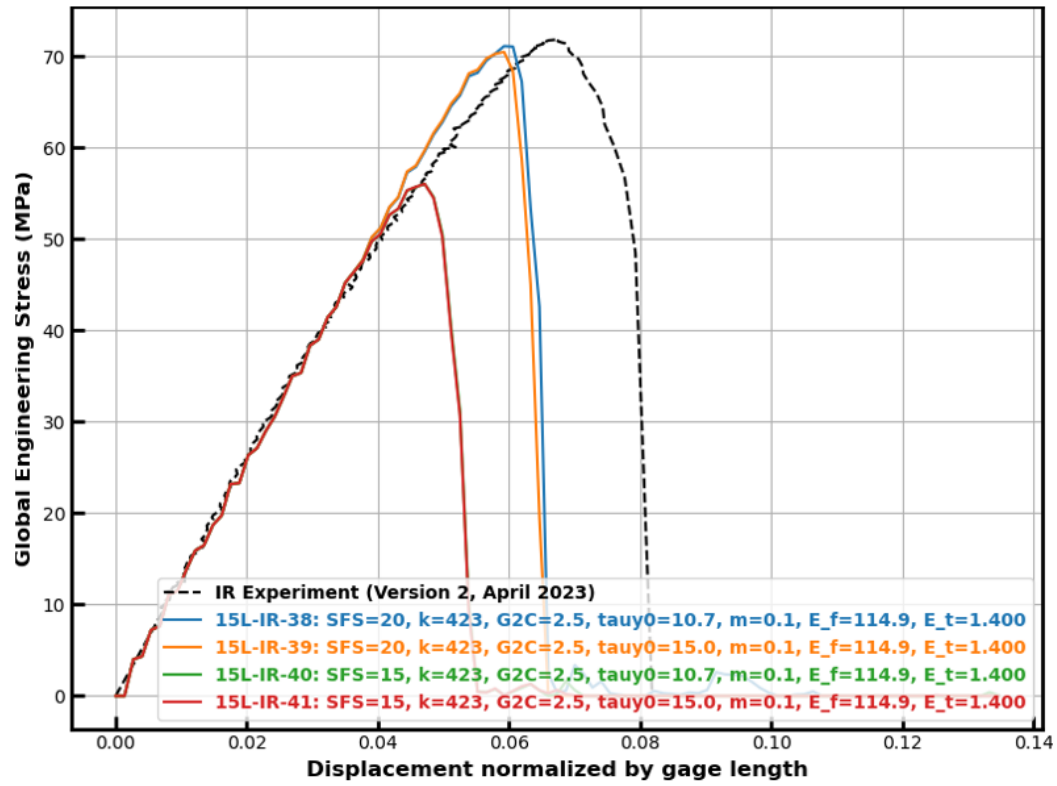


Fig. C-6 Effect of changing SFS in the traction–separation law. The red and orange curves had the same parameters except SFS = 15 MPa in the red simulation and SFS = 20 MPa in the orange simulation.

List of Symbols, Abbreviations, and Acronyms

EMS	elemental macroscale
FE	finite element
HR	high rate
IR	intermediate rate
LR	low rate
SF	scale factor
SFS	shear failure strength
SHPB	split-Hopkinson pressure bar
SMS	sub-mesoscale
UD	unidirectional
UHMWPE	ultra-high-molecular-weight polyethylene
UofSC	University of South Carolina

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