

# **Rapid Fatigue Assessment of Additively Manufactured Short-Fiber Thermoplastics**

by

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## Abstract

Short-fiber-reinforced thermoplastics (SFTs) manufactured via additive manufacturing–compression molding (AM-CM) provide a unique combination of highly aligned fibers (>80%) and low residual porosity (<2%). These characteristics make them promising candidates for fatigue-critical structural applications in aerospace, automotive, and wind energy systems. Despite growing industrial adoption, rapid methodologies for fatigue characterization and computational frameworks that link process-induced microstructures to cycle-dependent performance remain limited. This dissertation addresses these challenges by developing an experimentally validated, multiscale framework that integrates passive infrared thermography (IRT), micro-computed tomography ( $\mu$ -CT), finite-element (FE) homogenization, and machine learning surrogates for carbon fiber/acrylonitrile butadiene styrene (CF-ABS) SFTs processed via AM-CM.

First, on the experimental side, a multi-indicator IRT cyclic step loading protocol is developed and validated as an accelerated alternative to conventional stress-life (S-N) testing. By monitoring four thermal indicators, the proposed protocol predicts the high-cycle fatigue strength (HCFS) within  $\pm 4\%$  of conventional S-N results using only three specimens in five hours, reducing testing time by approximately  $96\times$ . Systematic parametric investigations further establish that HCFS increases by 17.3% as loading frequency rises from 5 to 20 Hz due to suppression of viscoelastic creep rather than thermal effects, and decreases by 19.2% as the stress ratio increases from  $R = 0.10$  to  $R = 0.75$ . Fatigue fracture entropy (FFE) is further demonstrated to remain invariant across the tested frequency range, providing a thermodynamic basis for frequency-corrected fatigue limit estimation.



Second, porosity is investigated as a fatigue-sensitive damage state variable through interrupted fatigue experiments combined with stage-wise  $\mu$ -CT imaging. Specimens spanning 1.41%–2.86% initial void content exhibit a 24.4% reduction in HCFS. Above the fatigue limit, void fraction increases by 232%–370% due to localized pore growth near fiber ends and matrix-rich regions. Stage-resolved FE homogenization based on experimentally derived microstructural distributions predicts a 2%–4% relative stiffness degradation, consistent with experimental measurements.

Third, to bridge microstructure and mechanical response,  $\mu$ -CT fiber arrangements are encoded as topology-aware weighted interaction graphs and processed by a hybrid graph neural network alongside a long short-term memory (GNN–LSTM) surrogate trained on nonlinear finite element (FE) homogenization data. The surrogate accurately predicts nonlinear stress–strain trajectories ( $R^2 = 0.993$ ) with a mean error below 4% across several microstructures while assembling coupon-scale responses in just 60 seconds, representing a  $100\times$  computational speedup over direct FE simulations. This enables rapid evaluation of microstructure-dependent constitutive behavior that would otherwise require computationally intensive nonlinear FE analyses.

Finally, the framework is extended to macroscale fatigue life prediction via a coupled thermomechanical transient implementation of matrix constitutivity that incorporates viscoelasticity and temperature-dependent stiffness degradation within a continuum damage mechanics framework. A cycle-jump acceleration algorithm reduces computational cost by  $100\times$  while maintaining less than 2% error in damage evolution.

Together, these contributions establish an integrated pathway from accelerated experimental characterization to an accelerated surrogate-based multiscale fatigue life prediction, thereby enabling more efficient qualification, design, and deployment of additively manufactured thermoplastic composites for fatigue-critical structural applications.

### Artificial Intelligence (AI) Use Disclosure Statement

In preparing this dissertation, the following Artificial Intelligence (AI) tools were used: Claude and Grammarly to improve grammar, sentence flow, and readability.

The author acknowledges full responsibility for the intellectual content of this work and has ensured that all AI-assisted sections have been reviewed and revised for accuracy and appropriate academic style. All AI-generated content was reviewed and validated for relevance, appropriateness, and accuracy before incorporation into the final document to maintain the scholarly integrity of this research.

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Every effort has been made to ensure this document is accessible to readers using screen readers and other assistive technologies. If any part of this dissertation is found to be inaccessible, please contact the author or the Auburn University Graduate School so that the issue may be addressed.

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## List of Abbreviations

|                          |                                                                 |
|--------------------------|-----------------------------------------------------------------|
| $\Delta T_{\text{stab}}$ | Stabilized Temperature Rise                                     |
| $\mu$ -CT                | Micro-computed Tomography                                       |
| $\phi$                   | Azimuthal fiber angle (measured from deposition direction)      |
| $\sigma_a$               | Stress amplitude                                                |
| $\sigma_{\text{max}}$    | Peak (maximum) applied stress                                   |
| $\sigma_{\text{min}}$    | Minimum applied stress                                          |
| $\theta$                 | Polar fiber angle (measured from specimen axis)                 |
| $D(N)$                   | Damage variable at given load cycle $N$                         |
| $R$                      | Stress ratio, $R = \sigma_{\text{min}}/\sigma_{\text{max}}$     |
| $R_\theta$               | Initial Heating Rate                                            |
| $R_c$                    | Cooling Rate                                                    |
| $S_2$                    | Second Harmonic Dissipation Signal                              |
| $T_g$                    | Glass transition temperature                                    |
| 3D-RUC                   | Three-Dimensional Repeating Unit Cell                           |
| AF                       | Above-Fatigue-limit ( $\mu$ -CT scan stage: post fatigue limit) |
| AM                       | Additive Manufacturing                                          |
| BF                       | Below-Fatigue-limit ( $\mu$ -CT scan stage: pre fatigue limit)  |

BT Before-Test ( $\mu$ -CT scan stage: pristine specimen)

CAF Constant amplitude fatigue

CDM Continuum Damage Mechanics

CF-ABS Carbon fiber-Acrylonitrile Butadiene Styrene

CM Compression molding

DMA Dynamic mechanical analysis

E(N) Elastic modulus at given load cycle N

ECM Extrusion Compression Molding

FE Finite Element

FFE Fatigue fracture entropy

FODs Fiber-Orientation Distributions

FPGD Pseudo-Grain Damage

FRP Fiber-reinforced polymer

GNN Graph Neural Network

HCFS High-Cycle Fatigue Strength

IRT Infrared thermography

LSTM Long Short-Term Memory

MTS Materials Testing System (servo-hydraulic test frame)

MWIR Mid-Wave Infrared (camera)

PAD Pore Aspect Ratio Distribution



PBC    Periodic Boundary Condition

PMCs   Polymer Matrix Composites

POD   Pore Orientation Distribution

PVD   Pore Volume Distribution

ROI    Region of Interest

S-N    Stress-Life

SEM   Scanning Electron Microscopy

SFTs   Short-fiber reinforced thermoplastics

UMAT   User Material subroutine (Abaqus)

UMATHT   User Material Heat Transfer subroutine (Abaqus)

## **Chapter 1**

### **Introduction**

#### **1.1 Background**

Short-fiber-reinforced thermoplastics (SFTs) produced via additive manufacturing - compression molding (AM-CM) represent a technologically significant yet incompletely characterized material class. The AM-CM process, developed at Oak Ridge National Laboratory (ORNL), combines pellet-extrusion deposition with subsequent hot-press consolidation to yield parts with greater than 60% fiber alignment within  $0^{\circ}$ – $20^{\circ}$  of the deposition direction and residual porosity below 2% [1–5]. This combination of microstructural control and defect mitigation is difficult to achieve through either process AM and CM in isolation, and has motivated direct industrial deployment for example, AM-CM SFTs are currently used in the AMERICA wind blade tip program at ORNL, where large-format additive stiffeners enhance blade fatigue life (Figure 1.1), and by ORNL in collaboration with OSHKOSH to produce a concrete truck chute subjected to sustained cyclic loading in service.

Three converging industry forces underpin the structural case for AM-CM SFTs. First, stricter emissions regulations from the International Civil Aviation Organization (ICAO) and fuel-economy mandates are accelerating the adoption of lightweight materials across aerospace, automotive, and wind-energy sectors – a combined advanced-composites market projected to reach USD 77.29 billion by 2032 at a compound annual growth rate of 7.08% [6–9], where SFTs offer a favorable strength-to-weight ratio without the end-of-life recycling penalties of thermoset composites [10–14]. Second, the AM-CM process enables complex component geometries —internal stiffener networks and variable wall sections

—that are unattainable through injection molding alone, thereby broadening the design space for components subjected to cyclic loading [15–18]. Third, and most critically for this dissertation, the thermoplastic ABS matrix in the carbon fiber-acrylonitrile butadiene styrene (CF-ABS) system studied here is inherently viscoelastic: under cyclic loading, molecular chain mobility produces time-dependent energy dissipation that manifests as surface self-heating. This phenomenon simultaneously constrains fatigue resistance at elevated loading frequencies and provides a real-time thermographic proxy for the internal damage state, making AM-CM SFTs a mechanistically challenging yet diagnostically rich material for the infrared thermography (IRT) framework developed in this dissertation.



**Figure 1.1:** Segment of the wind blade tip from the AMERICA program, manufactured via the AM-CM process at ORNL. Large-scale AM stiffeners are incorporated to enhance the blade's fatigue performance under sustained cyclic service loading.

## 1.2 Motivation

Realizing the full structural potential of AM-CM SFTs requires understanding how their process-induced microstructure, defined by fiber orientation, spatial clustering, and residual porosity, governs damage initiation, progression, and failure under cyclic loading. Translating this understanding into an industrially deployable form demands two complementary capabilities: (i) a rapid experimental characterization methodology that captures the fatigue response in hours rather than weeks, and (ii) a physically grounded, computationally efficient modeling framework that links micro-computed tomography ( $\mu$ -CT) resolved microstructure to cycle-dependent structural performance. Neither capability

currently exists for AM-CM SFTs, and their combined absence constitutes the primary barrier to reliable fatigue qualification and deployment of this material class.

Despite this growing industrial adoption, several critical gaps hinder the reliable deployment of AM-CM SFTs in high-stakes structural applications. These gaps span experimental characterization, microstructural understanding, and predictive modeling. The scope of this work must be stated before enumerating them: the framework is developed and validated at the coupon scale under uniaxial tensile fatigue loading for a single fiber-matrix system (20 wt.% carbon fiber in ABS, AM-CM processed). It does not claim to replace building-block certification testing, to generalize beyond the validated loading envelope without retraining, or to imply component-scale applicability without additional scaling studies. Within these bounds, the following five gaps define the specific unresolved problems this dissertation addresses.

**Gap 1 – Lack of validated rapid fatigue characterization methods for AM-CM SFTs:**

Traditional stress-life (S-N) fatigue testing is resource-intensive, typically requiring dozens of specimens and multiple weeks of continuous testing per loading condition [19]. While IRT has emerged as a promising rapid alternative for continuous-fiber composites, its applicability to AM-CM SFTs — whose controlled fiber alignment and low residual porosity may alter self-heating signatures relative to conventionally injection-molded SFTs — has not been examined. Consequently, the comparative reliability of the four principal IRT-based fatigue-limit indicators — stabilized temperature rise ( $\Delta T_{\text{stab}}$ ), initial heating rate ( $R_{\theta}$ ), cooling rate ( $R_c$ ), and second harmonic dissipation signal ( $S_2$ ) has not been established for this material class.

**Gap 2 — Unknown influence of loading frequency on fatigue behavior:**

ASTM D7791 restricts cyclic loading frequency to 5 Hz or below to minimize self-heating effects in thermoplastic specimens, yet structural components in aerospace, automotive,

and wind-energy applications routinely experience substantially higher loading frequencies in service. The interplay among loading frequency, viscoelastic energy dissipation, hysteretic self-heating, and failure morphology has not been investigated in AM-CM SFTs, leaving a disconnect between laboratory characterization practices and real-world service conditions unresolved.

**Gap 3** — Incomplete understanding of porosity evolution under cyclic loading:

Process-induced porosity acts as a stress concentrator at fiber ends and within fiber clusters, promoting early damage initiation at these locations. Although the AM-CM process reduces global porosity relative to as-deposited preforms, residual pores persist and evolve under cyclic loading. The rate, spatial pattern, and three-dimensional morphology of this evolution and its quantitative relationship to the measured fatigue limit have not been tracked in AM-CM SFTs using interrupted  $\mu$ -CT imaging.

**Gap 4** — Absence of a computationally efficient, topology-preserving surrogate for quasi-static response:

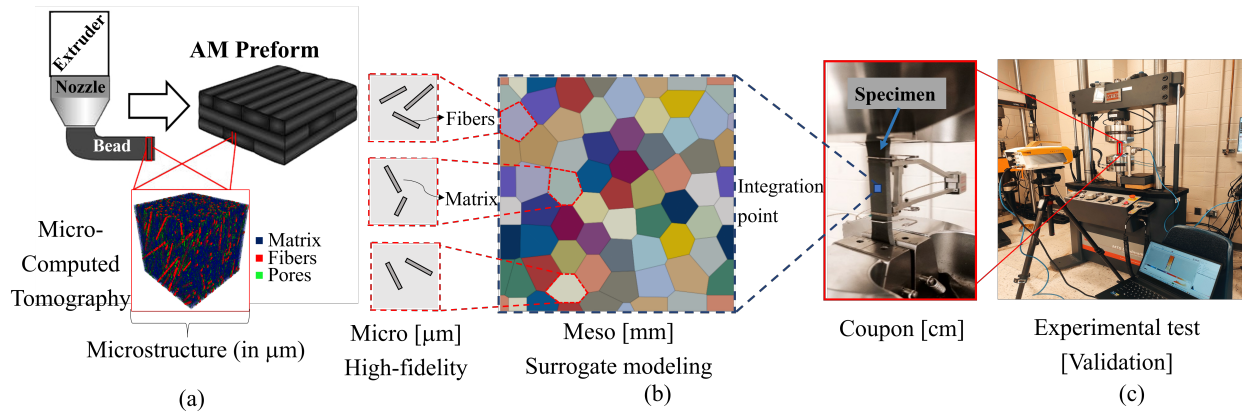
Full finite element (FE) homogenization of every discrete fiber neighborhood in a realistic specimen volume is computationally intractable, while mean-field approaches discard the topological information — fiber clustering, resin-rich zones, fiber-end stress concentrations — that govern both nonlinear deformation and progressive stiffness degradation. Image-based graph neural network (GNN) surrogates, operating on voxelized microstructures, additionally discard the discrete fiber-interaction graph topology, which is the natural representation of shear-lag-governed load transfer in SFTs and is directly accessible from  $\mu$ -CT fiber centerline data. No topology-preserving surrogate capable of accommodating variable fiber count per cell and encoding shear-lag-informed pairwise interactions as weighted graph edges has been demonstrated for AM-CM SFTs.

**Gap 5** — Absence of a computationally efficient of a cycle-resolved fatigue lifetime model sensitive to both microstructure and loading conditions:

Extending quasi-static modeling to fatigue life prediction introduces qualitatively different challenges: cell-level stiffness degrades cycle-by-cycle in a manner that depends jointly on fiber interaction topology, loading frequency, stress ratio, peak stress, and cumulative loading history, none of which are encoded in a surrogate trained exclusively on monotonic loading data.

### 1.3 Research Objectives

This dissertation addresses the five gaps identified above through an integrated, hierarchical methodology that combines IRT-based fatigue characterization,  $\mu$ -CT microstructural tracking, and a multiscale surrogate modeling framework (Figure 1.2). The five research objectives, each directly mapped to a corresponding gap, are as follows:



**Figure 1.2:** Multiscale framework linking AM-CM fabrication,  $\mu$ -CT-resolved microstructure, and mesoscale Voronoi surrogate modeling, validated against coupon-scale fatigue testing. (a) Extrusion-based fabrication and  $\mu$ -CT reconstruction (matrix, fibers, pores). (b) Micro-to-meso mapping of fiber-matrix topology onto Voronoi integration points. (c) Coupon-scale experimental validation setup.

- i. *Validate IRT-based rapid fatigue characterization for AM-CM SFTs (Gap 1, Chapter 3):*

Assess the efficacy of passive IRT techniques —  $\Delta T_{\text{stab}}$ ,  $R_\theta$ ,  $R_c$ , and  $S_2$ —for rapid estimation of the high-cycle fatigue strength (HCFS) of 20 wt.% CF-ABS SFTs manufactured via AM-CM, and compare IRT-derived fatigue limits against traditional S-N results to quantify gains in testing speed and specimen efficiency.

ii. *Investigate the influence of loading frequency on fatigue limit and damage mechanisms (Gap 2, Chapter 3):*

Conduct accelerated fatigue characterization at 5, 10, 15, and 20 Hz using a passive IRT staircase protocol, and interpret frequency-dependent fatigue trends through displacement accumulation, hysteretic energy dissipation, fatigue fracture entropy (FFE), and SEM fracture morphology.

iii. *Characterize the role of process-induced porosity on cyclic fatigue performance (Gap 3, Chapter 4):*

Use  $\mu$ -CT imaging at three interrupted fatigue stages — before testing, below the fatigue limit, and above the fatigue limit — to track pore evolution in AM-CM SFTs with varying initial porosity levels, and correlate microstructural progression with IRT-measured fatigue limits and stiffness degradation.

iv. *Develop a physics-informed graph neural network-long short-term memory (GNN–LSTM) surrogate for quasi-static constitutive response (Gap 4, Chapter 5):*

Reconstruct AM-CM SFT microstructures from  $\mu$ -CT data, discretize into Voronoi-based fiber-interaction cells, and train a hybrid GNN–LSTM architecture in which: (i) fibers are represented as graph nodes whose features encode length, orientation, and spatial position extracted from  $\mu$ -CT; (ii) pairwise fiber–fiber load-transfer efficiency is encoded as shear-lag-informed edge weights; and (iii) the LSTM decoder captures path-dependent plasticity and damage evolution under monotonic loading. The surrogate is designed to achieve  $R^2 \approx .98$  accuracy relative to FE homogenization while reducing computational cost by more than two orders of magnitude.

v. *Extend the damage model to fatigue lifetime prediction (Gap 5, Chapter 6):*

Develop a coupled thermomechanical user material subroutine for transient heat transfer (UMAT/UMATHHT) in Abaqus, incorporating viscoelasticity, temperature-dependent moduli, and a four-variable continuum damage mechanics (CDM) fatigue evolution law. Use the damage model to predict the cycle-dependent effective stiffness matrix as a joint function of fiber topology and fatigue loading conditions — cycle count  $N$ , frequency  $f$ , stress ratio  $R$ , and peak stress  $\sigma_{\max}$ .

All five objectives limited to the coupon level, for 20 wt.% CF-ABS SFTs under uniaxial tensile fatigue loading processed via AM-CM. Extension to other material systems, loading modes, or structural scales is identified as future work in Chapter 7.

## 1.4 Thesis Structure

This dissertation is structured to progress systematically from foundational experimental characterization through microstructural analysis to multiscale computational prediction, with each chapter corresponding to a peer-reviewed publication or manuscript in preparation. Cross-chapter dependencies are noted explicitly below.

Chapter 2 reviews the literature on SFT manufacturing, fatigue behavior and damage mechanisms, IRT-based characterization, and multiscale modeling approaches, establishing the theoretical foundation for Chapters 3–6. It motivates why GNN architectures are the natural choice for fiber-topology encoding and why the quasi-static surrogate in Chapter 5 requires explicit loading-condition augmentation before it can serve as a fatigue predictor in Chapter 6.

Chapter 3 addresses Gaps 1 and 2, establishing IRT as a validated rapid alternative to conventional S-N testing and then using that validated framework to reveal how loading frequency governs viscoelastic deformation, hysteretic dissipation, and failure morphology. The stiffness-degradation trends identified here motivate the damage-driver formulation used in the CDM law of Chapter 6.



Chapter 4 addresses Gap 3, tracking pore nucleation and growth in three dimensions across interrupted fatigue stages and linking that evolution to stage-resolved stiffness degradation. The IRT-based porosity estimator developed here feeds directly into the surrogate training pipeline of Chapter 5.

Chapter 5 addresses Gap 4, translating  $\mu$ -CT-resolved microstructures into Voronoi-based fiber-interaction cells and training a GNN–LSTM surrogate on the resulting FE-homogenized stress–strain trajectories. The resulting architecture is extended in Chapter 6 to the fatigue loading regime.

Chapter 6 addresses Gap 5, extending the Chapter 5 surrogate to fatigue lifetime by replacing its static FE training data with simulations from a coupled UMAT/UMATHT subroutine. The retrained surrogate predicts the full six-by-six cycle-dependent effective stiffness matrix as a function of fiber topology and loading condition, enabling damage-index prediction at both the cell and coupon scales.

Chapter 7 synthesizes the key findings, critically evaluates the limitations of the proposed framework, and proposes eight specific directions for future work organized by scientific priority and implementation readiness.

## **Chapter 2**

### **Literature review**

#### **2.1 Introduction**

The fatigue behavior of SFTs manufactured via AM–CM is governed by a hierarchy of interdependent phenomena — viscoelastic dissipation in the thermoplastic matrix, shear-lag stress transfer between fibers and matrix, and three-dimensional evolution of process-induced porosity under cyclic loading — that together determine service life. This chapter reviews the relevant literature in materials science, experimental mechanics, thermodynamics, CDM, and machine learning, identifying at the close of each section the specific gap that motivates this dissertation’s contributions.

#### **2.2 Composite Materials**

##### **2.2.1 Overview of Composite Materials**

Within the broad family of fiber-reinforced polymer matrix composites (PMCs), SFTs occupy a strategically important niche: they combine the lightweight, high-specific-strength performance characteristics of continuous-fiber systems with the high-volume manufacturability and end-of-life recyclability that thermoset-matrix composites cannot offer [10, 11]. Unlike continuous-fiber laminates, whose in-plane mechanical properties are dominated by the fiber axial modulus, SFT properties depend critically on fiber length, orientation, and spatial arrangement — microstructural variables governed almost entirely by the manufacturing process — and these variables control both static and cyclic mechanical

performance [20, 21]. This process-microstructure-property dependence defines the central scientific problem addressed in this dissertation: how the AM-CM process controls the microstructural architecture of 20 wt.% CF-ABS SFTs, and how that architecture governs fatigue damage initiation, progression, and eventual failure [1, 2, 22].

### **2.2.2 Short Fiber-Reinforced Thermoplastics**

This study centers on a two-phase SFT system - specifically, 20 wt.% CF-ABS manufactured via the AM-CM process at ORNL. The constituent geometry and fiber orientation convention used throughout this work are illustrated in Figure 2.1.

#### *(i) Matrix:*

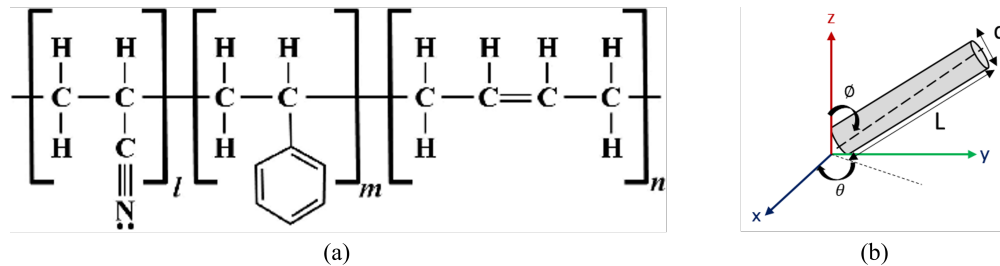
The thermoplastic matrix, ABS, binds and spatially positions the short carbon fibers, facilitating load transfer between phases while maintaining structural integrity [10]. ABS is a terpolymer of acrylonitrile, butadiene, and styrene (Figure 2.1(a)); it provides chemical resistance, impact toughness, and thermal processability well-suited to the AM-CM consolidation step. Its thermoplastic nature, enabling repeated softening and reshaping upon heating without cross-linking, enhances recyclability relative to thermoset-matrix composites. Most significantly for this dissertation, ABS exhibits pronounced viscoelastic behavior under cyclic loading: time- and temperature-dependent molecular chain mobility dissipates energy, manifesting as surface self-heating, a phenomenon central to the IRT-based fatigue characterization methodology in Chapter 3 and to the thermomechanical constitutive model in Chapter 6.

#### *(ii) Reinforcement Fibers:*

The CF-ABS system studied here uses high-tenacity chopped carbon fibers (Kaltex K20-HTU), with a nominal diameter of approximately  $8\text{ }\mu\text{m}$  and as-processed lengths ranging from 25 to  $350\text{ }\mu\text{m}$ . The fiber geometry is represented in Figure 2.1(b), where the

aspect ratio  $l/d$ , azimuthal angle  $\phi$ , and polar angle  $\theta$  are defined. Several parameters govern SFT mechanical behavior:

- Fiber Aspect Ratio: The ratio of fiber length to fiber diameter ( $l/d$ , Figure 2.1(b)) governs stress transfer efficiency via shear-lag load transfer. Higher aspect ratios improve strength and stiffness but increase susceptibility to fiber breakage under the high shear conditions encountered during extrusion [17, 18].
- Fiber Volume Fraction: The CF-ABS system studied here contains approximately 20 wt.% (approximately 13 vol.%) carbon fiber, influencing composite stiffness, tensile strength, and local stress redistribution under both static and cyclic loading [17, 18].
- Fiber Orientation Tensor: Characterized by azimuthal and polar angles ( $\phi$ ,  $\theta$ ) extracted from  $\mu$ -CT reconstructions (Chapter 4) and illustrated in Figure 2.1(b), the fiber-orientation distributions (FODs) govern elastic anisotropy and fatigue damage initiation pathways [23–29]. In AM-CM processed CF-ABS, approximately 60% of fibers lie within  $0^\circ$ – $30^\circ$  of the deposition direction [18, 30, 31].



**Figure 2.1:** Constituents of AM-CM CF-ABS SFTs: (a) Chemical structure of the ABS matrix (terpolymer of acrylonitrile, butadiene, and styrene), and (b) Semi-axes and orientation conventions for a geometric representation of a short fiber, with aspect ratio  $l/d$ , azimuthal angle  $\phi$ , and polar angle  $\theta$  (defined in Section 2.2).

### (iii) Fiber/Matrix Interface:

The fiber–matrix interface governs load-transfer efficiency and resistance to interfacial debonding and fiber pull-out, widely reported as the dominant fatigue damage mechanisms

in short-fiber thermoplastic composites [32, 33]. In the AM-CM process specifically, fiber ends are exposed after extrusion-induced chopping due to the absence of a post-chopping sizing treatment, resulting in weak interfacial bonding at fiber termini and high local stress concentrations consistent with classical shear-lag predictions [32, 33]. These stress concentrators are expected to act as primary nucleation sites for fatigue-driven interfacial damage and void formation under cyclic loading, consistent with synchrotron tomographic evidence of fiber-end debonding and cavitation in short-fiber PA66 (Figure 2.3(b)) [33]; whether the same mechanisms dominate in AM-CM SFTs is examined via  $\mu$ -CT and SEM fractography in Chapter 4.

## **2.3 Manufacturing Processes and Microstructural Effects**

### **2.3.1 Manufacturing Techniques for SFTs**

The mechanical performance of SFTs under cyclic loading is strongly governed by the processing-induced microstructure—FODs, fiber-length distributions (FLDs), and residual porosity—which collectively determine elastic anisotropy and fatigue resistance [34, 35]. The three principal manufacturing routes reviewed below differ fundamentally in the degree of fiber alignment and void content they produce, and this contrast provides the principal motivation for selecting the AM-CM process for the CF-ABS system studied in this dissertation (Figure 2.2).

#### *(i) Injection Molding:*

Injection molding melts thermoplastic feedstock and forces it into a mold cavity under high shear stresses, inducing complex three-dimensional flow fields that determine the resulting FODs and FLDs [22, 36]. Fibers aligned with the primary flow direction enhance fatigue resistance through efficient axial load transfer, whereas random or transverse orientations reduce strength, increase interfacial stress concentrations, and complicate fatigue life prediction [22, 36]. A fundamental limitation of injection molding is the inherent

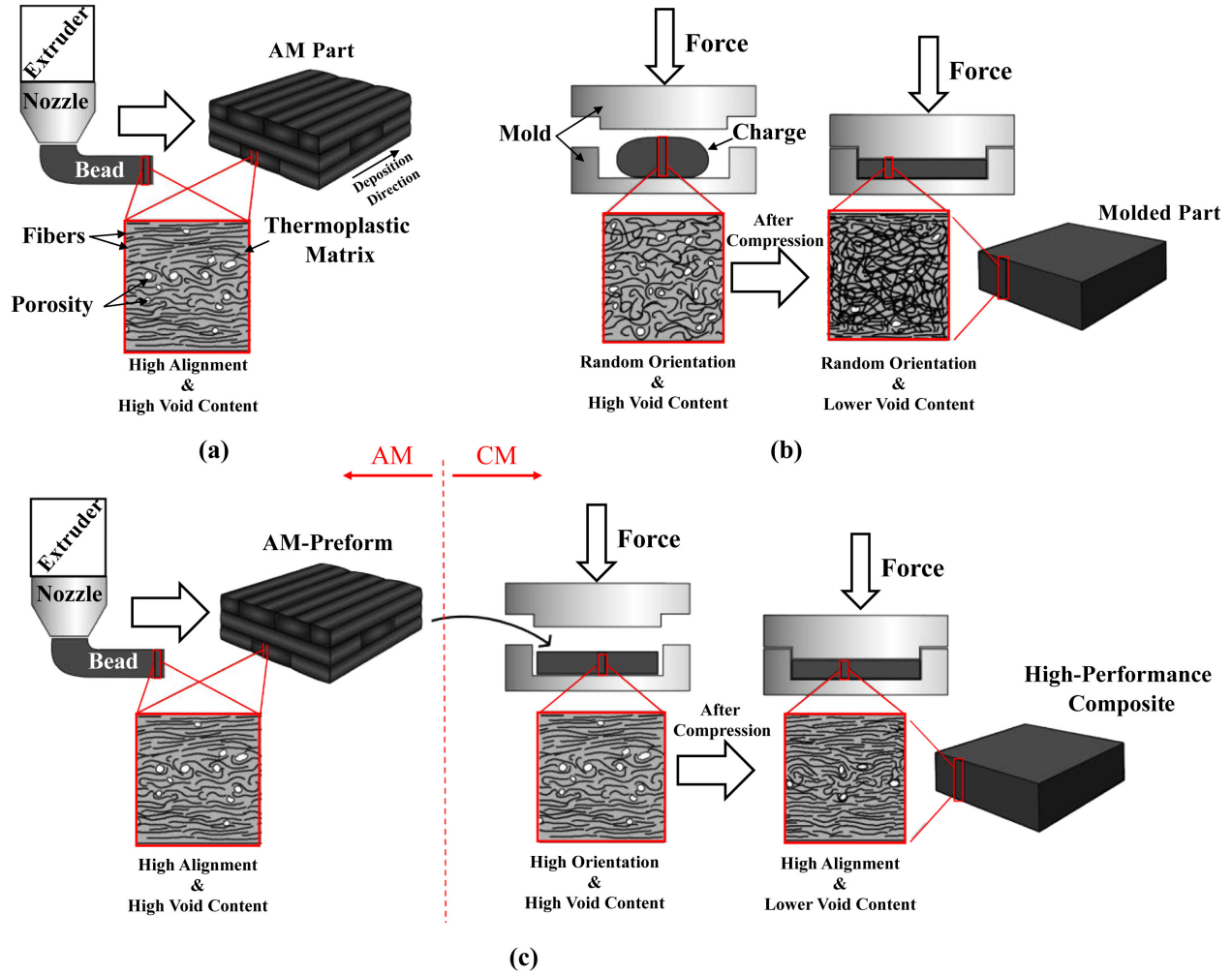
difficulty of achieving the high, spatially uniform fiber alignment required for fatigue-critical structural applications, particularly at component scales and wall thicknesses relevant to aerospace and wind-energy structures.

*(ii) Compression Molding and Extrusion Compression Molding (ECM):*

Compression molding compresses a preheated polymer-fiber mixture into a mold under controlled temperature and pressure, producing parts with lower void content and reduced porosity compared with as-deposited preforms. ECM extends this approach by extruding pelletized feedstock prior to the molding step, improving fiber length distribution control [1, 37, 38]. While both methods achieve low porosity, they typically yield non-homogeneous fiber-orientation distributions, with fiber-rich and resin-rich zones that introduce local stress concentrations and reduce fatigue resistance [37, 38]. Critically, neither method achieves the high, spatially controlled fiber alignment attainable through the AM-CM hybrid process.

*(iii) Additive Manufacturing and Integrated AM-CM:*

AM enables precise fiber alignment through nozzle-induced shear flow. When paired with CM in the AM-CM process, this hybrid technique leverages AM's microstructural control and CM's porosity reduction [1, 39], as illustrated schematically in Figure 2.2. In the specific ORNL process used for this research, a KUKA robotic arm extrudes 20 wt.% CF-ABS at approximately 1100–1200 rpm nozzle speed and 280 mm/s traverse speed [1]. The as-deposited preform is subsequently compression-molded at 523 K for 4 minutes, reducing global porosity to levels comparable to those of standalone CM while simultaneously retaining over 60% of fibers within 0°–20° of the deposition direction [1, 2]. This simultaneous achievement of controlled fiber alignment and low residual porosity, unattainable by either AM or CM in isolation, defines the microstructural quality that motivates the characterization and modeling approaches developed in this dissertation.



**Figure 2.2:** Schematic of the AM-CM process, illustrating the integration of additive deposition and compression consolidation for enhanced microstructural control: (a) AM preform deposition, (b) standalone CM, and (c) hybrid AM-CM process [1]. The AM-CM route achieves both high fiber alignment and low void content simultaneously, which motivates its selection for the CF-ABS system studied in this dissertation. The ORNL AM-CM process parameters are reviewed in Section 2.3.1 [1].

### 2.3.2 Microstructural Characterization via $\mu$ -CT

High-resolution X-ray  $\mu$ -CT is the standard tool for three-dimensional microstructural characterization of SFTs. For AM-CM SFTs,  $\mu$ -CT enables extraction of the following descriptors within representative sub-volumes:

- i. Fiber descriptors: FLD and FOD, quantified through azimuthal ( $\phi$ ) and polar ( $\theta$ ) angles of each fiber centerline (see Figure 2.1(b) for angle conventions) [30, 40].
- ii. Pore descriptors: Pore Volume Distribution (PVD), Pore Aspect Ratio Distribution (PAD), and Pore Orientation Distribution (POD), described using ellipsoidal approximations for computational efficiency [41–43].

These descriptors serve as inputs to numerical homogenization models and data-driven surrogates. A windowing approach based on the convergence of constituent volume fractions [40] ensures that the analyzed sub-volume is statistically representative of the bulk microstructure.

A capability of  $\mu$ -CT employed in this dissertation is interrupted fatigue scanning, by pausing cyclic loading at defined fatigue stages and re-scanning the same gauge volume with fiducial-marker-assisted volume registration, porosity evolution can be tracked in three dimensions on the same physical specimen without introducing additional cyclic damage. To the best of the author's knowledge, no published study has applied this approach to AM-CM SFTs, leaving the three-dimensional pore nucleation and growth kinetics under fatigue loading uncharacterized for this material class.

## 2.4 Fatigue Damage in SFTs

### 2.4.1 Overview of Fatigue Behavior

Unlike metallic alloys, which exhibit a well-defined endurance limit governed by the nucleation and propagation of a single dominant crack, SFTs undergo spatially distributed,



multi-modal damage accumulation driven by their inherently heterogeneous microstructure [23, 24, 26]. Fatigue degradation progresses simultaneously through matrix microcracking, fiber–matrix interfacial debonding, and fiber pull-out mechanisms that are spatially coupled, mutually reinforcing, and strongly exacerbated by process-induced porosity and viscoelastic self-heating [28, 44]. SFTs consequently lack a sharply defined endurance limit in the classical sense; instead, they are characterized by a HCFS that is sensitive to microstructural variability, loading conditions, and testing frequency. The HCFS, conventionally measured over  $10^6$  to  $10^8$  cycles, is a practical durability indicator but resource-intensive to determine by conventional S-N methods, a limitation that motivates the IRT-based rapid characterization framework developed in Chapter 3 and reviewed in Section 2.5.

## 2.4.2 Factors Influencing Fatigue Behavior

### *(i) Stress Ratio and Mean Stress:*

The stress ratio  $R = \sigma_{\min}/\sigma_{\max}$  and the associated mean stress significantly influence SFT fatigue life. Tensile stress ratios ( $R > 0$ ) promote fiber-bridged crack growth, whereas compressive cycling ( $R < 0$ ) accelerates matrix cracking and fiber–matrix interfacial damage. Studies on short-fiber composites report fatigue life reductions of 20–25% under fully reversed loading ( $R = -1$ ) compared with  $R = 0.1$  [45, 46]. All fatigue experiments in this dissertation adopt  $R = 0.1$ , ensuring that stress-ratio effects do not confound comparisons across Chapters 3–6.

### *(ii) Loading Frequency and Viscoelastic Effects:*

Loading frequency affects the fatigue behavior of thermoplastics such as ABS through viscoelastic mechanisms. In viscoelastic materials, cyclic loading produces a phase lag between applied stress and measured strain, resulting in energy dissipation per cycle that increases with both frequency and stress amplitude. The peak strain rate under cyclic

loading can be estimated as [47]:

$$\dot{\epsilon}_{\max} = \frac{\sigma_a}{E(N)} \cdot 2\pi f \quad (2.1)$$

where  $\sigma_a$  is the stress amplitude,  $E(N)$  is the cycle-dependent elastic modulus, and  $f$  is the loading frequency. Equation 2.1 is a first-order scaling estimate, not a quantitative prediction: it assumes a linear-elastic strain amplitude and therefore neglects the frequency-dependent complex modulus that governs the true viscoelastic response. This equation is used here only to show that higher frequencies amplify the effective strain rate  $\dot{\epsilon}_{\max}$ , which in viscoelastic thermoplastics correlates with reduced time-dependent molecular mobility and a shift from a viscous to an elastic-dominant response.

This frequency sensitivity produces two competing effects. First, higher frequencies generate more heat per unit time owing to increased hysteretic dissipation, thereby elevating the specimen surface temperature. Second and more critically for CF-ABS, higher frequencies suppress viscoelastic creep accumulation by limiting the time available per cycle for molecular chain mobility and stress relaxation. This suppression reduces cumulative displacement and shifts failure from matrix-dominated cracking to fiber-dominated fracture, and is hypothesized to increase the fatigue limit — a hypothesis examined experimentally in Chapter 3.

Studies on glass-fiber-reinforced polyamide systems report that loading frequency can affect the fatigue limit by 5–15% across typical laboratory testing ranges [3, 42]. For CF-ABS specifically, the influence of cyclic loading frequency across the 5–20 Hz range — spanning ASTM-recommended laboratory frequencies ( $\leq 5$  Hz) and representative service frequencies had not been characterized prior to the experimental work presented in Chapter 3. Dynamic mechanical analysis (DMA) confirms the glass transition temperature ( $T_g \approx 374$  K) of CF-ABS is substantially above the surface temperatures anticipated under moderate fatigue loading of thermoplastic composites, ruling out thermal softening as a

driver of frequency-dependent fatigue behavior and confirming that any observed frequency sensitivity must be viscoelastic in origin [48, 49]. The constitutive basis for this viscoelastic response is formalized by the Prony-series model in Equation 2.7 (Section 2.6.5).

*(iii) Porosity and Stress Concentrations:*

Porosity introduces local stress intensification and disrupts fiber-matrix load transfer, with severity dependent on void content, spatial distribution, and shape [50, 51]. Even at low porosity levels ( $\approx 2\%$ ), fatigue life reductions of up to 30% have been documented in short fiber composite systems [4, 52]. Pores concentrate at fiber ends and within fiber clusters — already elevated-stress locations from shear-lag load transfer — creating combined stress intensification that dramatically accelerates damage initiation [53].

Under cyclic loading, pores evolve through growth, coalescence, and crack linkage.  $\mu$ -CT studies of thermoplastic composites have quantified increases in void volume fraction ranging from 15% to over 300% between pristine and post-fatigue states, depending on the applied stress amplitude [4, 52]. How this void evolution proceeds in AM-CM SFTs specifically — in terms of three-dimensional growth rate, spatial localization, and morphological change — and how initial void content quantitatively governs the measured fatigue limit remain uncharacterized for this material system: no published study has applied interrupted  $\mu$ -CT scanning to CF-ABS across multiple specimens with deliberately varied initial void content.

*(iv) Fiber Orientation:*

Fibers aligned with the loading axis improve load-transfer efficiency and fatigue resistance, whereas off-axis orientations promote interfacial debonding at misoriented fiber ends, reducing fatigue performance by up to 40% in highly misaligned configurations compared with the aligned baseline [54].

### 2.4.3 Damage Mechanisms and Fatigue Progression

Fatigue degradation in SFTs progresses through three overlapping stages, illustrated schematically in Figure 2.3(a) and supported by synchrotron tomographic evidence in Figure 2.3(b):

i. *Early Damage — Matrix Cracking Initiation (Stage I, Figure 2.3(a)):*

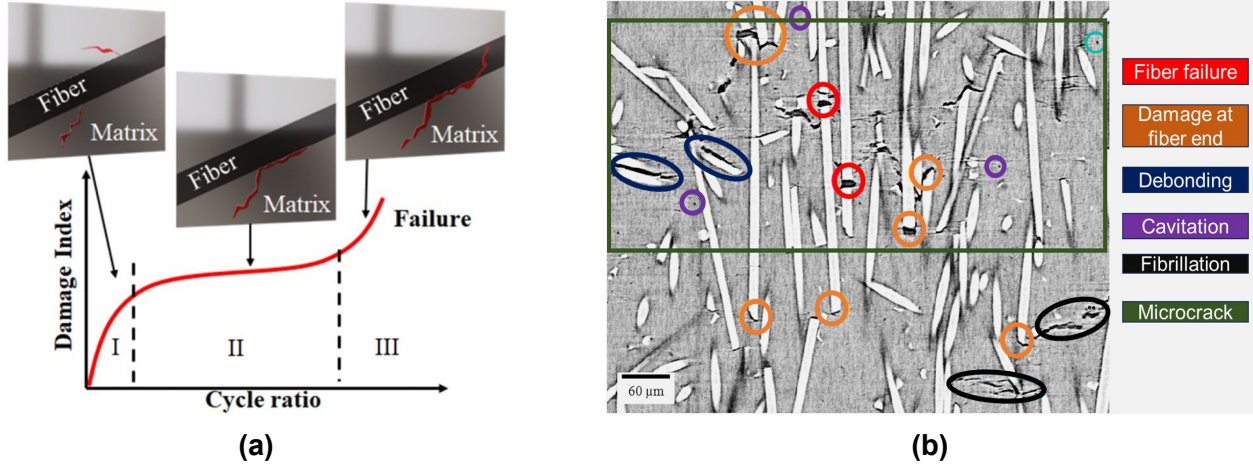
Fatigue initiation begins with matrix micro-cracking at stress concentrations near porosity sites and fiber ends. These cracks weaken load transfer between matrix and fibers and are detectable via  $\mu$ -CT as early as the pre-fatigue limit stage [23].

ii. *Gradual Degradation — Fiber-Matrix Debonding and Pull-Out (Stage II, Figure 2.3(a)):*

As cycle count increases, fiber-matrix debonding occurs as interfacial shear stresses exceed adhesion strength, leading to fiber pull-out that dissipates energy but reduces load-carrying capacity. This stage corresponds to the Phase II thermal plateau ( $\Delta T_{\text{stab}}$ ) monitored via IRT (Section 2.5.2) and captured by the CDM damage law in Equation 2.6 [55].

iii. *Critical Failure — Crack Coalescence and Fiber Fracture (Stage III, Figure 2.3(a)):*

Rapid crack coalescence, extensive debonding, and eventual fiber fracture mark the final stage, corresponding to the Phase III thermal spike in IRT measurements [56]. At higher frequencies (15–20 Hz), scanning electron microscopy (SEM) fractography reveals shorter fiber pull-out lengths and more frequent fiber breakage, consistent with elevated strain rates (Equation 2.1) limiting matrix relaxation time and promoting fiber-dominated fracture — in contrast to the extensive matrix cracking and long pull-out lengths characteristic of low-frequency (5–10 Hz) fatigue failure.



**Figure 2.3:** (a) Three-stage progressive damage index evolution over cycle ratio in SFT composites [32]: Stage I (matrix micro-cracking), Stage II (stable fiber-matrix debonding), and Stage III (crack coalescence and fracture), as described in Section 2.4.3. (b) Synchrotron X-ray microtomography of fatigue damage in short-fiber PA66, identifying fiber-end debonds, cavitation, fibrillation, and microcrack populations that serve as the micro-scale fatigue damage indicators (FDIs) tracked in Chapter 4 for AM-CM CF-ABS [33]. The three-stage trajectory in (a) is the physical basis for the stiffness degradation trajectory predicted by the GNN-LSTM surrogate in Chapter 6.

## 2.5 Fatigue Limit Assessment Using IRT

### 2.5.1 Traditional S-N Testing

The S-N curve remains a cornerstone of fatigue evaluation. For SFTs, a typical S-N dataset requires at least 15–18 specimens and multiple weeks of continuous testing, with variability from fiber orientation, porosity, and matrix properties complicating analysis [57]. Despite this high experimental cost, to the best of the author’s knowledge, no published S-N characterization exists for 20 wt.% CF-ABS manufactured via the ORNL AM-CM process, leaving the conventional fatigue limit of this specific material–process combination unestablished as a quantitative reference baseline.

### 2.5.2 Principles of IRT for Fatigue Assessment

IRT leverages infrared radiation from a specimen surface to monitor self-heating driven by fatigue damage [58]. Under cyclic loading, viscoelastic deformation and damage-related dissipative processes convert mechanical energy to heat, detectable by cooled

mid-wave infrared (MWIR) cameras with thermal sensitivities in the 20–50 mK range. Systems with megapixel spatial resolution can resolve the small temperature fluctuations (0.1–5 K) characteristic of fatigue-driven self-heating in thermoplastic composites [59], making them well-suited to the distributed damage signatures expected in heterogeneous AM-CM microstructures.

The thermal response under constant amplitude fatigue (CAF) exhibits three distinct phases: Phase I (rapid initial temperature rise), Phase II (stabilized mean temperature  $\Delta T_{\text{stab}}$ ), and Phase III (accelerating temperature rise to failure), directly analogous to the three mechanical damage stages in Figure 2.3(a). The Phase II  $\Delta T_{\text{stab}}$  increases monotonically with applied stress, forming the basis of IRT fatigue limit estimation. When combined with a staircase loading protocol — in which stress amplitude is increased in discrete increments, each maintained for a fixed number of cycles until thermal equilibrium is reached — the  $\Delta T_{\text{stab}}$  vs.  $\sigma_{\text{max}}$  relationship follows a bi-linear curve whose inflection point identifies HCFS from a single specimen [3, 60–62].

The local heat equation governing temperature evolution is [63–65]:

$$\rho C \left( \frac{\partial \theta}{\partial t} + \frac{\theta}{\tau_{\text{eq}}} \right) - k \left( \frac{\partial^2 \theta}{\partial x^2} + \frac{\partial^2 \theta}{\partial y^2} \right) = d_1 + s_{\text{the}} \quad (2.2)$$

where  $\theta = T - T_0$  is temperature variation,  $d_1$  is intrinsic dissipation,  $s_{\text{the}}$  is thermoelastic coupling, and  $\tau_{\text{eq}}$  is a heat loss time constant. IRT leverages the  $d_1$  term in Equation 2.2 as the primary damage proxy; this same dissipation quantity is the physical origin of the FFE measure defined in Equation 2.3.

### 2.5.3 Thermodynamic Framework: FFE

Cyclic self-heating reflects ongoing entropy production — a thermodynamic signature of irreversible material degradation — whose cumulative integral over the fatigue life defines

the fatigue fracture entropy as [63]:

$$\text{FFE} = \int_0^{t_f} \frac{\dot{E}_d}{T} dt \quad (2.3)$$

where  $\dot{E}_d$  is irreversible damage energy dissipated per unit time (the  $d_1$  term from Equation 2.2),  $T$  is instantaneous surface temperature, and  $t_f$  is time to failure. Naderi et al. [63] demonstrated FFE's loading-condition independence in metals, and subsequent studies extended this concept to fiber-reinforced composites.

FFE is particularly significant for the present research context. In thermoplastics like ABS, the viscoelastic energy dissipation is intrinsically rate-dependent, raising the open question of whether FFE retains its loading-condition independence in frequency-sensitive polymer-matrix systems — a question that prior literature has not addressed for any short-fiber thermoplastic composite. If confirmed, loading-condition independence would establish FFE as a frequency-invariant scalar descriptor of fatigue damage in viscoelastic composites, providing a thermodynamic basis for frequency-corrected fatigue limit estimation. Recent applications of FFE to fiber-reinforced polymer composites have extended the original metallic framework to heterogeneous, viscoelastic systems. Moghanlou et al. [66] demonstrated FFE's applicability to continuously reinforced thermoplastic composites during accelerated fatigue characterization, reporting near-constant FFE values across stress levels differing by up to 30% of  $\sigma_{\text{uts}}$ . Krairi et al. [67] incorporated thermodynamic dissipation arguments into a multiscale CDM framework for neat and SFTs, showing that cumulative entropy (Equation 2.3) is a more robust failure predictor than cycle count alone for strain-rate-sensitive matrices. These studies share a common limitation: none has systematically examined the rate-dependence of FFE across a range of loading frequencies in a short-fiber thermoplastic composite system, leaving open the fundamental question of whether FFE constitutes a genuinely rate-independent material property as demonstrated in metallic systems or an effective macroscale metric whose apparent constancy absorbs

frequency-dependent dissipation effects. This question is addressed directly by Chapter 3 of this dissertation.

## 2.5.4 IRT-Based Fatigue Limit Indicators

Several temperature-based indicators have been developed for IRT fatigue assessment, all grounded in the heat equation (Equation 2.2):

i.  $\Delta T_{stab}$  *Method*:

Pioneered by La Rosa and Risitano [58, 65], this method plots Phase II stabilized temperature against  $\sigma_{max}$  to yield a bi-linear curve defining HCFS. Step-loading protocols enable single-specimen HCFS estimation, validated against S-N curves for fiber-reinforced polymer (FRP) systems [3, 60–62]. This is the primary method used throughout Chapters 3 and 4 of this dissertation. While the  $\Delta T_{stab}$  method is the most established for estimating the high-cycle fatigue strength, its reliance on a fully stabilized Phase II thermal plateau may mask the initiation of early-stage micro-damage in materials with high process-induced microstructural variability, such as AM-CM SFTs.

ii. *Heating Rate ( $R_\theta$ )*:

The initial temperature rise rate at the start of each load step ( $R_\theta = \left. \frac{dT}{dt} \right|_{t=0}$ ) can be used to construct a bi-linear HCFS estimate analogous to  $\Delta T_{stab}$  [63, 68–72]. Originally developed for metals, its applicability to AM-CM SFTs is examined in Chapter 3.

iii. *Cooling Rate ( $R_c$ )*:

Proposed by Meneghetti [73], the cooling rate measured after interrupting fatigue at the Phase II plateau reflects thermal power loss per unit volume — a more fundamental damage indicator less susceptible to geometric effects than surface temperature itself. Whether this property translates into reduced sensitivity to geometric artifacts and the



spatially non-uniform self-heating characteristic of layered AM-CM microstructures is evaluated alongside  $\Delta T_{\text{stab}}$  and  $R_\theta$  in Chapter 3.

iv. *Second Harmonic Analysis ( $S_2$ ):*

Full-field temporal surface temperature data contain harmonic components related to thermoelastic and dissipative effects [61, 65, 74]:

$$S_m(t) = (S_0 + at) + S_1 \sin(\omega t + \phi) + S_2 \sin(2\omega t) \quad (2.4)$$

$S_m$  is the thermal signal (not radiometrically calibrated) in the time ( $t$ ) domain. In this equation,  $(S_0 + at)$  represents the increase in mean temperature, inclusive of ambient temperature effects, during cyclic mechanical loading in terms of radiometric signal,  $\omega$  is the angular frequency of the mechanically imposed cyclic load,  $\phi$  is the phase shift of the first harmonic component,  $S_1$  and  $S_2$  are related to the amplitude of the first harmonic component and the second Fourier harmonic component, respectively. Here,  $S_1$  corresponds to the signal variation associated with the thermoelastic effect, while  $S_2$  is proportional to the amplitude of the intrinsic dissipation  $d_1$  in Equation 2.2.  $S_2$  exhibits threshold behavior at the fatigue limit, providing a complementary, spatially resolved damage indicator evaluated in Chapter 3.

Existing literature often treats these IRT indicators as interchangeable, yet their relative sensitivities to damage initiation, viscoelastic background dissipation, and specimen-geometry artifacts may differ substantially in materials with high microstructural heterogeneity. Whether  $S_2$ , with its harmonic decomposition separating thermoelastic from dissipative contributions, offers superior early-warning capability relative to  $\Delta T_{\text{stab}}$  in AM-CM SFTs has not been established in the literature.

No published study has quantified the gains in accuracy, specimen efficiency, or testing speed achievable by applying IRT-based staircase protocols to AM-CM SFTs, or compared

these four indicators against a conventional S-N baseline for this material system. These represent the key unresolved practical questions motivating Chapter 3.

### 2.5.5 Stiffness Degradation and Temperature Correlation

IRT is paired with mechanical measurement tools to correlate surface thermal response with volumetric stiffness degradation [64, 75–77]. The stiffness-based damage index is defined as:

$$D(N) = 1 - \frac{E_N}{E_0} \quad (2.5)$$

where  $E_N$  is stiffness after  $N$  cycles and  $E_0$  is initial stiffness. The three-stage evolution of  $D(N)$  (Equation 2.5) mirrors the damage stages in Figure 2.3(a), and provides the physical basis for the autocatalytic and initiation-driven terms in the CDM law of Equation 2.6. Montesano et al. [64] demonstrated a direct correlation between temperature evolution and stiffness loss. Establishing this IRT–stiffness correlation for AM-CM SFTs, where process-induced microstructural variability and thermoplastic viscoelasticity complicate the thermal response, is a necessary prerequisite for using IRT as a validated proxy for the internal damage state in this material and constitutes a primary validation objective of Chapter 3.

## 2.6 Fatigue Damage Modeling

### 2.6.1 Overview

Three primary approaches exist: progressive models that track stiffness degradation (via Equation 2.5); phenomenological models that leverage energy dissipation metrics (via Equation 2.3); and micromechanical models that link microstructural features to macroscale behavior. For AM-CM SFTs specifically, accurate fatigue models must account for coupled thermomechanical effects: viscoelastic self-heating, temperature-dependent stiffness

reduction, and irreversible creep strain accumulation that are not typically addressed in constitutive frameworks developed for thermoset-matrix composites.

### 2.6.2 Progressive Damage Models

Progressive models track damage through measurable mechanical degradation. Stiffness degradation [78], a cornerstone approach, quantifies damage by tracking changes in the stress-strain hysteresis loop via the damage index  $D(N)$  (Equation 2.5). De Monte et al. [25] identified a three-stage pattern — rapid initial decline, steady-state progression, and accelerated failure, correlated with thermal effects observable via IRT (Figure 2.3(a)). Progressive damage models calibrated for thermoset composites are not formulated to account for the coupled thermomechanical effects inherent in thermoplastic fatigue. Specifically, they ignore the feedback loop between self-heating and temperature-dependent softening of stiffness, which leads to non-conservative life estimates for SFTs operating at service-relevant frequencies. Whether this three-stage pattern holds for AM-CM SFTs is examined via stiffness degradation data in Chapter 3; if confirmed, it forms the physical basis for the stiffness trajectory targeted by the GNN–LSTM surrogate in Chapter 6.

### 2.6.3 Phenomenological Models and FFE

Phenomenological models predict fatigue life based on macroscopic behavior. Hysteretic energy dissipation models relate fatigue lifetime to the area enclosed by the stress-strain hysteresis loop per cycle. Risitano et al. [58] introduced the concept that failure occurs when irreversible deformation energy reaches a material-dependent limit, whose formal expression is the FFE integral (Equation 2.3). Khonsari and colleagues [68, 72, 79] formalized FFE as a material property, demonstrating loading-condition independence in metallic systems. No systematic FFE evaluation has been reported for AM-CM CF-ABS across multiple loading frequencies, and the question of whether FFE retains its

rate-independence in a viscoelastic short-fiber thermoplastic matrix, where frequency-dependent molecular mobility introduces rate sensitivity absent in metallic systems, has not been addressed in the open literature. Establishing this is a prerequisite for using FFE as a frequency-invariant indicator of fatigue damage in this material class.

#### 2.6.4 Micromechanical and Continuum Damage Mechanics Models

Micromechanical models bridge microstructural features to macroscopic fatigue behavior. Kammoun et al.'s First Pseudo-Grain Damage (FPGD) model [80] uses mean-field homogenization to simulate anisotropic damage in pseudo-grains and has been validated on polyamide-based SFTs. Despringre et al. [81] developed a multiscale visco-damage model for a 30% glass-fiber-reinforced Polyamide 66 (PA66-GF30) composite, capturing three-stage damage kinetics consistent with Figure 2.3(a), which was implemented in Abaqus.

A particularly relevant CDM framework for this work is that of Nouri et al. [82], which proposes a thermodynamically motivated two-term damage evolution law:

$$\frac{dD_k}{dN} = \gamma_k D_k^{m_k} + \lambda_k Y_k \exp(-\delta_k N) \quad (2.6)$$

where  $Y_k$  is the thermodynamic energy release rate driving damage in mode  $k$ , and with material parameters  $\{\gamma_k, m_k, \lambda_k, \delta_k\}$ . The first term in Equation 2.6 represents autocatalytic damage propagation (Stage III in Figure 2.3a), as cracks multiply and coalesce; the second represents initiation-dominated damage (Stage I), driven by stored elastic energy that decays exponentially with cycle count. This formulation naturally produces the three-stage degradation behavior observed experimentally and captured by the damage index  $D(N)$  in Equation 2.5. The selection of the Nouri et al. CDM formulation for Chapter 6 is motivated by its physical completeness: unlike simpler power-law models, which represent

only a single damage regime, this two-term evolution law captures both the initiation-driven Stage I damage surge and the autocatalytic Stage III acceleration within a single thermodynamically consistent framework. Chapter 6 implements Equation 2.6 within a coupled thermomechanical UMAT/UMATHT subroutine in Abaqus, with four independent damage variables governing axial, transverse, in-plane shear, and out-of-plane shear degradation of the composite's transversely isotropic stiffness tensor.

### 2.6.5 Viscoelastic Constitutive Modeling for Thermoplastics

The ABS matrix in CF-ABS SFTs exhibits time- and temperature-dependent viscoelastic behavior under cyclic loading, as evidenced by DMA measurements of the frequency-dependent storage modulus and loss factor. Accurate thermomechanical fatigue simulation requires constitutive modeling that captures this behavior and the associated energy dissipation that drives self-heating (Equation 2.2).

The generalized Maxwell (Prony series) model is the standard approach for linear viscoelastic solids [83]. For Maxwell branch  $i$  and strain component  $j$ , the viscoelastic strain evolves recursively:

$$\varepsilon_{ij}^{\text{ve}}(t) = \varepsilon_{ij}^{\text{ve}}(t^-) + \Delta t \cdot p_i [\varepsilon_j^{\text{el}}(t) - \varepsilon_{ij}^{\text{ve}}(t^-)] \quad (2.7)$$

where  $p_i$  is the relaxation rate (inverse relaxation time) fitted from DMA data. The viscous energy dissipated per increment,  $W_{\text{visco}}$ , serves as the volumetric heat source in the thermal problem (the  $d_1$  term in Equation 2.2). Chapter 6 fits a three-term Prony series for the ABS matrix and implements it in the UMAT subroutine, allowing the model to capture frequency-dependent self-heating and the resulting thermal softening. Chapter 3 identifies this same mechanism as a candidate driver of the frequency-dependent fatigue limit observed in AM-CM SFTs (Section 2.4.2).

## 2.7 Multiscale Modeling and Surrogate Frameworks

### 2.7.1 Multiscale Homogenization Approaches

Fatigue prediction in SFT composites requires capturing multi-scale interactions across fiber ( $\mu\text{m}$ ), bead/mesoscale (mm), and coupon (cm) levels. Mean-field homogenization approaches, including Mori-Tanaka and related inclusion-based models, offer computational efficiency by spatially averaging reinforcement contributions within an equivalent homogeneous matrix [80, 84–87]. However, because these formulations rely on spatial averaging, they cannot explicitly represent fiber-fiber interactions, resin-rich pockets, or localized damage hotspots observable in  $\mu\text{-CT}$ -resolved microstructures [88–90]. While mean-field models provide reasonable estimates of global elastic properties, they remain fundamentally limited in capturing microstructure-driven nonlinear response and progressive stiffness degradation ( $D(N)$ , Equation 2.5). Specifically, mean-field homogenization is computationally efficient but fundamentally blind to the local fiber clustering that governs failure in AM-CM materials. Experimental and computational evidence in the SFT literature consistently shows significant variability in local effective stiffness between fiber-dense and matrix-rich regions at identical global volume fractions [88, 89] — variability that dictates damage nucleation sites and that mean-field spatial averaging suppresses by construction. Analytical extensions to the Mori-Tanaka framework, including multi-phase inclusion modifiers [84], orientation-averaging corrections [86], and two-step homogenization schemes [87] — reduce but cannot eliminate this deficiency. At AM-CM bead interfaces specifically, fiber populations from adjacent extruded beads intersect at angles determined by the deposition raster strategy, creating locally chaotic, multi-directional fiber arrangements that violate the dilute-inclusion, spatially-uncorrelated assumption underpinning all mean-field formulations. No closed-form mean-field variant can represent the discrete connectivity of fibers across a bead boundary, because this connectivity is a topological, not statistical, feature of the AM-CM microstructure. This topological character

is precisely what graph-structured representations capture natively, and what motivates the GNN approach of Section 2.7.3. Full finite element models explicitly resolve local stress concentrations from  $\mu$ -CT data but are computationally intractable for realistic specimen volumes with thousands of fibers, particularly under nonlinear fatigue-damage cycling. This dual limitation —the topology-blindness of mean-field approaches and the computational intractability of full-FE models at the specimen scale—defines the modeling gap that the GNN–LSTM surrogate frameworks of Chapters 5 and 6 are designed to address.

## 2.7.2 Voronoi Tessellation for Mesoscale Discretization

Voronoi tessellation provides a physically motivated approach to decomposing heterogeneous composite microstructures into spatially distinct, non-overlapping cells. When seeded from fiber-interaction neighborhood centroids derived from a moving-sphere sampling procedure applied to  $\mu$ -CT fiber coordinates (Section 2.3.2), the resulting Voronoi cells naturally adapt to the underlying fiber density: fiber-dense regions produce smaller cells, while matrix-rich regions yield larger cells. This topology-adaptive partitioning preserves the intrinsic structural consistency of the fiber distribution without requiring user-defined mesh parameters and provides complete volumetric coverage for subsequent FE homogenization and surrogate evaluation.

Chapter 5 combines topology-adaptive Voronoi tessellation with GNN-based encoding of the fiber interaction graph — enabling the surrogate to capture load-redistribution effects of local clustering, fiber-end stress concentrations (consistent with Figure 2.3b), and resin-rich zones that mean-field approaches cannot represent (Section 2.7.1). The Voronoi tessellation produces a partition whose cells are the natural unit of analysis for a graph-based surrogate: each cell contains a finite, variable number of fibers, whose geometric relationships govern load transfer within the cell. The fiber population within a Voronoi cell constitutes a graph — nodes are fibers, edges are pairwise interactions weighted by proximity and orientation (Equation 2.8), and the cell’s effective constitutive response is a

function of this graph’s topology. This observation is the key physical insight motivating the GNN architecture of Chapter 5: whereas conventional surrogates map scalar statistical descriptors (mean fiber orientation, volume fraction) to effective properties, a GNN operates directly on the fiber graph, preserving the discrete interaction topology that governs local load redistribution. In this framework, the Voronoi tessellation defines the graph structure from the  $\mu$ -CT fiber coordinates; the GNN learns the mechanically significant mapping from that topological structure to the effective local constitutive response.

### 2.7.3 GNN for Composite Microstructure Modeling

GNNs are a class of deep learning architectures designed to operate on graph-structured data, making them well-suited to representing discrete fiber interaction networks in SFT composites [91–94]. In a composite fiber graph, each fiber is represented as a node with features encoding its geometry (aspect ratio  $l/d$ , angles  $\phi$  and  $\theta$ , Figure 2.1b) and spatial location, while edges encode pairwise interaction weights based on proximity and orientation quantities directly motivated by shear-lag theory of load transfer in SFTs [95–101].

GNNs update node embeddings through message-passing operations that aggregate weighted information from neighboring nodes, capturing multi-fiber load redistribution effects that cannot be represented by pairwise edge weights alone. Stacked graph convolutional layers iteratively propagate these effects across the interaction network, analogous to equilibrium iterations in FE analysis.

Dai et al. [93] demonstrated the use of GNNs to predict effective properties of polycrystalline materials. Image-based convolutional neural network (CNN) approaches have also been proposed for predicting composite microstructure properties [91–94], yet this work argues that they are physically inappropriate for SFTs. Voxelizing microstructures for CNNs discards the discrete fiber graph topology—the very mathematical structure that represents shear-lag load transfer. By choosing a GNN architecture, this work frames the



surrogate not as an empirical regression tool but as a data-driven numerical implementation of shear-lag load-transfer physics, grounded in the Nairn shear-lag formulation [95]. The fiber-graph approach of Chapters 5 and 6 preserves explicit fiber-level geometry and interaction information, enabling topology-sensitive constitutive mappings.

In Chapter 5, GNN edge weights are physically informed by the Nairn shear-lag formulation [95]:

$$w_{pq} = \exp\left(-\frac{d_{pq}}{L_c}\right) (0.90 |\mathbf{t}_p \cdot \mathbf{t}_q| + 0.10) \quad (2.8)$$

where  $d_{pq}$  is the minimum segment-to-segment distance between fibers  $p$  and  $q$ ,  $L_c$  is the shear transfer length, and  $\mathbf{t}_p, \mathbf{t}_q$  are unit orientation vectors (defined using the conventions in Figure 2.1b). The two-component orientation factor in Equation 2.8 captures both the dominant cosine-dependent axial shear-lag coupling (0.90 term) and a residual orientation-independent transverse stress concentration (0.10 term) confirmed by parametric two-fiber FE analysis in Appendix D of Chapter 5.

#### 2.7.4 LSTM Networks for Path-Dependent Mechanical Evolution

LSTM networks are designed for sequence modeling tasks in which the output at any time step depends on the full history of prior inputs [102]. LSTM units maintain hidden and cell state vectors that evolve through gated update operations, enabling selective retention or forgetting of information over long sequences — making them well-suited to capturing history-dependent processes such as progressive fatigue damage accumulation (Equation 2.6) and elasto-plastic hardening.

Chen et al. [103] demonstrated LSTM networks for accelerating elasto-plastic analysis of heterogeneous materials, showing that LSTM hidden states can serve as surrogates for internal state variables, such as plastic strain and damage  $D_k$  (Equation 2.6), without requiring explicit tracking across increments. In Chapters 5 and 6, the LSTM processes the loading history as a sequence — strain increments in Chapter 5 (quasi-static) and cycle-count snapshots paired with loading condition parameters in Chapter 6 (fatigue) —

with the hidden state serving as a surrogate for accumulated matrix plasticity, damage variables, and thermal history. The GNN embedding (Section 2.7.3) is provided as a fixed conditioning signal at every sequence step, enabling the LSTM to modulate its damage accumulation trajectory based on the local fiber interaction topology of each Voronoi cell (Section 2.7.2).

### 2.7.5 Physics-Informed Machine Learning for Composites

Physics-informed machine learning (PIML) augments data-driven surrogate models with physical constraints to improve generalization, enforce thermodynamic admissibility, and reduce training data requirements [104]. Relevant constraints for composite surrogate constitutive modeling include: monotonic stiffness degradation (reflecting thermodynamic irreversibility of fatigue damage, consistent with Equation 2.6); trajectory smoothness (preventing physically implausible oscillations in  $D(N)$ ); initial stiffness consistency (anchoring the surrogate to known elastic behavior); and symmetry of the predicted stiffness tensor.

In Chapters 5 and 6, these constraints are enforced through a composite physics-informed loss function:

$$\mathcal{L} = \mathcal{L}_{\text{Huber}} + 0.05 \mathcal{L}_{\text{mono}} + 0.001 \mathcal{L}_{\text{smooth}} + 0.02 \mathcal{L}_{\text{zero}} + 0.3 \mathcal{L}_{\text{aux}} + 0.5 \mathcal{L}_{\text{peak}} \quad (2.9)$$

combining a primary strain/cycle-weighted Huber loss with auxiliary penalty terms for monotonic degradation, trajectory smoothness, zero-stress initial condition, and auxiliary physics supervision on mechanically interpretable scalar targets (initial modulus, peak stress, half-life stiffness retention, and terminal stiffness). The weights in Equation 2.9 were selected by sensitivity analysis as detailed in Chapter 5. Such regularization constrains the surrogate to physically admissible regions of the constitutive response space, thereby improving generalization to microstructural configurations underrepresented in the

training data — a critical property for AM-CM SFTs, where process-induced microstructural variability yields a wide range of fiber topologies.

### 2.7.6 Key Distinctions Between Static and Fatigue Surrogate Inputs

The quasi-static surrogate of Chapter 5 and the fatigue surrogate of Chapter 6 share the same GNN encoder (Section 2.7.3) and Voronoi assembly architecture (Section 2.7.2), but differ fundamentally in input, output, and the physical phenomena they must represent. Understanding these distinctions clarifies why the quasi-static surrogate cannot simply be applied at each cycle count as a fatigue prediction tool. A significant limitation in the current surrogate literature is the implicit assumption that quasi-static constitutive surrogates can be extended to fatigue prediction by treating cycle count as an additional input; this dissertation argues that such an extension is physically unjustified without augmenting the input space to account for frequency-dependent viscoelastic dissipation and mean-stress-driven void growth.

In the quasi-static case, the LSTM input encodes the monotonic strain trajectory and the GNN embedding encodes fiber topology; the output is a scalar stress at each strain increment. The ABS matrix damage is deterministic given the strain history: the same topology and strain path always produce the same response. In the fatigue case, the same topology under two different loading conditions  $(f_1, R_1, \sigma_{\max,1})$  and  $(f_2, R_2, \sigma_{\max,2})$  will produce fundamentally different stiffness trajectories  $C(N)$  even at the same cycle count  $N$ , because:

- (i) the viscoelastic energy dissipation rate, and hence steady-state temperature— depends explicitly on loading frequency through the Prony-series relaxation (Equation 2.7);
- (ii) the mean stress, set by  $\sigma_{\max}$  and  $R$ , governs void growth kinetics independently of the cyclic amplitude; and

- (iii) cumulative damage is path-dependent — the damage state at cycle  $N$  reflects the entire prior loading history through Equation 2.6, not just the current applied stress.

A quasi-static surrogate trained on monotonic trajectories encodes none of these dependencies and cannot reproduce the characteristic three-stage (rapid onset → stable plateau → accelerated terminal) fatigue stiffness degradation shown in Figure 2.3a. A physics-aware fatigue surrogate therefore requires a fundamentally augmented input representation that explicitly encodes loading frequency, stress ratio, and mean stress alongside fiber topology and an output representation that captures the full anisotropic stiffness tensor rather than a scalar stress response. These are not incremental changes to surrogate architecture; they reflect the qualitatively different physics that cycle-resolved fatigue prediction must represent, as detailed in Chapter 6.

## 2.8 Research Gaps and Industrial Relevance

AM-CM SFTs are already deployed in fatigue-critical structural roles, making the gaps identified below consequential rather than academic. Large-format AM-CM stiffeners are in active use in the AMERICA wind blade tip program at ORNL, where components are subjected to billions of fatigue cycles over a service life of 20–30 years. The OSHKOSH concrete truck chute represents a second industrial deployment operating under sustained cyclic loading in a demanding environment.

Beyond these current applications, the thermoplastic recyclability of CF-ABS aligns with automotive end-of-life directives, and the AM-CM process enables rapid design iteration and geometric complexity unattainable through injection molding at comparable scale—attributes that are accelerating the adoption of AM-CM SFTs in automotive, aerospace, and renewable energy structural programs. In each of these sectors, the absence of a rapid, physics-based fatigue qualification methodology is a direct barrier to component certification and safe deployment at scale.

The foregoing review reveals five specific gaps between the current state of the literature and the requirements for reliable fatigue characterization and life prediction of AM-CM SFTs. The following synthesis positions each gap against the specific body of evidence reviewed in the preceding sections, explicitly contrasting the limitations of prior work with the contributions of this dissertation.

**Gap 1** — IRT validated for metals and thermosets, not for AM-CM SFTs:

Section 2.5 established that  $\Delta T_{\text{stab}}$ ,  $R_\theta$ ,  $R_c$ , and  $S_2$  have been validated as fatigue limit indicators for metallic alloys [58, 65] and thermoset-matrix continuous-fiber composites [59, 60]. However, none of these studies examined AM-CM processed SFTs, whose layered bead architecture, controlled FOD, and ABS matrix viscoelasticity alter self-heating signatures in ways that existing calibrations cannot predict. Chapter 3 addresses this gap through a comparative four-indicator study validated against S-N data.

**Gap 2** — Frequency effects on thermoplastic SFT fatigue remain uncharacterized above 5 Hz:

Section 2.4.2 reviewed viscoelastic frequency sensitivity in PA66 and PPS systems [48, 49], and ASTM D7791 constrains laboratory testing to  $\leq 5$  Hz on precisely these grounds. Yet no published study has characterized the competing effects of hysteretic self-heating versus creep suppression on the fatigue limit of AM-CM across the 5–20 Hz range spanning laboratory and service frequencies. Whether FFE retains its loading-condition independence in this viscoelastic system — a question absent from the prior literature for any short-fiber thermoplastic — is examined directly in Chapter 3, with the goal of establishing a thermodynamic framework for frequency-corrected fatigue limit estimation in this class of material.

**Gap 3** — Porosity characterized as a static defect; its cyclic evolution untracked:

Section 2.4.2 reviewed Eshelby-based stress concentration models and  $\mu$ -CT studies that quantify initial porosity distributions [50, 53]. These treat porosity as a fixed microstructural parameter. No study has tracked the three-dimensional growth, coalescence, and redistribution of individual voids across the fatigue life of an AM-CM SFT specimen using interrupted  $\mu$ -CT (Section 2.3.2). Without this evolution data, the quantitative link between process-induced void morphology and the fatigue limit cannot be established, limiting both porosity-aware process optimization and the calibration of void-evolution damage models. Chapter 4 is designed to provide this data for the first time.

**Gap 4** — No topology-preserving surrogate exists for AM-CM SFT quasi-static response:

Section 2.7.1 demonstrated that mean-field models, even with multi-phase modifiers, are blind to local fiber topology, and Section 2.7.3 established that CNN-based surrogates discard the discrete fiber graph that represents shear-lag load transfer. The graph-based GNN approach reviewed in Section 2.7.3 has been demonstrated for polycrystalline metals [93] but not for discontinuous-fiber thermoplastic composites, where variable fiber counts per cell, orientation distributions, and process-induced topological variability pose qualitatively different representation challenges. Chapter 5 addresses this gap by developing a shear-lag-informed GNN–LSTM surrogate to be validated against  $\mu$ -CT-resolved FE homogenization data.

**Gap 5** — Surrogate models encode microstructure or loading conditions, never both:

Section 2.7.6 established that quasi-static surrogates cannot predict cycle-resolved stiffness degradation without explicitly encoding loading frequency (governing the viscoelastic dissipation rate, Equation 2.7), stress ratio (governing mean-stress-driven void growth), and cumulative damage history (Equation 2.6). Existing fatigue surrogates in the literature either parameterize loading conditions without accounting for microstructural topology [84] or encode topology without accounting for loading-condition dependence. No framework

jointly maps  $\mu$ -CT fiber topology and the full loading quadruplet  $(N, f, R, \sigma_{\max})$  to the cycle-dependent stiffness matrix. Chapter 6 closes this gap with an extended GNN–LSTM architecture that simultaneously encodes topology via graph convolutions and loading history via an LSTM decoder conditioned on all four loading parameters.

## 2.9 Summary

This chapter has reviewed the state of the art across five interlocking research domains: SFT manufacturing and microstructural control; fatigue damage mechanisms and their governing factors; IRT- and thermodynamics-based fatigue assessment; continuum damage and viscoelastic constitutive modeling; and multiscale, graph-based surrogate modeling. Across each domain, the literature is broad and methodologically mature for metallic alloys, thermosets, and select short-fiber thermoplastic systems such as glass-fiber and carbon-fiber reinforced polyamide, but consistently stops short of the process–microstructure–fatigue coupling specific to AM-CM SFTs.

Taken together, the critical synthesis of Section 2.8 identifies five specific gaps that persist despite this breadth: IRT indicators unvalidated for AM-CM SFTs; frequency-dependent fatigue behavior uncharacterized above 5 Hz; porosity evolution untracked in three dimensions under cyclic loading; the absence of a topology-preserving quasi-static constitutive surrogate; and the absence of a surrogate that jointly encodes microstructural topology and full fatigue loading conditions. These five gaps, grounded in the specific limitations identified across the reviewed literature, define the scope and motivate the contributions developed in Chapters 3–6.

## Chapter 3

### Rapid Fatigue Characterization via Infrared Thermography: Validation and Parametric Study

#### 3.1 Introduction

This chapter addresses Gaps 1 and 2 from Chapter 2: the absence of validated IRT-based fatigue-limit indicators for AM-CM SFTs, and the uncharacterized effect of loading frequency on their fatigue behavior. Conventional S-N testing requires 15–18 specimens and several weeks of continuous testing, a cost incompatible with the rapid characterization this material class demands.

Passive IRT offers an efficient alternative, using the self-heating response under cyclic loading as a non-invasive proxy for the evolving damage state. Four indicators from the literature —  $\Delta T_{\text{stab}}$ ,  $R_{\theta}$ ,  $R_c$ , and  $S_2$  — are evaluated here for AM-CM SFTs for the first time, whose controlled fiber alignment and low residual porosity may alter their self-heating signature relative to injection-molded counterparts. Using two AM-CM panels differing only in bead extrusion speed, this chapter validates these indicators against conventional S-N and stiffness-degradation benchmarks (Section 3.3) and applies them to characterize loading frequency, stress ratio, and fiber orientation effects (Section 3.4).

#### 3.2 Materials and Methods

##### 3.2.1 Material Preparation

This study investigated two material systems: neat ABS and ABS reinforced with 20 wt.% chopped carbon fibers. Two CF-ABS panels were manufactured via the AM-CM

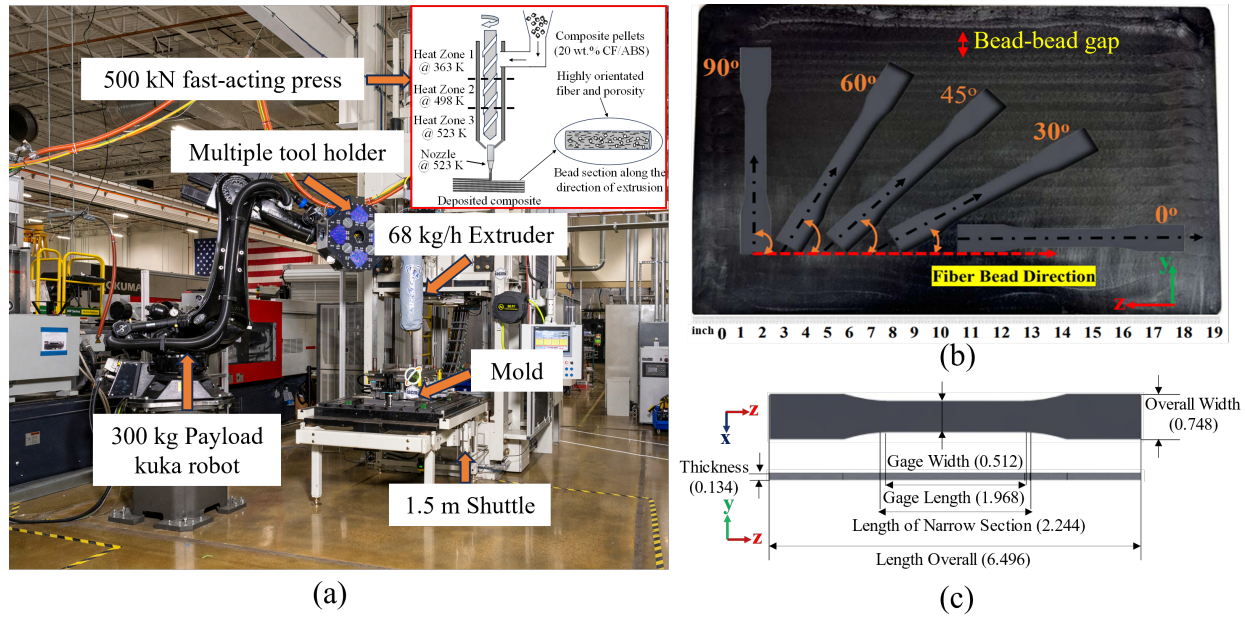


process at ORNL, differing exclusively in bead extrusion speed. **Panel A** employed a standard 1x bead speed (extrusion speed equal to the bed traverse speed  $\approx 1200$  rpm) and serves as the IRT validation panel; **Panel B** employed a reduced 0.9x bead speed (i.e. 1100 rpm) and is used for systematic parametric investigations of loading frequency, stress ratio, and fiber orientation.

The reinforcement phase consisted of high-tenacity (HT) Kaltex K20-HTU chopped carbon fibers with a nominal filament diameter of  $8\text{ }\mu\text{m}$  and as-processed lengths ranging from 25 to  $350\text{ }\mu\text{m}$ . In the first step of the AM-CM process, ABS pellets and chopped carbon fibers were blended and deposited using a single-screw extruder mounted to a KUKA robotic arm. The arm operated at a motor speed of 1200 rpm (Panel A) and a deposition nozzle speed of 280 mm/s, with a constant 9.88 mm standoff between the nozzle tip and the substrate surface. The extruder comprised four independent heating zones, with temperature increasing progressively from 363 K in Zone 1 to 523 K in Zone 4 (Figure 3.1a), yielding a highly aligned AM preform whose fiber architecture is governed by the deposition kinematics.

In the second step, the as-deposited preform was transferred to a 250-ton fast-acting hot press (Carver Press, Model 3895.4NE10000) for compression molding at 523 K for 4 minutes. This consolidation step produced flat composite panels with nominal dimensions of  $450\text{ mm} \times 300\text{ mm} \times 3.5\text{ mm}$  (Figure 3.1b). The AM-CM process uniquely combines AM's capacity for preferential fiber alignment with CM's ability to reduce porosity, enhancing mechanical performance relative to either process alone [1].

Specimens were machined at different angles relative to the bead direction ( $0^\circ$ ,  $30^\circ$ ,  $45^\circ$ ,  $60^\circ$ , and  $90^\circ$ ) using abrasive waterjet machining following ASTM D638 Type I specimen dimensions (Figure 3.1c) [105]. Prior to all mechanical testing, specimen surfaces were verified to be within the required flatness and dimensional tolerance limits.

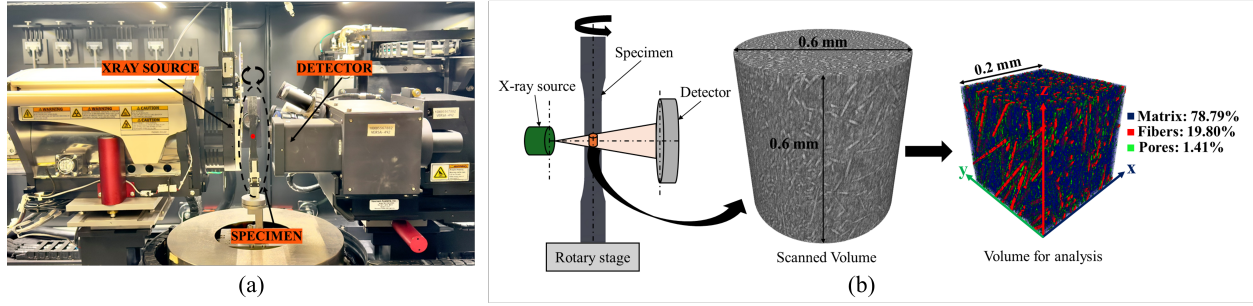


**Figure 3.1:** (a) Robotic arm and fast-acting press used in the AM-CM process at ORNL, (b) schematic of AM-CM composite panel with fiber bead direction and differently oriented specimens, and (c) ASTM D638 Type I specimen dimensions used for waterjet cutting and subsequent quasi-static and fatigue testing.

### 3.2.2 Microstructural Characterization

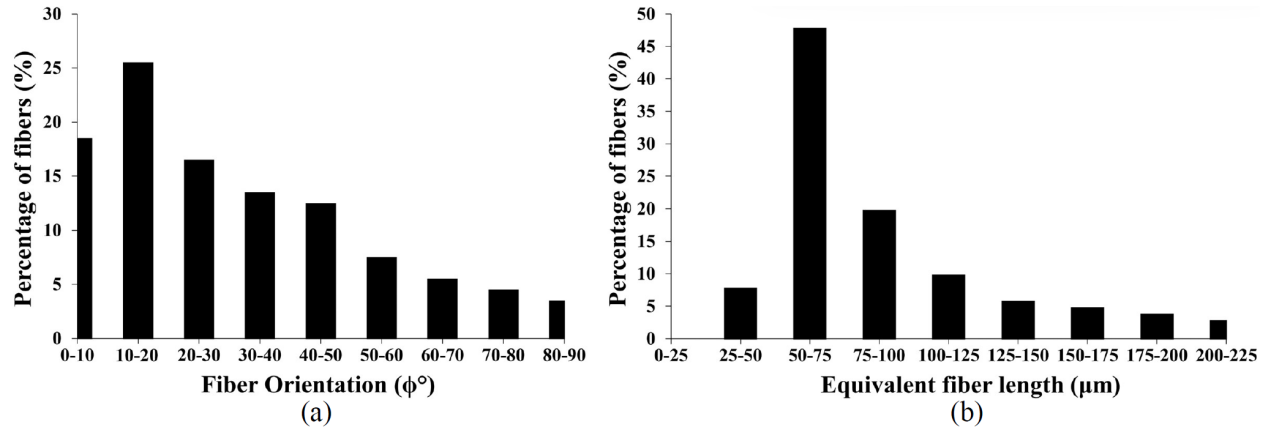
Three-dimensional microstructural characterization was performed using high-resolution X-ray  $\mu$ -CT on a Zeiss Xradia 620 Versa system at Auburn University (Figure 3.2a). Each specimen was mounted on a precision rotary stage oriented perpendicular to the incident X-ray beam, at a source-to-sample distance of 28 mm and a sample-to-detector distance of 36 mm (Figure 3.2b). Projection data were acquired at an accelerating voltage of 140 kV and a beam power of 21 W, using a  $4\times$  scintillator objective lens with  $2 \times 2$  pixel binning, yielding an isotropic voxel resolution of  $0.6 \times 0.6 \times 0.6 \mu\text{m}^3$ .

Volumetric reconstruction was performed using filtered back-projection algorithms with non-local means denoising and intensity-based threshold segmentation. FODs and FLDs were extracted quantitatively using Avizo 9.3.0 with the automated XFiber tracking module. Porosity characterization in Dragonfly PRO (Version 3.5) revealed a global void content of approximately 2% for Panel A, with the majority of pores smaller than the nominal fiber



**Figure 3.2:** (a) Zeiss Xradia 620 Versa system at Auburn University, and (b) schematic of the scanning process.

diameter ( $8 \mu\text{m}$ ). For Panel A, the print parameters resulted in  $\approx 60\%$  fiber alignment within  $0^\circ$ – $30^\circ$  of the deposition direction, with a typical fiber length of  $50$ – $75 \mu\text{m}$  in the bead direction (Figure 3.3). For Panel B ( $0.9\times$  bead speed), optimized print parameters yielded up to  $80\%$  fiber alignment within  $0^\circ$ – $30^\circ$ , with a typical fiber aspect ratio of  $5$ – $7$  and an average fiber diameter of  $8 \mu\text{m}$ .



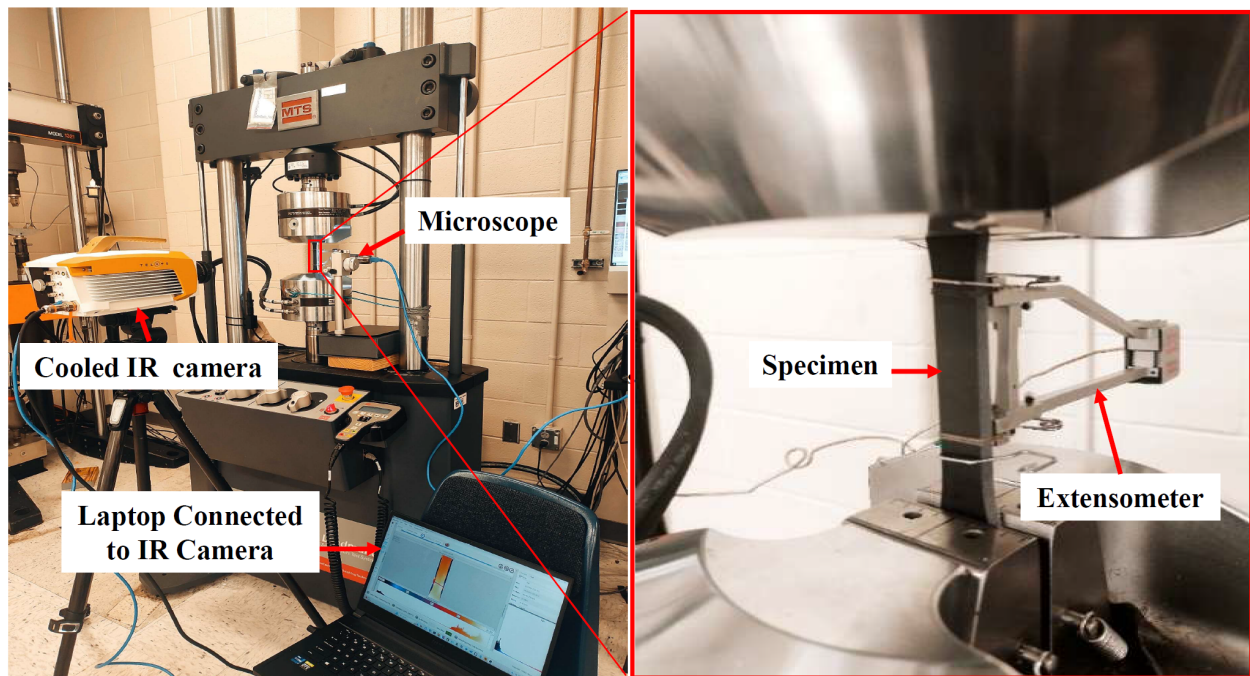
**Figure 3.3:** Panel A: (a) Statistical distribution of fiber orientations, and (b) statistical distribution of fiber lengths measured from  $\mu$ -CT.

### 3.2.3 Quasi-Static Testing

All quasi-static and fatigue tests for  $0^\circ$  bead-aligned specimens were performed using a material testing system (MTS) Landmark servohydraulic universal test frame (Model 370.25, 100 kN capacity), as depicted in Figure 3.4. Quasi-static tensile tests were conducted at a  $2 \text{ mm/min}$  displacement-controlled loading rate to determine the baseline mechanical

properties of each specimen set. Specimen strains were monitored using an extensometer with a 5 cm gauge length.

For Panel A (1x bead speed), five specimens were evaluated, yielding a mean ultimate tensile strength ( $\sigma_{uts}$ ) of  $64.52 \pm 2.17$  MPa, failure strain ( $\epsilon_f$ ) of  $0.82 \pm 0.01\%$ , and initial elastic modulus ( $E_0$ ) of  $8.32 \pm 0.02$  GPa. These values established the baseline stress amplitudes for the subsequent IRT staircase and S-N fatigue testing on Panel A. The consistency of properties across five replicates confirmed uniform FOD and FLD along the primary bead deposition direction.



**Figure 3.4:** Experimental setup for in-situ surface temperature measurements, featuring a cooled IR camera connected to a laptop with Reveal Infrared (IR) software, integrated with a Universal Testing Machine (UTM) system and a 5 cm gauge-length extensometer.

### 3.2.4 Fatigue Testing Approach

#### IRT cyclic step Loading:

Tension-tension fatigue was conducted with a stress ratio  $R = 0.1$  under sinusoidal load-controlled mode, with maximum and minimum loads determined as percentages of

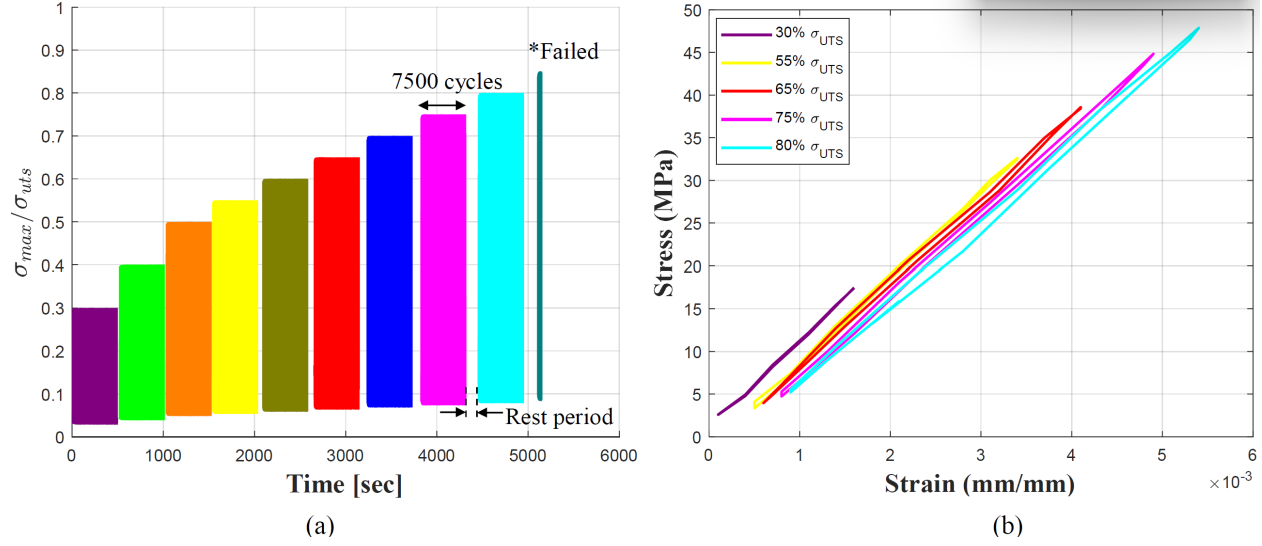
the average  $\sigma_{\text{uts}}$  from quasi-static testing. The loading frequency for IRT staircase tests was maintained at 15 Hz. Grip pressure was consistently maintained at approximately 200 psi to prevent specimen slippage.

A Telops Spark M150 MWIR camera equipped with an InSb-cooled detector ( $640 \times 512$  pixel resolution, 50 mm lens, noise-equivalent temperature difference (NETD) of 20 mK, spectral range 3–5.4  $\mu\text{m}$ ) was used for all in situ temperature measurements. Thermal images were captured at a 100 Hz acquisition frequency, yielding multiple temperature measurements per load cycle and enabling harmonic analysis to characterize anelastic dissipative effects, as described in Eq. 2.4 [72]. The region of interest (ROI) was restricted to a 13 mm  $\times$  13 mm area centered around the specimen failure zone. All thermographic data were extracted using Reveal IR software and processed in MathWorks MATLAB software (MATLAB ver. R2022b).

Figure 3.5 shows the staircase cyclic loading profile at constant  $R = 0.1$  and 15 Hz, following the approach outlined in [5, 61, 64, 76]. HCFS is identified as the inflection point of the bi-linear  $\Delta T_{\text{stab}}$  versus  $\sigma_{\text{max}}$  curve. The step size ( $N_{\text{step}}$ ) was set to 7,500 cycles, determined from trial tests to ensure a well-defined Phase II stabilized plateau at every load level (Figure 3.5a). A minimum of three replicates was tested at each condition. After each load step, testing was stopped, and the specimen was allowed to cool to ambient room temperature (the ‘rest period’ in Figure 3.5a). Following each rest period, a static test was performed to estimate stiffness degradation as a function of the number of applied load cycles.

### **Traditional S-N Testing:**

In parallel with the IRT staircase testing, conventional S-N reference data were generated for Panel A CF-ABS specimens. CAF tests were conducted at maximum stress levels of 70%, 65%, 60%, 55%, 50%, and 35%  $\sigma_{\text{uts}}$  at 5 Hz under  $R = 0.1$ , in compliance with ASTM D7791 [105] to prevent macroscopic self-heating effects that would confound



**Figure 3.5:** Staircase loading profile to determine HCFS rapidly: (a) early increments of 10%  $\sigma_{uts}$  followed by 5%  $\sigma_{uts}$  increments to  $\sigma_{max}$  at  $R = 0.1$  and 15 Hz; rest periods allow cooling to ambient temperature after each step load. (b) Hysteresis energy at a given load level at  $N = 5000$  cycles.

the stiffness measurements. Three replicates were tested at each load level. Specimens surviving  $3 \times 10^6$  cycles were treated as run-out, consistent with literature [62, 77].

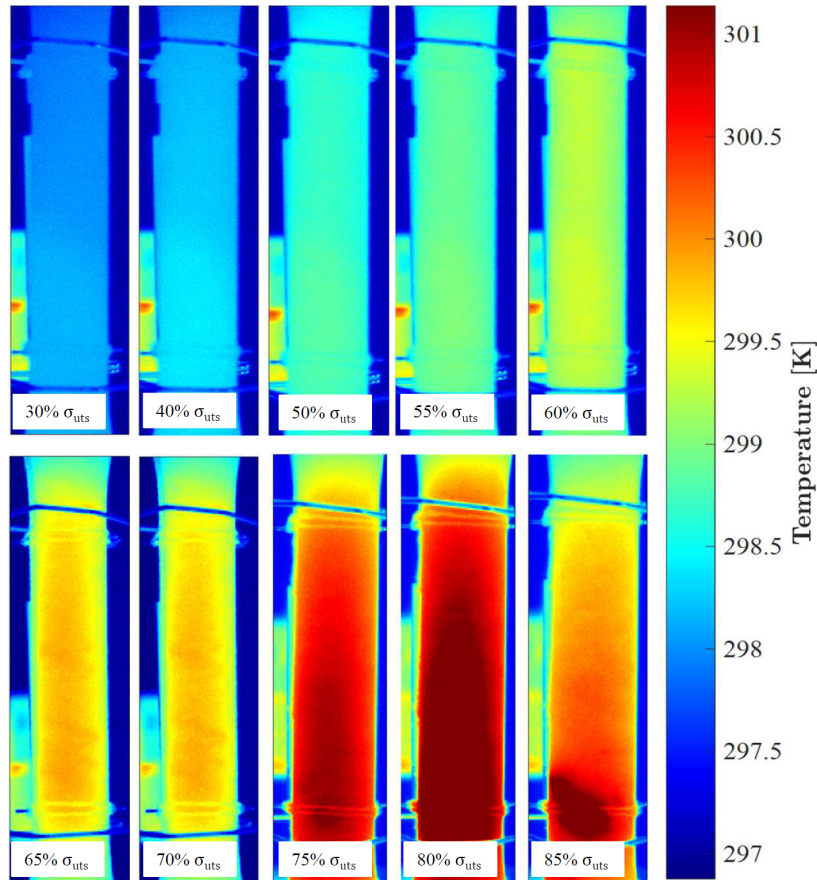
### 3.3 IRT Indicator Validation

#### 3.3.1 Cyclic Temperature Stabilization and Stiffness Degradation

Figure 3.6 shows the representative full-field surface temperature evolution of a 20 wt.% CF-ABS specimen under staircase fatigue loading (Figure 3.5). Each thermogram corresponds to the stabilized Phase II temperature at the indicated load level, with the region of maximum temperature within the gage section identified from the full-field data. The temporal evolution of this maximum temperature is plotted in Figure 3.7a for each applied step; the temperature at the start of each step is ambient room temperature after the intervening rest period. At higher applied load levels, the distinctive Phase II-stabilized plateau is absent, indicating rapid irreversible damage growth. The specimen ultimately failed at 85%  $\sigma_{uts}$ , and the spatial location of the maximum temperature coincides precisely



with the final failure site, confirming that thermal localization is a reliable precursor to structural failure in AM-CM SFTs.



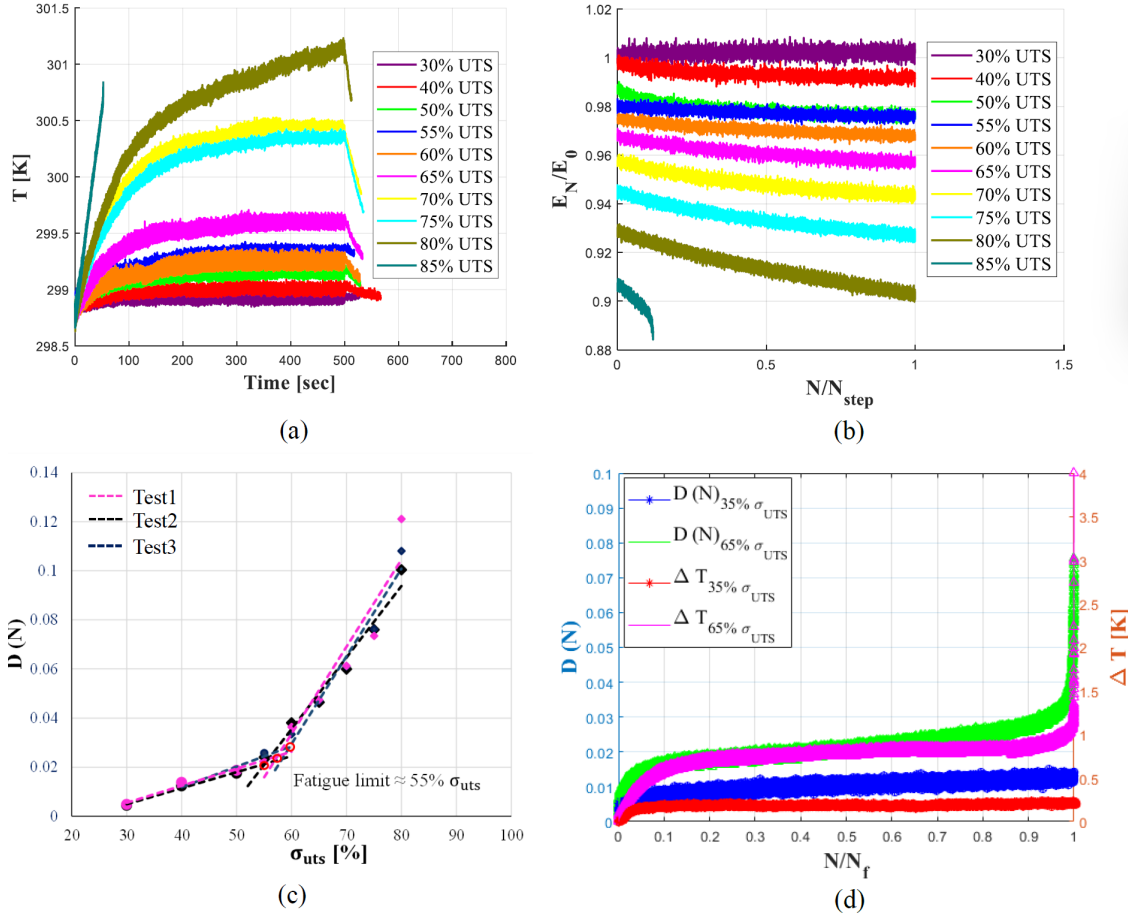
**Figure 3.6:** Change in specimen surface temperature profile of a CF-ABS specimen with increasing loading cycles from the start of the experiment to failure. The applied load level is indicated in each sub-figure.

An extensometer was used throughout the fatigue testing to correlate the temporal evolution of surface temperature resulting from self-heating under fatigue loading with the corresponding degradation of volumetric stiffness. The extensometer provides a conductive heat dissipation pathway; however, the maximum mean temperatures consistently coincide with the location of damage incipience and eventual final failure. Figure 3.7b depicts the stiffness degradation of the test specimen under step loading. The stiffness degradation represents a characteristic progressive damage behavior wherein the damage magnitude gradually increases before final failure (approximately 12% in this case) [64]. Figure 3.7d

illustrates the temporal temperature and stiffness data for two applied CAF levels, namely 35%  $\sigma_{\text{uts}}$  and 65%  $\sigma_{\text{uts}}$ . The data are plotted against the normalized life  $N/N_f$  of the specimen, where  $N_f$  denotes the failure life for the corresponding applied CAF. For 35%  $\sigma_{\text{uts}}$  CAF,  $N_f$  was chosen to be  $3 \times 10^6$  cycles, the maximum number corresponding to a run-out test. Surface temperatures were recorded throughout the CAF tests. The two load levels have been selected to illustrate the damage-temperature correlation for two load cases, one below and the other above the fatigue limit. It is observed that the two parameters are closely correlated, similar to the results presented in [77]. Nevertheless, while surface temperature is a viable measure of fatigue, specific heat dissipation per unit volume could offer a more accurate indicator, given that surface temperatures typically depend on loading frequency and specimen geometry. Process defects in AM-CM composites frequently produce thermal hot spots. In the current examination of phenomenological models, findings from pristine specimens have been compiled for analysis, supported by the uniform temperature across the gage section, as shown in Figure 3.6.

A note on the damage mechanisms in SFTs: fiber-matrix interfacial friction followed by debonding has been recognized as the dominant failure mode in the selected SFTs, as corroborated by others [106–108]. Theoretically, the fiber ends of a chopped short fiber have a very high stress concentration factor; these fiber ends act as heat sources upon cyclic load application. With increasing load cycles, debonding at the fiber-matrix interface progresses, and damage incipience occurs at the fiber ends. This debonding mode progresses in a stable manner over time, as represented by phase II of the temperature evolution curve at each load step. Eventually, a significant number of fiber-matrix debonds occur, leading to final failure accompanied by a temperature surge (phase III). SEM conducted on the failed surfaces confirms that fiber matrix debonding is the predominant damage mode, as elaborated in section 3.4.7.



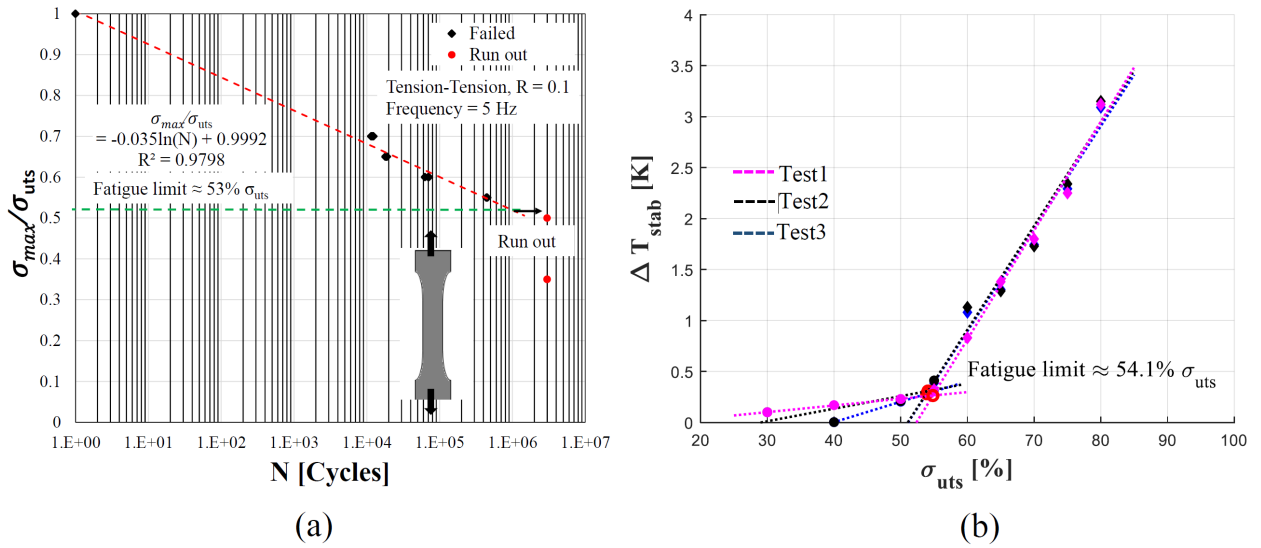


**Figure 3.7:** (a) Maximum surface temperature evolution of a 20 wt.% CF-ABS specimen under staircase loading with rest periods between steps. (b) Stiffness degradation measured by an extensometer under staircase loading. (c) Damage evolution under staircase loading showing bilinear behavior similar to  $\Delta T_{stab}$ . (d) Damage and temperature correlation for CAF at 35%  $\sigma_{uts}$  and CAF at 65%  $\sigma_{uts}$  at 5 Hz.

### 3.3.2 Fatigue Limit Comparison: IRT versus S-N Curve

The temperature evolution plots in Figure 3.7a show how  $\Delta T_{stab}$  varies with  $\sigma_{max}$ . Up to an applied  $\sigma_{max} = 50\% \sigma_{uts}$ , the temperature remained uniform across the specimen surface (see Figure 3.6). However, as the load level increases, a distinct ‘hot zone’ emerges, corresponding to the location of damage incipience in the specimen, followed by eventual failure (Figure 3.6). The temperature stabilizes over a brief range of cycles before failure. Figure 3.8b illustrates the temperature increase plotted against the maximum applied stress, revealing a clear point at which the increase in dissipated heat is more

pronounced, representing an approximate fatigue limit of 54%  $\sigma_{uts}$ . In addition to IR fatigue testing, conventional S-N curve results are shown in Figure 3.8a, yielding a fatigue limit of approximately 53%  $\sigma_{uts}$  at 5 Hz, very close to that obtained from IRT. However, it should be noted that, to obtain the S-N curve for the 20% CF-ABS panels, 18 specimens were tested (three replicates at each load level) over more than two weeks. On the other hand, the IRT fatigue testing was conducted using only three specimens in a total of 5 hours. Thus, the IRT approach provides an accelerated testing framework for rapidly estimating the fatigue limit.

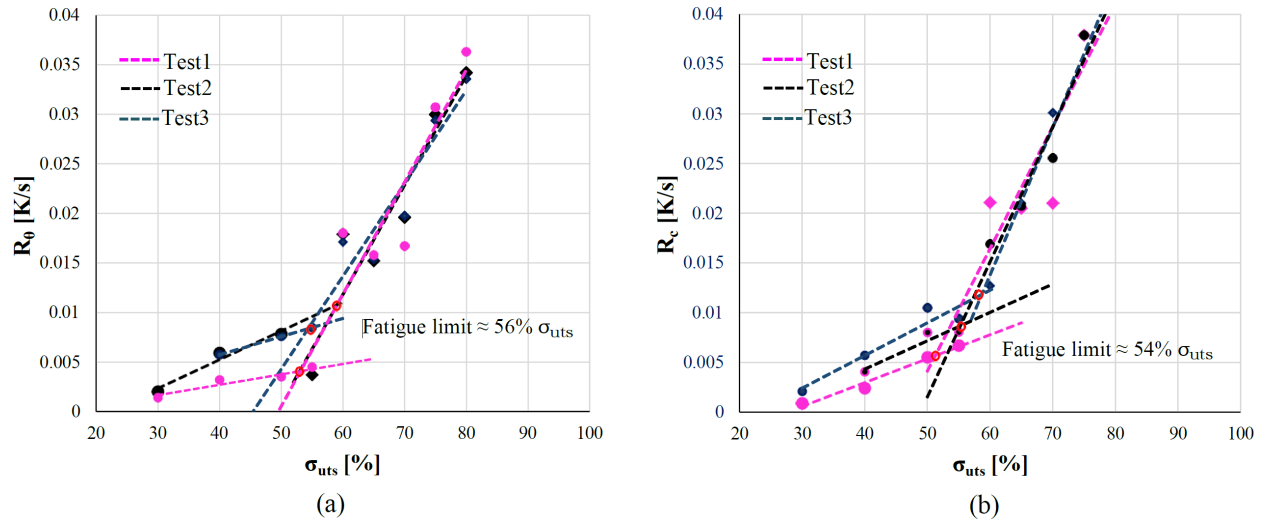


**Figure 3.8:** (a) S-N curve-based fatigue limit estimation at 5 Hz. (b) Bi-linear  $\Delta T_{stab}$  approach to fatigue limit estimation at 15 Hz.

### 3.3.3 Rate of Heating ( $R_\theta$ ) and Cooling Index ( $R_c$ )

The initial  $R_\theta$  and the  $R_c$  are barometers of the state of damage in a specimen, as discussed in Section 2.5.4. Methodically, the initial temperature rise is measured at the start of every new load step, and the tests are stopped after each loading cycle to measure the cooling rate. Figure 3.9 depicts the estimation of fatigue limit using these measured  $R_\theta$  and  $R_c$ , adopting the bi-linear approach described for  $\Delta T_{stab}$  in Figure 3.8 b. The analysis reveals a consistent trend: the material's temperature rate gradually increases at low

stress levels. However, as the applied stress magnitude increases, the rate of damage development is also expected to increase, as evidenced by increasingly pronounced temperature fluctuations. The  $R_c$  also captures this effect. These results are particularly useful for designing experiments to assess a component's remaining life. Since heating and cooling rates depend on the state of damage in a system, these indicators could potentially yield valuable information about the state of damage in a structure with an unknown load history [71, 73]. The fatigue limits predicted by  $R_\theta$  and  $R_c$  are relatively close, 56%  $\sigma_{uts}$  and 54%  $\sigma_{uts}$ , respectively. The  $R_\theta$  and  $R_c$  values diverge for load levels that cause significant damage within the load step; in this case, at load levels beyond 70%  $\sigma_{uts}$ .



**Figure 3.9:** Bi-linear approach to fatigue limit estimation using: (a)  $R_\theta$  approach, (b)  $R_c$  approach.

### 3.3.4 Second Harmonic Analysis ( $S_2$ )

As outlined in Eq. 2.4, harmonic analysis of temporal temperature data is a commonly employed method to discern the onset and progression of damage [62, 65]. Specifically, the  $S_1$  is associated with the thermoelastic stress analysis (TSA) effect, while the  $S_2$  captures the influence of dissipative mechanisms. The choice of a temperature data acquisition rate (100 Hz) and loading frequency (15 Hz) facilitated harmonic analysis of the thermal signals. Figure 3.10 depicts the evolving  $S_2$  signals in the vicinity of the final failure location, starting

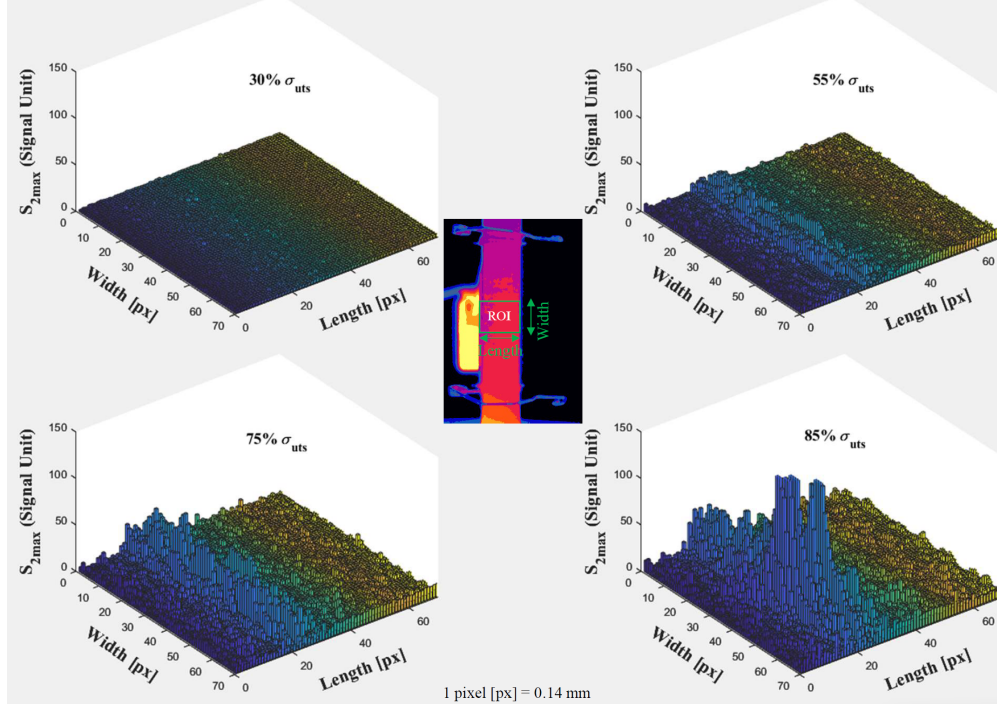
from 30%  $\sigma_{uts}$  till eventual failure at 85%  $\sigma_{uts}$ . Harmonic analysis of the temperature signals was conducted at each load level to ensure the specimen had reached the steady-state phase II region.

A noteworthy observation is a steady increase in the radiometric temperature signal throughout each loading stage (see Figure 3.11a). This trend is primarily influenced by the viscoelastic properties inherent in the matrix material [65]. A significant spike in the signal becomes apparent when damage mechanisms are initiated, with  $S_2$  exhibiting pronounced variations when stress exceeds 55% of  $\sigma_{uts}$ . The 98<sup>th</sup> percentile of  $S_2$  over the chosen ROI is chosen for further analysis to exclude the influence of vibration or other effects that might influence the temperature signals. Residuals of the 98<sup>th</sup> percentile  $S_2$  signal were evaluated following the approach recommended in [74], as shown in Figure 3.11b.

Analyzing the signal dynamics over individual sub-steps reveals a generally consistent trend: the 98<sup>th</sup> percentile  $S_2$  residuals exhibit threshold behavior, below 55%  $\sigma_{uts}$ , and no significant  $S_2$  residual signals are present. This indicates that the thermographic parameters are independent of the number of cycles at low stress levels. The identified threshold of 55%  $\sigma_{uts}$  represents the material's fatigue limit using the described harmonic analysis. Conversely, using  $S_{2max}$  versus  $\sigma_{max}$  plots overestimates the fatigue limit, yielding 58%  $\sigma_{uts}$ .

### 3.3.5 Comparative Analysis of IRT Methods with Stiffness Degradation

As noted in Section 3.1, establishing a correlation between IRT-observable surface temperatures and volumetric stiffness degradation is a prerequisite for validating IRT-based fatigue limit characterization. Figure 3.12 illustrates damage ( $D(N)$ ) correlation with the derived fatigue limits for the chosen staircase loading at 15 Hz frequency, considering  $\Delta T_{stab}$ ,  $S_{2max}$ ,  $R_\theta$ , and  $R_c$ . All IRT methods yield consistent estimates of the fatigue limit and exhibit a certain degree of scatter while comparing well with volumetric stiffness degradation (Table 3.1). The close fatigue limit values obtained using  $\Delta T_{stab}$ ,  $R_\theta$ , and

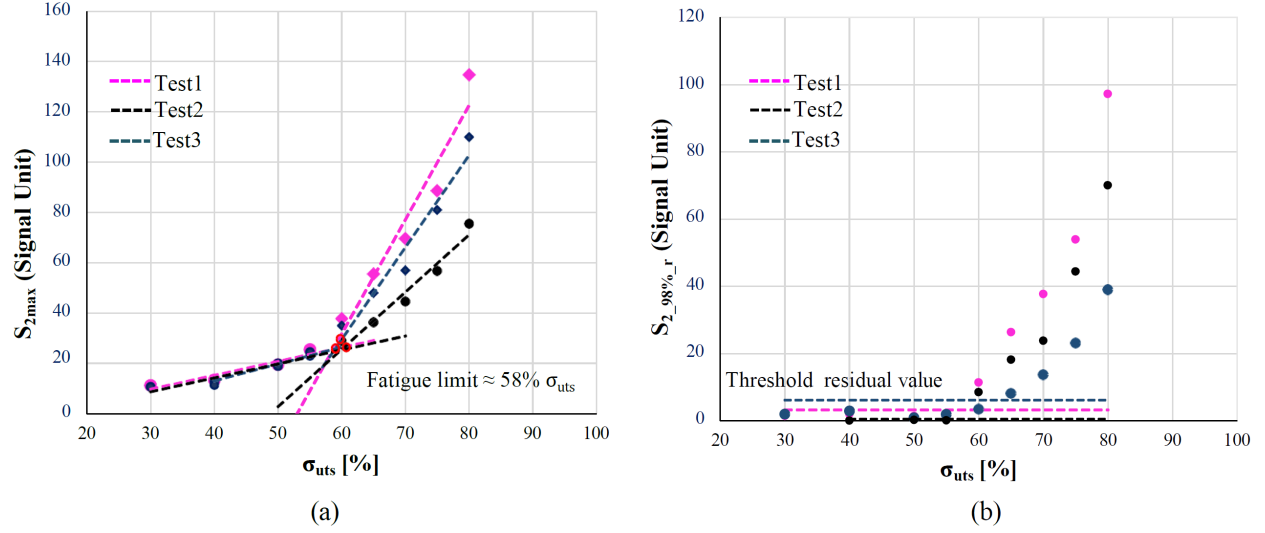


**Figure 3.10:** Surface map of the thermographic  $S_2$  signal.

$R_c$  can be attributed to their dependence on temperature change and energy dissipation, which also aligns with the close fatigue limit value obtained by the  $D(N)$  method. On the other hand,  $S_{2max}$  is more sensitive to thermomechanical coupling and microstructural changes, such as matrix cracking or fiber realignment. These changes may not be as pronounced in the early stages, resulting in a higher fatigue limit obtained using this method than others. An average fatigue limit of approximately  $54\% \sigma_{uts}$  was found across all IRT methods, demonstrating their reliability and robustness.

**Table 3.1:** Summary of comparison of all IRT approaches (all values as  $\% \sigma_{uts}$ ).

| Sample Number                 | $\Delta T_{stab}$ | $D(N)$           | $R_\theta$       | $R_c$            | $S_{2max}$       |
|-------------------------------|-------------------|------------------|------------------|------------------|------------------|
| 1                             | 54.92             | 54.40            | 54.90            | 51.70            | 58.10            |
| 2                             | 53.50             | 55.00            | 55.10            | 53.80            | 59.30            |
| 3                             | 54.10             | 58.30            | 58.00            | 58.10            | 57.80            |
| Average ( $\% \sigma_{uts}$ ) | $54.10 \pm 0.78$  | $55.56 \pm 2.25$ | $56.05 \pm 1.73$ | $54.47 \pm 3.24$ | $58.41 \pm 0.79$ |

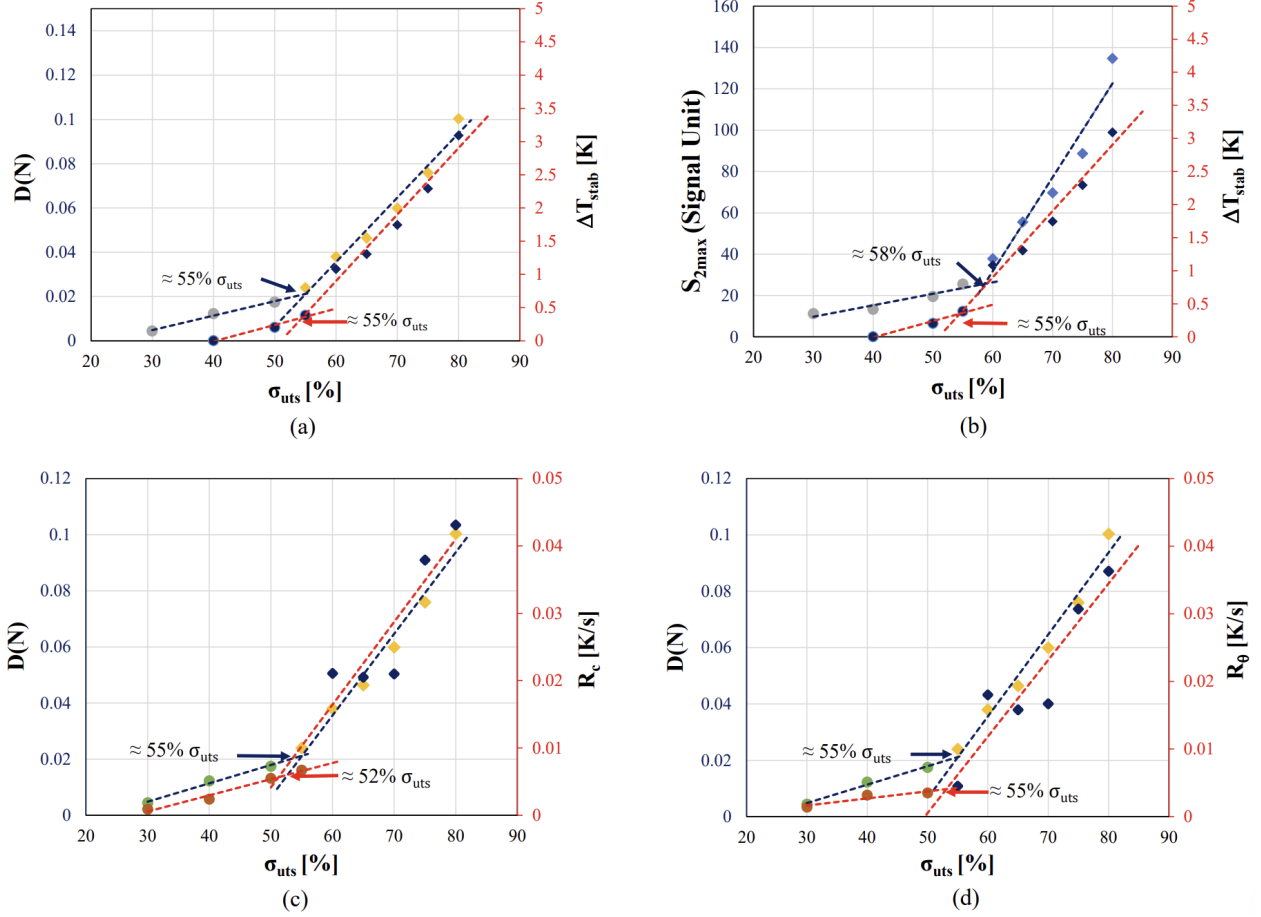


**Figure 3.11:** Fatigue limit estimation using  $S_2$ : (a) bi-linear approach with  $S_{2max}$  versus  $\sigma_{max}$ , and (b) residuals of the 98<sup>th</sup> percentile  $S_2$  signal.

Having established the accuracy and consistency of the four IRT indicators on Panel A, the validated framework is applied in the following sections to Panel B for systematic parametric characterization of loading frequency, stress ratio, and fiber orientation effects.

### 3.4 Parametric Study

With the four IRT indicators validated against S-N and stiffness degradation data on Panel A, the framework is applied in this section to Panel B (0.9x bead speed) for systematic parametric characterization. Three loading and microstructural variables are investigated: (i) loading frequency, (ii) stress ratio, and (iii) fiber bead orientation. Loading frequency receives particular attention: ASTM D7791 restricts fatigue testing of thermoplastics to  $\leq 5$  Hz to minimize self-heating artifacts, yet structural components in aerospace, automotive, and wind-energy applications routinely experience substantially higher cyclic frequencies in service. Whether this restriction is overly conservative for the well-aligned AM-CM SFTs system and how frequency governs the fatigue limit and damage mechanisms constitute the primary foci of Section 3.4.2.

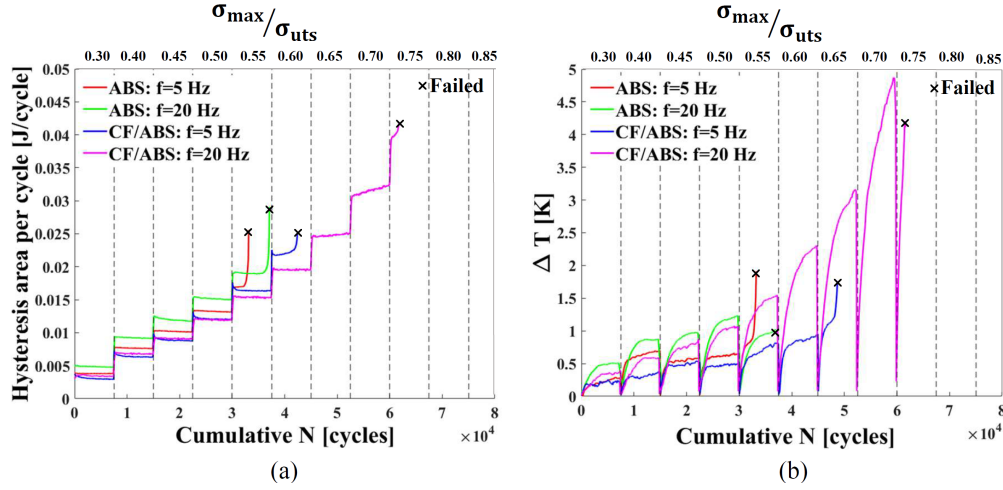


**Figure 3.12:** Comparison of all IRT approaches: (a) damage accumulation over  $\Delta T_{stab}$ , (b)  $S_{2max}$  over  $\Delta T_{stab}$ , (c) damage accumulation over  $R_c$ , (d) damage accumulation over  $R_\theta$ .

### 3.4.1 Comparison of Pure ABS and CF-ABS Under Cyclic Loading

The temperature rise observed in pure ABS and CF-ABS under cyclic loading at  $R = 0.1$  for 5 Hz and 20 Hz was compared to isolate the contributions of fiber-matrix interactions versus the pure matrix response.

For pure ABS, DMA and differential scanning calorimetry (DSC) confirmed a glass transition temperature of approximately 105 °C. At room temperature (25 °C), energy dissipation under fatigue arises primarily from internal molecular friction, mechanical damage, and creep effects. At 20 Hz, molecular chains are forced to respond more rapidly than at 5 Hz, leading to higher internal friction and greater heat generation (Figure 3.13b).



**Figure 3.13:** Comparison of pure ABS and CF-ABS composite at 5 Hz and 20 Hz,  $R = 0.1$ : (a) hysteresis energy loss per cycle, and (b) representative surface temperature evolution with cycle.

In CF-ABS, carbon fibers restrict ABS chain mobility, altering the energy-dissipation balance. At 5 Hz, the longer cycle duration allows greater matrix deformation, and frictional interactions at fiber-matrix interfaces — especially at the unsized fiber ends, which act as stress concentrators — contribute to localized heating that, once fatigue damage initiates, exceeds that of pure ABS. At 20 Hz, fibers carry a larger share of the applied load, reducing matrix strain energy dissipation (Figure 3.13a), though interface friction remains active. These contrasting energy dissipation mechanisms at 5 Hz and 20 Hz motivate the systematic investigation of frequency-dependent fatigue behavior in AM-CM SFTs presented in Section 3.4.2.

### 3.4.2 Effect of Loading Frequency on Fatigue Limit

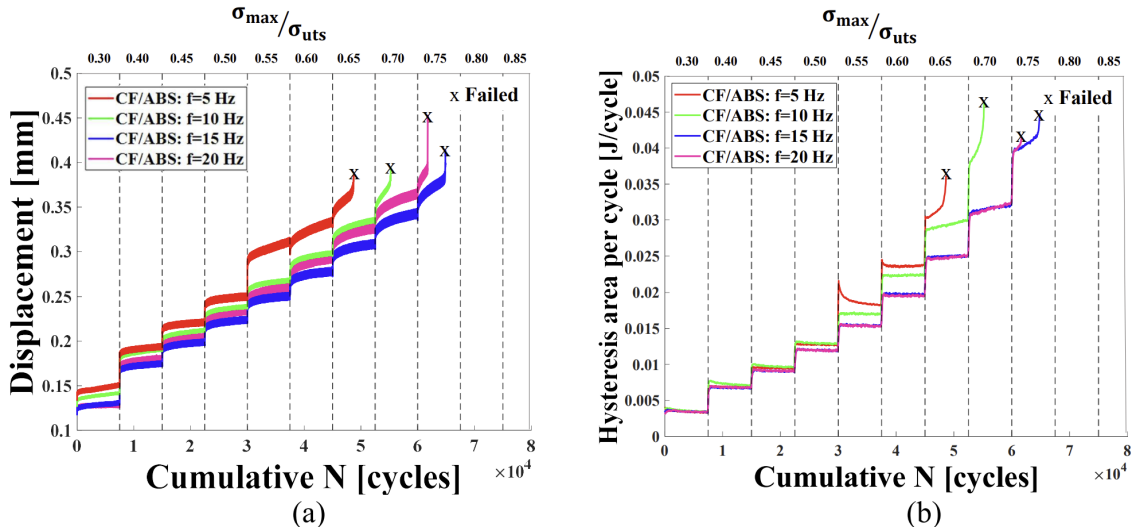
The influence of loading frequency was investigated by subjecting CF-ABS specimens to interrupted staircase fatigue tests at 5, 10, 15, and 20 Hz at constant  $R = 0.1$ . The mechanistic framework underlying frequency effects is rooted in the viscoelastic, strain-rate-sensitive nature of the ABS matrix. The peak strain rate under cyclic loading is given by [3]:

$$\dot{\epsilon}_{\max} = \frac{\sigma_a}{E(N)} \cdot 2\pi f \quad (3.1)$$



where  $\sigma_a$  is the stress amplitude,  $E(N)$  is the cycle-dependent elastic modulus, and  $f$  is the loading frequency. Higher frequencies amplify the effective strain rate, which, in viscoelastic thermoplastics, correlates with reduced times for molecular chain rearrangement and stress relaxation.

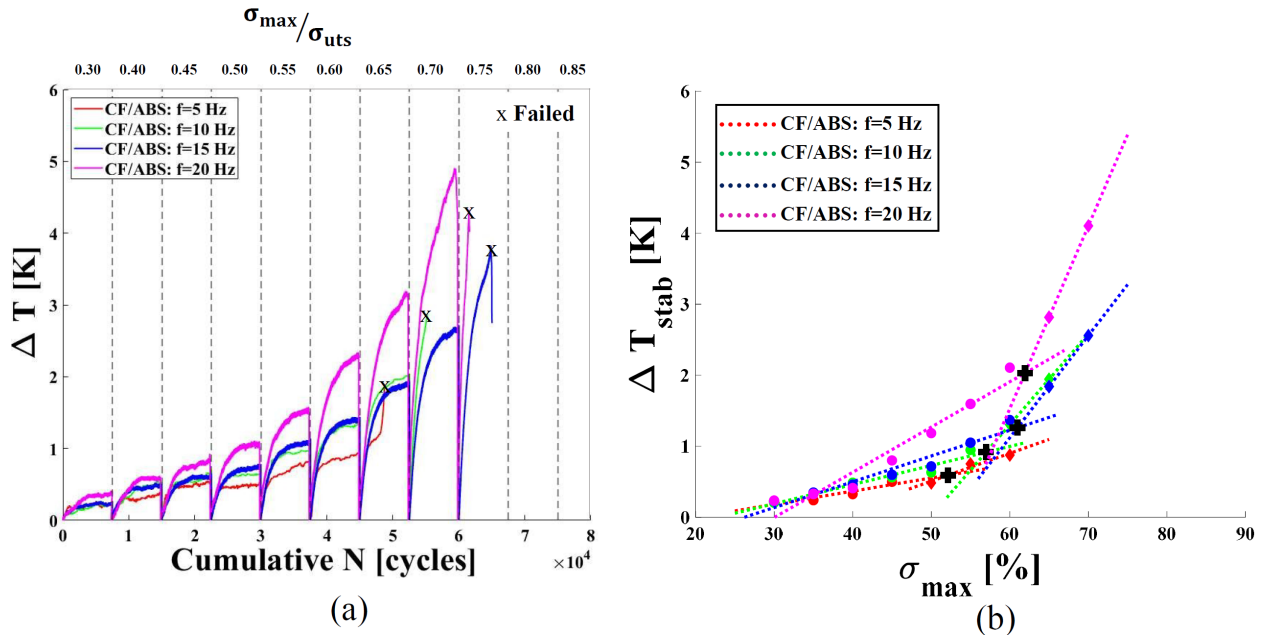
This frequency sensitivity manifests through two competing mechanisms. On one hand, higher frequencies increase the energy dissipation rate, elevating the surface temperature. On the other hand, and more critically, higher frequencies suppress viscoelastic creep deformation by limiting the available time per cycle for chain mobility. To confirm that creep suppression, rather than thermal softening, is the operative mechanism, DSC was performed on the CF-ABS system, yielding a glass transition temperature of  $T_g \approx 374$  K (see Appendix A). Since the measured fatigue surface temperatures remained in the range 301–303 K even at 20 Hz — approximately 73 K below  $T_g$  — thermal softening and macroscopic polymer flow can be conclusively excluded as contributors to the observed frequency-dependent behavior. The results are therefore consistent with a predominantly viscoelastic response [3].



**Figure 3.14:** CF-ABS composite response at 5, 10, 15, and 20 Hz,  $R = 0.1$ : (a) displacement for a given stress level versus number of cycles, (b) damage progression.

Figure 3.14a shows that specimens tested at 5 Hz and 10 Hz exhibit substantially higher cumulative displacement than those at 15 Hz and 20 Hz for the same applied stress. At

lower frequencies, longer cycle durations allow more extensive creep and time-dependent viscoelastic flow in the ABS matrix, leading to greater displacement accumulation and earlier fatigue damage initiation. At higher frequencies, the reduced cycle time limits matrix relaxation, confining deformation predominantly to elastic modes. Damage progression (Figure 3.14b) confirms that damage onset is delayed at higher frequencies, consistent with the suppression of time-dependent deformation.



**Figure 3.15:** CF-ABS fatigue behavior at 5, 10, 15, and 20 Hz,  $R = 0.1$ : (a) temperature increment versus cycles for each stress level, (b) fatigue limit estimation via bi-linear  $\Delta T_{stab}$  for each frequency.

Using the bi-linear  $\Delta T_{stab}$  approach validated in Section 3.3, the fatigue limit increases monotonically with frequency, from  $52.14 \pm 0.71\% \sigma_{uts}$  at 5 Hz to  $61.14 \pm 0.85\% \sigma_{uts}$  at 20 Hz (Figure 3.15b, Table 3.2). This represents a  $\approx 17\%$  relative increase in fatigue limit over the tested frequency range, driven by suppression of viscoelastic matrix deformation rather than thermal effects. This monotonic trend is reported only over the tested range (5–20 Hz); it should not be extrapolated beyond 20 Hz. Mohammadi et al. [109] recently reported that the apparent fatigue limit of a 3D-printed short-carbon-fiber-reinforced PA12 composite increases with frequency up to 15 Hz but then decreases at 25 Hz, attributing the reversal to a shift in the balance between viscoelastic creep suppression and frequency-driven

self-heating. Since the present study tested only up to 20 Hz and did not include a higher-frequency condition, it cannot be determined whether the CF-ABS system investigated here would exhibit a similar reversal beyond 20 Hz; this remains an open question for future work rather than a conclusion supported by the present data.

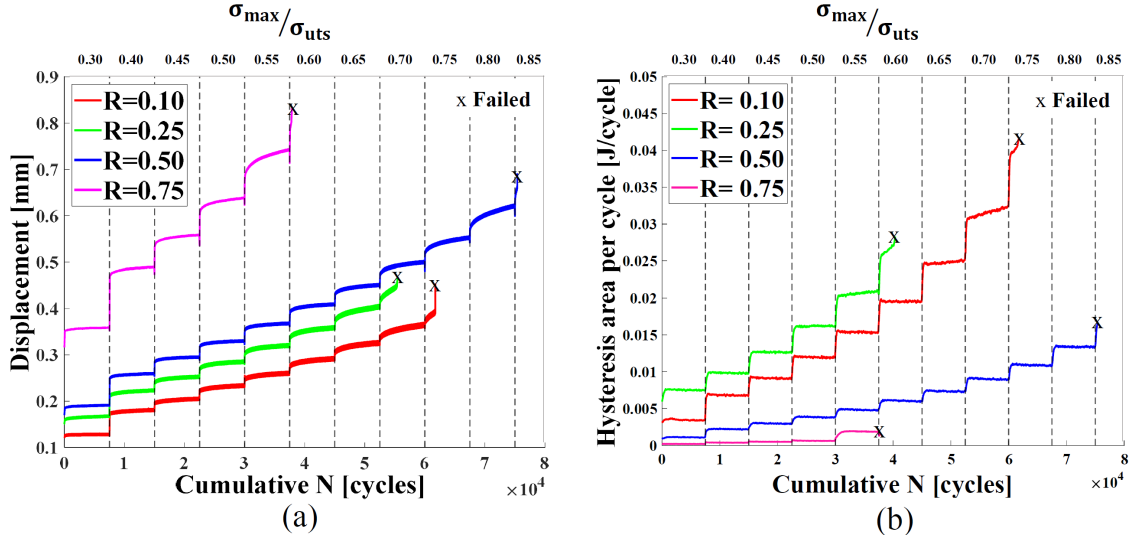
**Table 3.2:** Fatigue limit as a function of loading frequency for CF-ABS at  $R = 0.1$ .

| Frequency | Fatigue Limit [% $\sigma_{\text{uts}}$ ] |
|-----------|------------------------------------------|
| 5 Hz      | $52.14 \pm 0.71$                         |
| 10 Hz     | $56.98 \pm 0.25$                         |
| 15 Hz     | $59.14 \pm 1.08$                         |
| 20 Hz     | $61.14 \pm 0.85$                         |

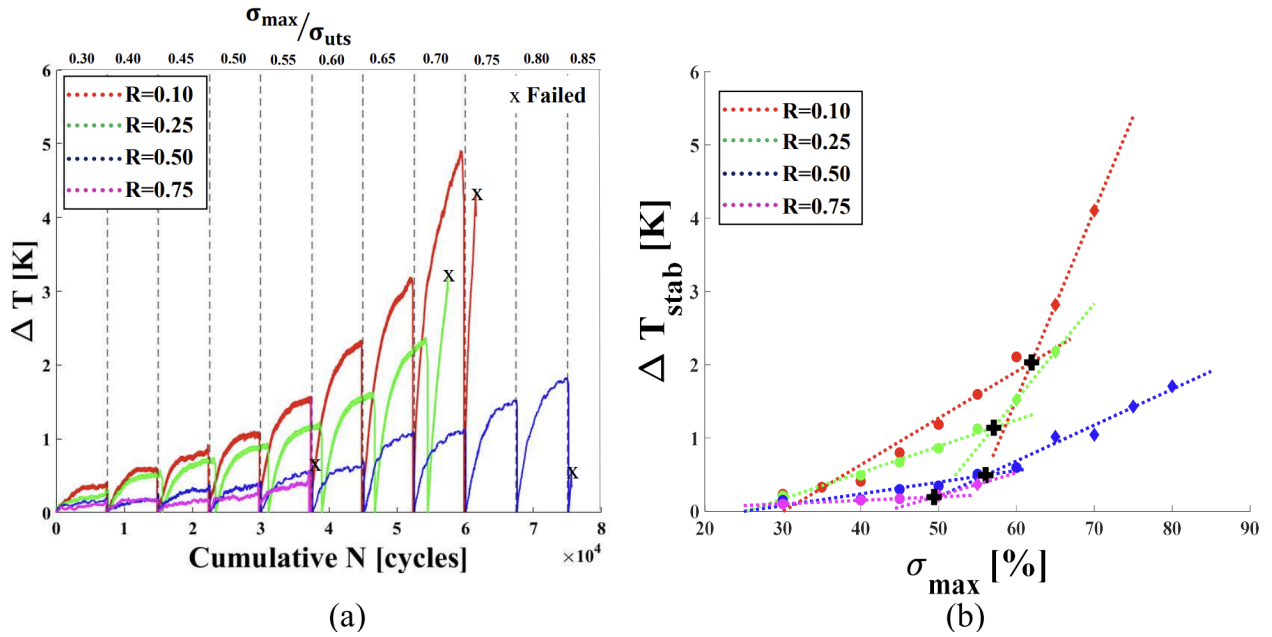
### 3.4.3 Effect of Stress Ratio on the Fatigue Limit

Staircase IRT fatigue tests were performed at 20 Hz across four stress ratios:  $R = 0.10$ , 0.25, 0.50, and 0.75. Increasing  $R$  elevates the mean stress ( $\sigma_m = \frac{1}{2}(\sigma_{\text{max}} + \sigma_{\text{min}})$ ) while reducing the cyclic stress amplitude ( $\Delta\sigma = \sigma_{\text{max}} - \sigma_{\text{min}}$ ). Despite the lower cyclic amplitude at high  $R$ , the sustained mean stress accelerates time-dependent damage mechanisms — creep, stress relaxation, and fiber–matrix debonding — at a rate that outpaces the benefit of the reduced cyclic driving force, leading to a net reduction in the fatigue limit. This behavior is consistent with the modified Goodman mean-stress dependence observed in viscoelastic polymer composites, where mean stress effects are amplified by molecular chain mobility and irreversible creep accumulation [45, 46].

Temperature fluctuations are lower at higher  $R$  because the smaller hysteresis loop area at high  $R$  leads to less internal friction and lower heat generation per cycle. Conversely, at lower  $R$ , a larger cyclic stress variation drives greater viscoelastic and plastic deformation, contributing to a greater temperature rise. The fatigue limit decreases progressively with increasing  $R$ , from  $61.14 \pm 0.85\%$  at  $R = 0.1$  to  $49.42 \pm 0.78\%$  at  $R = 0.75$  (Table 3.3).



**Figure 3.16:** CF-ABS composite response at  $R = 0.10, 0.25, 0.50$ , and  $0.75$ , frequency = 20 Hz: (a) displacement versus cycles for each stress level, (b) damage progression.



**Figure 3.17:** CF-ABS fatigue behavior at  $R = 0.10, 0.25, 0.50$ , and  $0.75$ , frequency = 20 Hz: (a) temperature increment for each stress level, (b) fatigue limit estimation via bi-linear  $\Delta T_{\text{stab}}$ .

### 3.4.4 Effect of Fiber Orientation on Fatigue Behavior

#### Quasi-Static Tensile Properties:

Quasi-static tensile tests were conducted on pure ABS and CF-ABS specimens with varying fiber orientations ( $0^\circ, 30^\circ, 45^\circ, 60^\circ, 90^\circ$ ) using the 100 kN MTS machine at 2 mm/min. Three replicates were tested for each orientation. Results are summarized in Table 3.4.

**Table 3.3:** Fatigue limit as a function of stress ratio for CF-ABS at 20 Hz.

| Stress Ratio $R$ | Fatigue Limit [% $\sigma_{\text{uts}}$ ] |
|------------------|------------------------------------------|
| 0.10             | $61.14 \pm 0.85$                         |
| 0.25             | $57.60 \pm 0.25$                         |
| 0.50             | $56.05 \pm 0.32$                         |
| 0.75             | $49.42 \pm 0.78$                         |

**Table 3.4:** Ultimate tensile strength and failure strain for various specimen orientations.

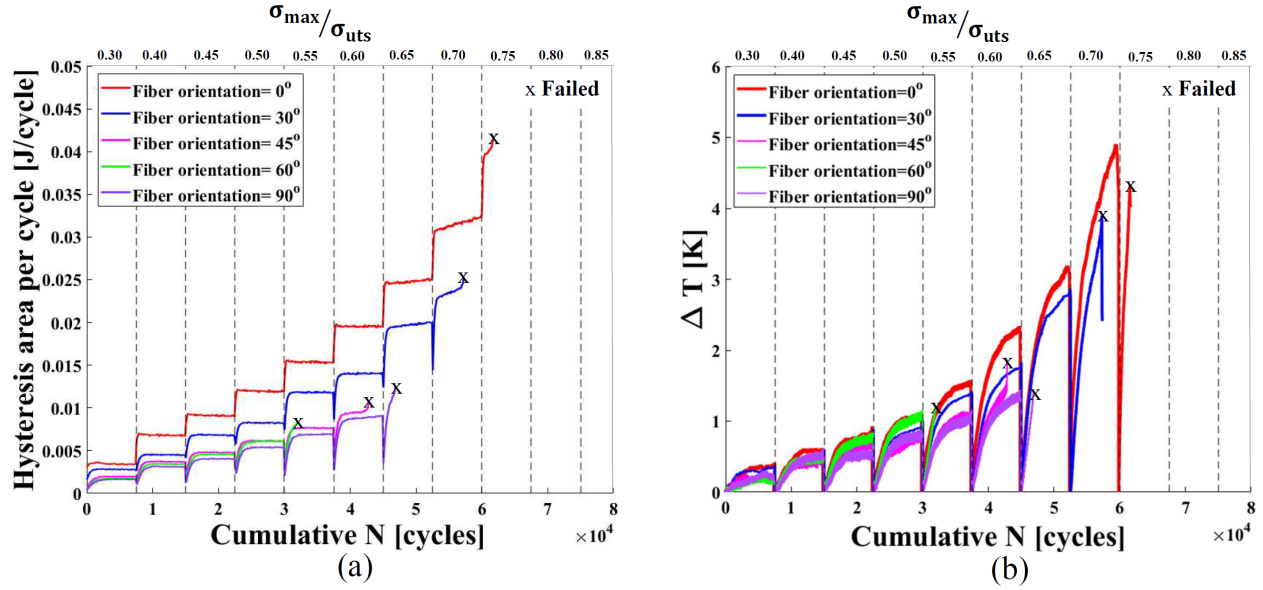
| Specimen              | $\sigma_{\text{uts}}$ [MPa] | $\varepsilon_f$ [%] |
|-----------------------|-----------------------------|---------------------|
| Pure ABS              | $54.000 \pm 1.810$          | $1.320 \pm 0.050$   |
| 0° fiber orientation  | $87.320 \pm 1.240$          | $0.730 \pm 0.003$   |
| 30° fiber orientation | $61.720 \pm 0.770$          | $0.910 \pm 0.001$   |
| 45° fiber orientation | $44.600 \pm 0.190$          | $0.935 \pm 0.005$   |
| 60° fiber orientation | $43.320 \pm 1.490$          | $0.877 \pm 0.002$   |
| 90° fiber orientation | $42.420 \pm 1.180$          | $1.055 \pm 0.004$   |

Both  $\sigma_{\text{uts}}$  and  $\varepsilon_f$  exhibit strong dependence on fiber bead orientation (Table 3.4). 0°-aligned specimens achieve the highest  $\sigma_{\text{uts}}$  and lowest  $\varepsilon_f$ , reflecting efficient axial fiber load transfer and the resulting brittle-dominant composite behavior. As the specimen extraction angle deviates from 0°,  $\sigma_{\text{uts}}$  decreases monotonically while  $\varepsilon_f$  increases, with the transition from fiber-dominated to matrix-dominated response occurring between 30° and 45°. Notably,  $\sigma_{\text{uts}}$  for 45°, 60°, and 90° specimens falls below that of unreinforced ABS, indicating that at these orientations, the misaligned fiber ends act as stress concentrators that actively reduce the composite's tensile capacity relative to the unfilled matrix.

#### *Fatigue Testing of Oriented Specimens:*

All oriented specimens were subjected to interrupted staircase fatigue loading at 20 Hz and  $R = 0.1$ . Results are shown in Figure 3.18 and Table 3.5.

The 0° specimens exhibit the slowest damage accumulation and highest fatigue limit (62%  $\sigma_{\text{uts}}$ ), owing to efficient fiber-mediated load transfer and crack bridging. Off-axis specimens (45°, 60°, 90°) show rapid damage progression and lower fatigue limits than pure ABS, as misaligned fibers cannot efficiently share the load, leading to accelerated



**Figure 3.18:** CF-ABS fatigue behavior at 20 Hz,  $R = 0.1$ , for five fiber orientations: (a) damage progression versus cycles, (b) representative surface temperature evolution.

**Table 3.5:** Fatigue limit for various fiber orientations at 20 Hz,  $R = 0.1$ .

| Specimen                     | Fatigue Limit [% of $\sigma_{uts}$ ] |
|------------------------------|--------------------------------------|
| Pure ABS                     | $51.850 \pm 0.740$                   |
| $0^\circ$ fiber orientation  | $61.950 \pm 0.850$                   |
| $30^\circ$ fiber orientation | $56.040 \pm 1.080$                   |
| $45^\circ$ fiber orientation | $50.820 \pm 0.710$                   |
| $60^\circ$ fiber orientation | $36.180 \pm 0.250$                   |
| $90^\circ$ fiber orientation | $38.810 \pm 0.780$                   |

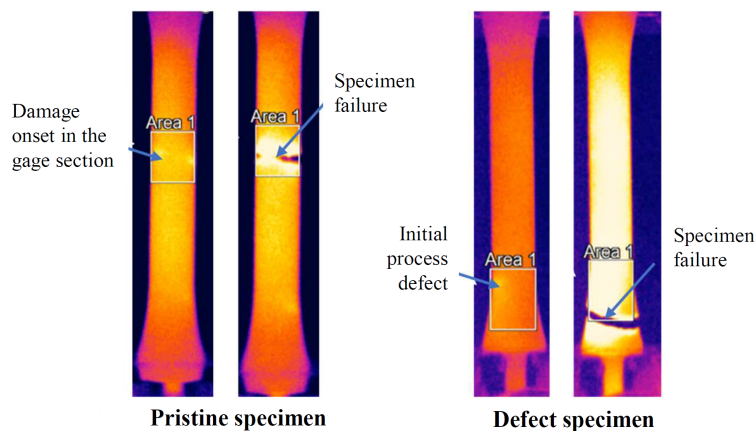
matrix cracking and fiber-matrix debonding. The temperature profiles further support this: while  $0^\circ$  specimens display the highest temperature rise from concentrated self-heating at fiber ends, this does not compromise their superior fatigue performance relative to other orientations.

This orientation dependence is consistent with observations described by Amjadi and Fatemi [110] for short-fiber-reinforced thermoplastics: as the fiber angle is rotated with respect to the loading direction, the fiber ends act as increasingly severe local stress concentrators, and the fatigue limit decreases accordingly. The results obtained here show this same qualitative nature —  $0^\circ$  specimens sustain the highest fatigue limit and

60°/90° specimens fall below even unreinforced ABS (Table 3.5) — and are qualitatively consistent with the SEM-confirmed fiber-matrix debonding failure mode identified for the AM-CM CF-ABS system in this chapter (Section 3.4.7).

*IRT for Process Defect Detection:*

A key advantage of IRT beyond fatigue limit estimation is its ability to localize incipient damage before catastrophic failure. Figure 3.19 depicts IR thermograms for two CF-ABS specimens — one pristine, one with an initial process defect. For the pristine specimen, fatigue damage initiation and final failure occurred within the gauge section without early hot-spot formation. For the specimen with a process defect, a hot spot formed within a few hundred load cycles and later became the site for damage initiation and final failure. Critically, the defect specimen failed after far fewer load cycles than the pristine specimen. This demonstrates IRT's value for rapid classification of process defects in AM-CM composites, thereby motivating the systematic characterization of porosity effects on fatigue in Chapter 4.



**Figure 3.19:** Thermograms illustrating the effect of process defects on fatigue damage onset and final failure in 20 wt.% CF-ABS.

### 3.4.5 Validation of Frequency-Dependent Fatigue Limits via Constant Amplitude Tests

To provide independent validation of the IRT-derived frequency-dependent fatigue limits, CAF tests were performed at 60%  $\sigma_{uts}$  for both 5 Hz and 20 Hz. This stress level was chosen deliberately: 60%  $\sigma_{uts}$  lies above the 5 Hz fatigue limit (52%  $\sigma_{uts}$ ) but below the 20 Hz fatigue limit (61%  $\sigma_{uts}$ ), as established by the IRT staircase results in Table 3.2. The 5 Hz specimen was therefore expected to fail before run-out, while the 20 Hz specimen was expected to survive. As predicted, the 20 Hz specimen completed  $3 \times 10^6$  cycles without failure, whereas the 5 Hz specimen failed within 16,000 cycles. This outcome confirms that the staircase IRT methodology reliably predicts endurance thresholds under frequency-varying loading conditions. Collectively, these results demonstrate that fatigue life in AM-CM SFTs is governed predominantly by time-dependent viscoelastic behavior rather than by thermal degradation, thereby reinforcing the role of loading frequency as a design-critical parameter for fatigue-sensitive structural applications.

### 3.4.6 Energy Dissipation and FFE

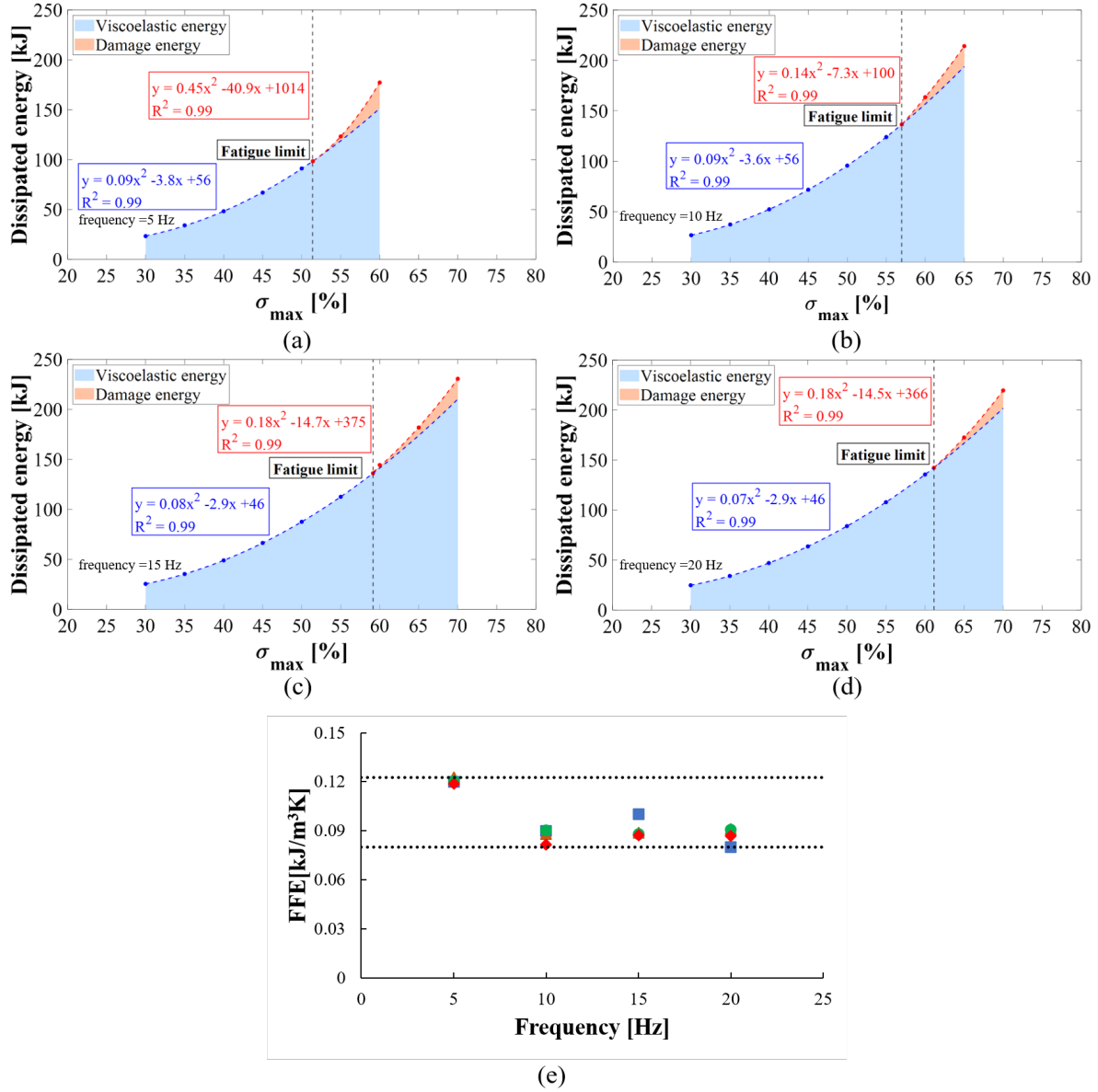
The viscoelastic energy dissipation extracted from hysteresis loops at each stress level exhibited a clear dependence on loading frequency (Figure 3.20). The energy per cycle was calculated as the area enclosed within the stress-strain hysteresis loop using numerical integration. The FFE was estimated as [66]:

$$FFE = \int_0^{t_f} \frac{\dot{E}_d}{T} dt \quad (3.2)$$

where  $\dot{E}_d$  is the irreversible damage energy dissipated per unit time,  $T$  is the instantaneous surface temperature (in K), and  $t_f$  is the time to failure.

At lower frequencies (5–10 Hz), higher mean stresses trigger greater matrix deformation and time-dependent viscoelastic energy loss (Figure 3.20a–b). At higher frequencies





**Figure 3.20:** Total viscoelastic energy dissipation versus applied stress at 5 Hz (a), 10 Hz (b), 15 Hz (c), and 20 Hz (d), showing higher viscoelastic dissipation at lower frequencies due to increased matrix flow, and lower dissipation at higher frequencies due to reduced relaxation time; (e) FFE versus loading frequency, exhibiting consistent values across all tested frequencies.

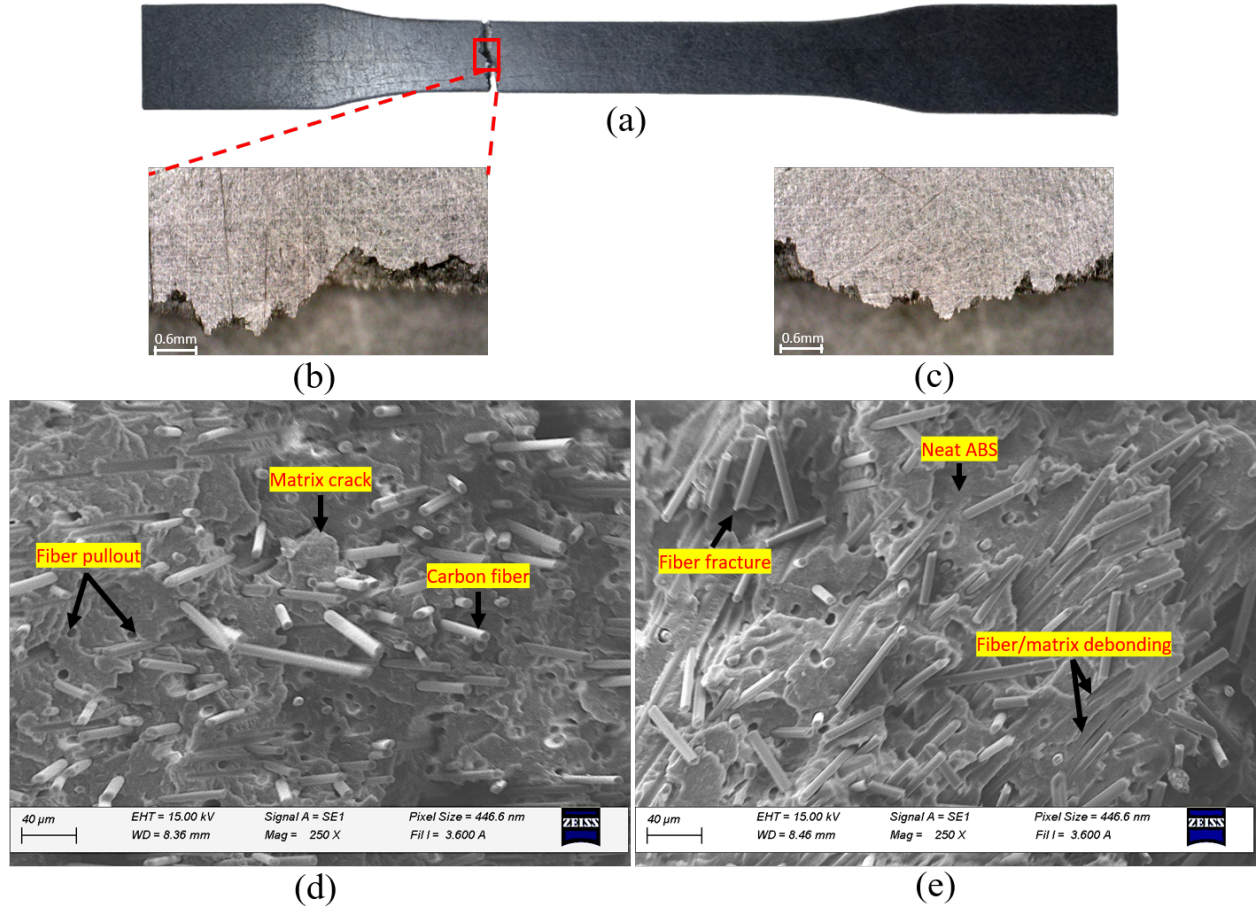
(15–20 Hz), the reduced relaxation time limits viscoelastic dissipation and suppresses structural degradation (Figure 3.20c–d). The damage energy component remains negligible below the fatigue threshold and rises sharply once the threshold is exceeded.

Importantly, as shown in Figure 3.20e, FFE values remained within a narrow  $\pm 15\%$  band across all tested frequencies, with a mean of  $0.0965 \text{ kJ/m}^3\text{K}$  and standard deviation of  $0.0144$ . This consistency — despite the viscoelastic energy dissipation exhibiting a strong frequency dependence — confirms that FFE is a rate-independent scalar descriptor of fatigue damage in AM-CM SFTs. FFE remained low during early load steps and rose sharply beyond the fatigue threshold, capturing the onset of irreversible degradation. This behavior validates FFE's role as a material property for characterizing fatigue damage, offering a loading-condition-independent quantitative indicator with practical utility for future fatigue diagnostics.

### **3.4.7 Microstructural Validation via SEM**

SEM of fractured specimens provided microstructural evidence corroborating the observed mechanical and thermal responses. All SEM micrographs in Figure 3.21 were taken from the central region of the macroscopic fracture surface, within approximately  $\pm 2.5 \text{ mm}$  of the mid-thickness plane in the gauge section, to avoid edge effects and ensure representative sampling of dominant failure mechanisms (Figure 3.21a). Across all specimens, the macroscopic fracture plane was flat and uniform (Figure 3.21b–c), enabling consistent comparison between low- and high-frequency cases.

At lower frequencies (5 Hz, 10 Hz), extensive fiber pull-out, matrix cracking, and interfacial debonding are evident in Figure 3.21d — consistent with a damage mechanism dominated by cyclic viscoelastic deformation and interfacial degradation over long cycle durations. At higher frequencies (15 Hz, 20 Hz), Figure 3.21e shows reduced matrix damage and more frequent fiber breakage, indicating stronger fiber-matrix load transfer and suppression of viscoelastic flow. The shorter pull-out lengths and brittle fiber fractures at high frequency reflect elevated strain rates that limit matrix relaxation and trigger fiber-dominated failure. These microstructural observations validate the rate-dependent transition in failure mechanisms inferred from macroscopic fatigue trends and thermographic analysis.



**Figure 3.21:** Macroscopic and microscopic fracture morphology at representative low and high frequencies: (a) macroscopic fracture surface at 5 Hz (red box:  $5 \times 5$  mm), (b) magnified SEM sampling region for 5 Hz, (c) magnified SEM sampling region for 20 Hz, (d) SEM image at 5 Hz showing fiber pull-out, matrix cracking, and interfacial debonding, (e) SEM image at 20 Hz showing fiber fracture and reduced matrix damage.

### 3.5 Conclusions

This chapter presented a comprehensive investigation of IRT-based rapid fatigue characterization for AM-CM 20 wt.% CF-ABS SFTs, encompassing validation of multiple IRT indicators and systematic parametric characterization of fatigue behavior. The key findings are as follows:

1. *IRT validation against S-N and stiffness degradation (Panel A, 1x bead speed):* All four IRT-based fatigue limit methods —  $\Delta T_{\text{stab}}$ ,  $R_{\theta}$ ,  $R_c$ , and  $S_2$  — yielded fatigue

limits within  $\approx 4\%$  of the traditional S-N-derived value ( $53\% \sigma_{\text{uts}}$ ), with an average across methods of  $54\% \sigma_{\text{uts}}$ . The IRT staircase approach required only 3 specimens and 5 hours of testing, versus 18 specimens and 2 weeks for the S-N curve — a  $\approx 100$ -fold reduction in testing time with one-sixth the specimen count. The  $\Delta T_{\text{stab}}$  bi-linear method provided the most consistent estimates; the  $S_{2\text{max}}$  method slightly overestimates the limit, with the  $S_2$  residuals approach providing a more reliable alternative.

2. *Frequency-dependent fatigue limit (Panel B, 0.9x bead speed)*: The fatigue limit of AM-CM SFTs increases monotonically with loading frequency, from  $52.14 \pm 0.71\% \sigma_{\text{uts}}$  at 5 Hz to  $61.14 \pm 0.85\% \sigma_{\text{uts}}$  at 20 Hz ( $\approx 17\%$  relative increase). DMA confirmed that the measured surface temperatures (301–303 K) remain well below  $T_g \approx 378$  K, ruling out thermal softening and confirming that the frequency effect is governed by the suppression of viscoelastic creep deformation at higher strain rates. CAF tests at  $60\% \sigma_{\text{uts}}$  independently validated these limits: the 5 Hz specimen failed within 16,000 cycles while the 20 Hz specimen survived  $3 \times 10^6$  cycles.
3. *Stress ratio and fiber orientation effects (Panel B, 0.9x bead speed)*: The fatigue limit decreases with increasing stress ratio, from  $61.14 \pm 0.85\%$  at  $R = 0.1$  to  $49.42 \pm 0.78\%$  at  $R = 0.75$ , reflecting mean stress-accelerated creep and fiber-matrix debonding. Fiber orientation proved equally critical:  $0^\circ$ -aligned specimens achieved  $62\% \sigma_{\text{uts}}$  through efficient load transfer, while  $60^\circ$  and  $90^\circ$  specimens fell to  $36\text{--}39\% \sigma_{\text{uts}}$ , performing below pure ABS at these orientations.
4. *FFE as a rate-independent material property*: FFE values remained consistent within  $\pm 15\%$  across all tested frequencies (mean =  $0.0965 \text{ kJ/m}^3\text{K}$ , std =  $0.0144$ ), confirming FFE as a rate-independent scalar descriptor of irreversible fatigue damage in AM-CM CF-ABS. This establishes FFE as a material property suitable for fatigue diagnostics independent of loading conditions.

5. *IRT for process defect classification*: IRT successfully detected incipient damage at process defect sites within a few hundred load cycles, identifying hot spots that later became failure initiation sites. This capability motivates a systematic investigation of the effects of porosity on fatigue, which is addressed in Chapter 4.

The IRT indicators developed and validated in this chapter —  $\Delta T_{\text{stab}}$ ,  $R_\theta$ ,  $R_c$ , and  $S_2$  — are all defined from a stabilized, steady-state thermal response within each staircase load step, and their calibration and validation here are correspondingly restricted to the high-cycle fatigue (HCF) regime in which such a stabilized Phase II response is actually reached. Near the failure stress, no genuine plateau develops, and the specimen effectively behaves as a low-cycle fatigue (LCF) loading within that step. This is consistent with thermographic studies of metals, where a similar three-phase pattern persists under LCF loading but the “stabilized” temperature tracks the hysteresis loop area rather than a true steady state, and the classical method can fail to identify Phase II at all at sufficiently high stress [111, 112]. These studies were conducted on metals rather than short-fiber thermoplastic composites, and an equivalent characterization for AM-CM SFTs has not, to the author’s knowledge, been established; the present chapter does not attempt to close this gap. Extending the framework to explicitly cover the LCF regime would require separate calibration under constant-amplitude high-stress loading rather than the staircase protocol used here, and is left for future work.

The integrated multi-indicator IRT framework established in this chapter — validated against conventional S-N and stiffness-degradation benchmarks and applied across a systematic parametric space of frequency, stress ratio, and fiber orientation — provides both a practical accelerated-testing methodology and a mechanistic understanding of the factors governing HCFS in AM-CM SFTs. The IRT thermograms additionally demonstrate that process-induced porosity concentrates thermographic damage signatures at specific defect locations well before macroscopic failure, motivating the systematic three-dimensional characterization of pore nucleation and growth under cyclic loading presented in Chapter 4.

## **Chapter 4**

### **Porosity Evolution and Its Effect on Fatigue Limit**

#### **4.1 Introduction**

Chapter 3 showed that process-induced defects act as preferential fatigue-initiation sites, with thermal hotspots emerging within a few hundred cycles. This raises two questions Chapter 3 could not answer: how does porosity magnitude quantitatively govern the fatigue limit, and how does void morphology evolve spatially during cyclic loading? Prior work has treated porosity as a fixed manufacturing characteristic rather than an evolving damage-state variable, leaving its evolution under fatigue — and its link to fatigue endurance — uncharacterized for AM-CM SFTs.

This chapter addresses Gap 3 (Section 2.8) by tracking void morphology in three dimensions across the fatigue life of three CF-ABS specimens spanning a range of initial porosity (1.41–2.86%), combining the IRT staircase protocol of Chapter 3 with repeated  $\mu$ -CT scanning of the same gauge volume. The resulting fatigue-stage-resolved microstructures both quantify the porosity–fatigue–endurance relationship and provide the geometric input — FODs, FLDs, PVDs, PADs, PODs — for the GNN–LSTM surrogate developed in Chapter 5.

#### **4.2 Materials and Methods**

##### **4.2.1 Specimen Selection via Ultrasonic C-Scan**

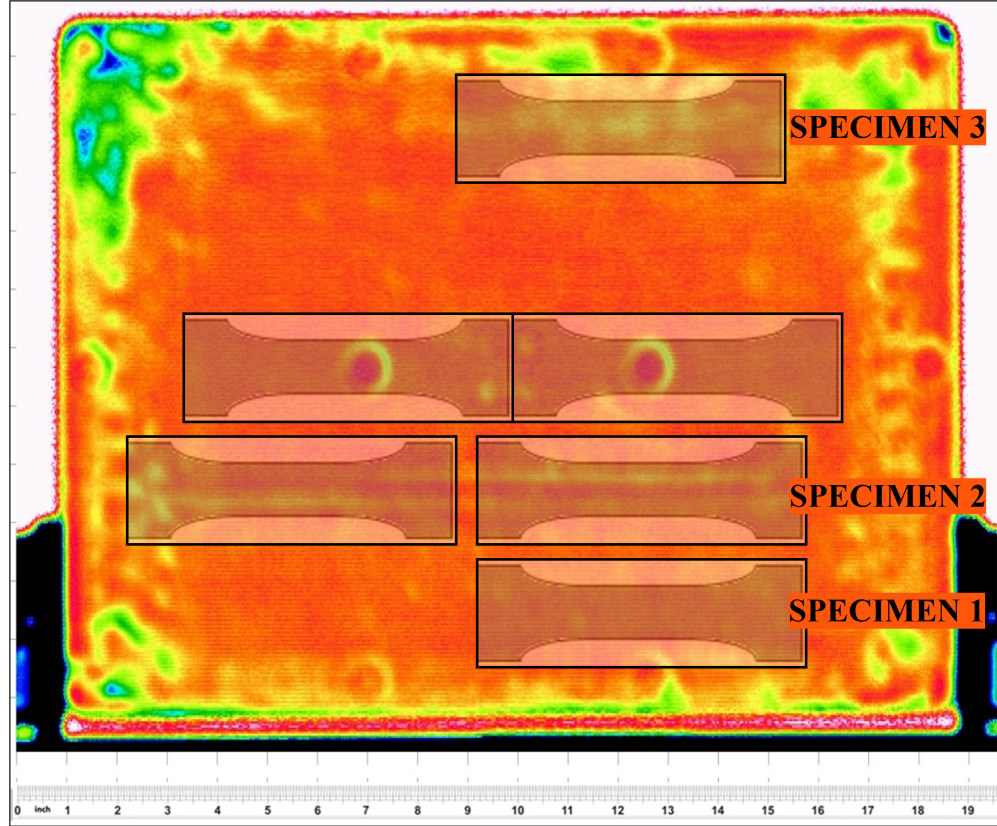
The material constituents and AM-CM fabrication process are those described in Section 3.2.1. Panel B specimens (0.9x bead speed) were selected for this investigation

because the optimized extrusion speed produces superior fiber alignment consistency — up to 80% of fibers within  $0^{\circ}$ – $30^{\circ}$  of the deposition direction — while the single-panel extraction strategy ensures that fiber-matrix chemistry and processing history are identical across all three specimens, isolating initial porosity as the sole variable. The compressed flat composite panels measured approximately 450 mm  $\times$  300 mm  $\times$  3.5 mm.

Although the hybrid AM-CM process enhances directional fiber alignment and mitigates bulk macro-void attachments, local process-induced microstructural variations, originating from differential consolidation pressure fields, spatial thermal gradients within the mold, and localized cooling zone variations near panel edges, produce spatially non-uniform porosity distributions across a single manufactured sheet. To map these variations and isolate coupons representing distinct defect states, ultrasonic C-scan inspection was executed on the AM-CM 20 wt.% CF-ABS panel prior to machining. Figure 4.1 illustrates the resulting non-destructive C-scan image, where the color mapping scheme indicates increasing relative attenuation and void content from red (low porosity) through yellow and green to blue (high porosity). As expected, higher relative attenuation and porosity are concentrated along the immediate boundaries of the panel edges due to lateral squeeze-flow pressure drops during consolidation. Three specimens were extracted from distinct interior sub-regions exhibiting systematically varied but locally stable porosity levels (yellow markers in Figure 4.1, deliberately avoiding the high-porosity edge zones arising from lateral squeeze-flow pressure gradients during compression molding. All specimens were machined precisely parallel to the bead deposition axis using abrasive waterjet cutting following the geometric profiles of ASTM D638 Type I coupons [22, 105].

#### **4.2.2 $\mu$ -CT Characterization**

High-resolution  $\mu$ -CT scanning was performed on all specimens using the Zeiss Xradia 620 Versa system and scanning configuration described in Section 3.2.2 (140 kV



**Figure 4.1:** Ultrasonic C-scan image of AM-CM 20 wt.% CF-ABS SFT panel (Courtesy: Kratos Inc.); blue/green/yellow hues indicate increasing porosity. Red boxes indicate the three selected specimens.

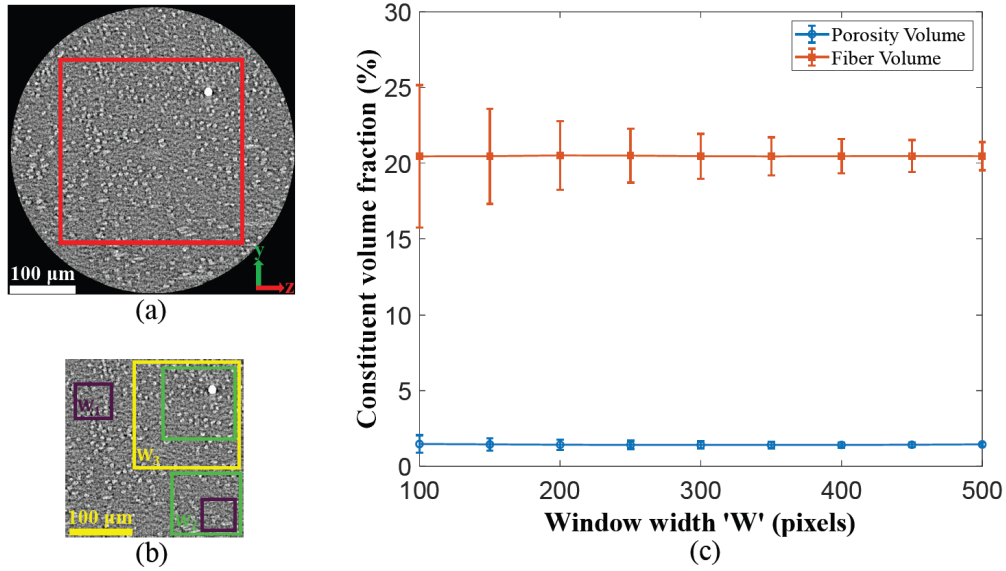
accelerating voltage, 21 W beam power,  $4\times$  objective lens,  $2 \times 2$  pixel binning), yielding an isotropic voxel resolution of  $0.6 \times 0.6 \times 0.6 \mu\text{m}^3$ .

To precisely track the same physical gauge volume across multiple fatigue-life milestones, a mechanical fiducial notch marker was engraved on each coupon before loading. The Scale-Invariant Feature Transform (SIFT) image registration algorithm was subsequently deployed during volume reconstruction to align and register the three-dimensional (3D) tomographic datasets from different testing intervals.

The primary analysis volume was defined as a right circular cylinder with a diameter of  $0.6 \approx \text{mm}$  and an axial height of  $0.6 \approx \text{mm}$ , comprising a stack of 997 image slices perpendicular to the specimen loading axis. Constituent phase volume fractions were extracted via automated grayscale intensity segmentation using Dragonfly PRO software (Version

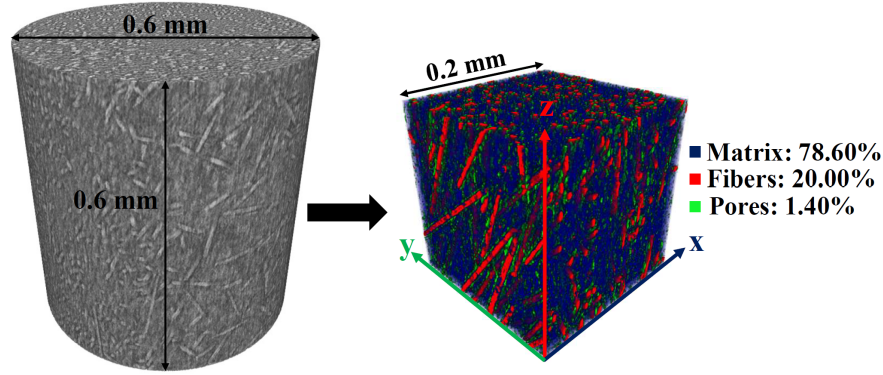


2022.2) to cleanly separate the chopped carbon fibers, the background ABS matrix, and the void domains. To ensure statistical convergence of the microstructural data, a windowing approach was employed to determine the minimum representative volume element (RVE) boundaries. As detailed in Figure 4.2(c), the calculated constituent volume fractions converge stably at a spatial cubic window width of 0.2 mm, which was subsequently adopted as the standard sub-volume bounding box for all downstream morphological extractions [113].



**Figure 4.2:** (a) Cross-section of  $\mu$ -CT slice image of Specimen 1, (b) windowing approach for sub-volume selection, and (c) constituent volume fractions measured across window sizes, showing convergence at 0.2 mm.

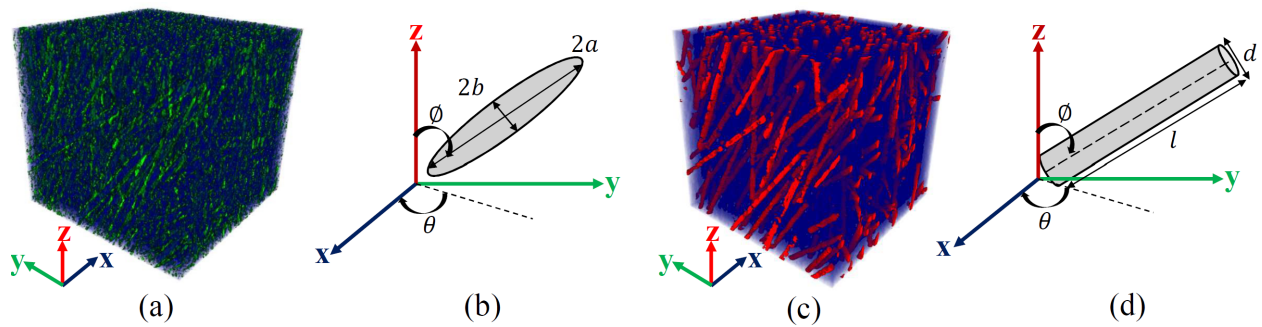
A Gaussian smoothing filter was applied to the reconstructed volumes to reduce boundary noise and suppress grayscale reconstruction prior to segmentation. Isolated voxels smaller than 1  $\mu$ m and anomalous pore clusters exhibiting strict integer-valued orientation vectors, indicative of back-projection reconstruction rather than physical voids, were excluded from the phase assignment. The combined effect of these regularization steps on the calculated phase volume fractions was verified to be negligible ( $<0.1\%$  change in total void fraction). Figure 4.3 shows the extracted, segmented representative sub-volume, illustrating the three material phases resolved at the discrete fiber scale.



**Figure 4.3:** Selection of sub-volume using the windowing approach, showing the 0.6  $\approx$  mm scanned cylinder (left) and the 0.2  $\approx$  mm representative sub-volume (right) segmented into matrix (blue), fibers (red), and pores (green).

#### *Microstructural Descriptors:*

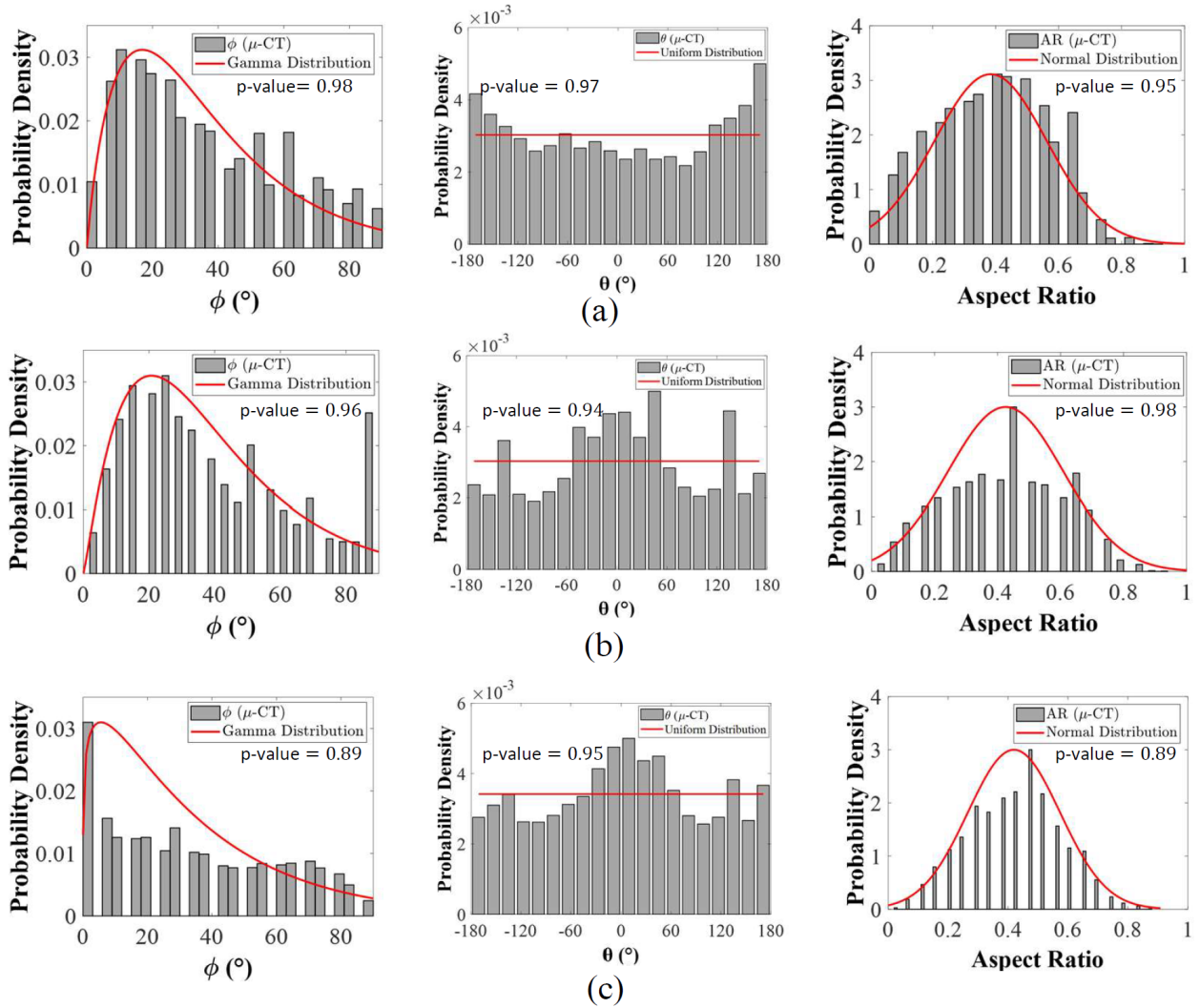
Figure 4.4 defines the coordinate frameworks and geometric descriptors used to characterize both the fiber and void phases throughout this research. The pore aspect ratio is defined as  $b/a$  (where  $b$  and  $a$  represent the smallest and largest calculated semi-axes of an equivalent ellipsoid, respectively), with spatial orientation mapped via the azimuthal angle  $\phi$  (measured within the  $x$ - $y$  plane) and the polar angle  $\theta$  (measured relative to the vertical  $x$ - $z$  axis). Reinforcement fibers are characterized using an identical reference convention, tracking the aspect ratio as  $l/d$ .



**Figure 4.4:** (a) Visualization of pores from  $\mu$ -CT, (b) semi-axes and orientation conventions for ellipsoidal pore representation ( $b/a$ ), (c) visualization of fibers from  $\mu$ -CT, (d) semi-axes and orientation conventions for cylindrical fiber representation ( $l/d$ ).

Irregular void morphologies were approximated as equivalent ellipsoids, and the carbon fiber reinforcement phase was modeled as right circular cylinders with a nominal diameter

of 8  $\mu\text{m}$ . Continuous probability density functions (PDFs) were fitted to the  $\mu\text{-CT}$  void and fiber descriptor datasets using chi-square goodness-of-fit tests, confirming statistically adequate fits across all specimens ( $p \geq 0.89$ ). The calibrated PDF parameters for the initial pore descriptors are listed in Table 4.1, and the corresponding experimental distributions are shown in Figure 4.5. Initial void volume fractions, measured from the Before-Test (BT) scans, were 1.41% for Specimen 1, 1.90% for Specimen 2, and 2.86% for Specimen 3.



**Figure 4.5:** Distribution of pore parameters from  $\mu\text{-CT}$ : orientation  $\phi$ , orientation  $\theta$ , and aspect ratio for (a) Specimen 1, (b) Specimen 2, and (c) Specimen 3. Fitted PDFs are overlaid with  $p$ -values confirming goodness of fit.

**Table 4.1:** Probability distribution functions for pore descriptors from  $\mu$ -CT.

| Parameter | Distribution | PDF                                                                                                               | Parameters                     |
|-----------|--------------|-------------------------------------------------------------------------------------------------------------------|--------------------------------|
| AR        | Normal       | $f(x \mu, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right)$ | $\mu = 0.42, \sigma = 0.18$    |
| $\phi$    | Gamma        | $f(x \alpha, \beta) = \frac{\beta^\alpha x^{\alpha-1} e^{-\beta x}}{\Gamma(\alpha)}$                              | $\alpha = 1.90, \beta = 18.67$ |

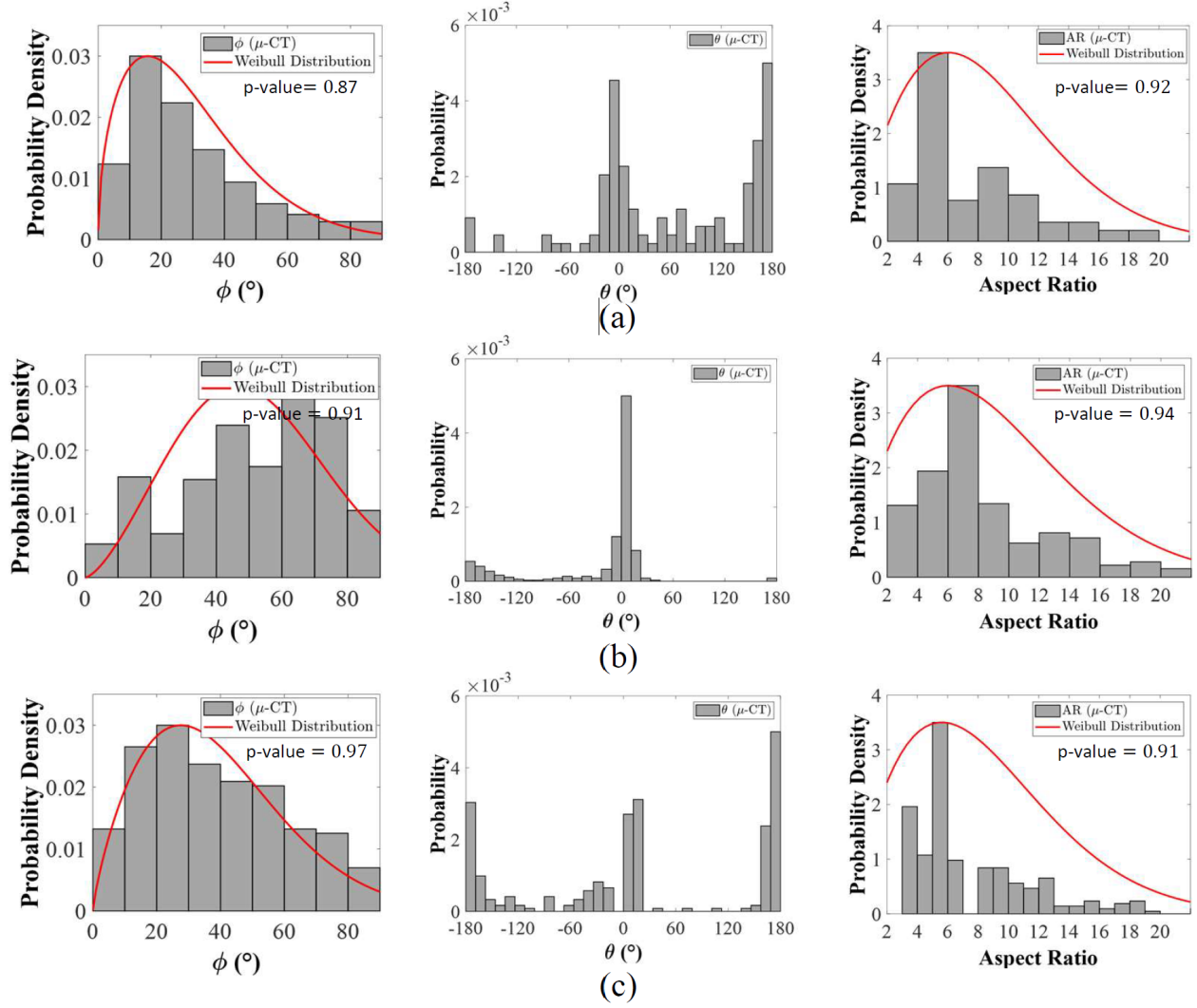
The baseline fiber descriptor arrays are illustrated in Figure 4.6 and summarized in Table 4.2. Specimen 1 demonstrated a sharp distribution containing 60% of reinforcement fibers aligned within  $0^\circ$ – $30^\circ$  of the primary longitudinal extrusion vector (bead-parallel axis,  $z$ -direction), exhibiting a peak fiber aspect ratio band between 5 and 10. This pronounced directional alignment, compared with the more uniformly dispersed fiber layouts in Specimens 2 and 3, matches the superior baseline mechanical properties recorded for Specimen 1. For downstream micromechanical finite element modeling, a constant polar orientation value of  $\theta = 0^\circ$  is assumed across the arrays to optimize solver efficiency without losing physical accuracy.

**Table 4.2:** Probability distribution functions for fiber descriptors from  $\mu$ -CT.

| Parameter | Distribution | PDF                                                                                                   | Parameters            |
|-----------|--------------|-------------------------------------------------------------------------------------------------------|-----------------------|
| AR        | Weibull      | $f(x a, b) = \frac{b}{a} \left(\frac{x}{a}\right)^{b-1} \exp\left[-\left(\frac{x}{a}\right)^b\right]$ | $a = 9.58, b = 1.78$  |
| $\phi$    | Weibull      | $f(x a, b) = \frac{b}{a} \left(\frac{x}{a}\right)^{b-1} \exp\left[-\left(\frac{x}{a}\right)^b\right]$ | $a = 32.26, b = 1.51$ |

### 4.2.3 Interrupted Fatigue Protocol

Quasi-static tensile characterization and fatigue tests were performed on the MTS Landmark servo-hydraulic test frame described in Section 3.2.4. Quasi-static tensile tests on Panel B  $0^\circ$ -aligned specimens confirmed baseline mechanical properties consistent with Chapter 3 Panel A results ( $\sigma_{\text{uts}} = 64.52 \pm 2.17$  MPa,  $E_0 = 8.32 \pm 0.02$  GPa), validating the use of Panel A-derived S-N and IRT reference data for comparison.



**Figure 4.6:** Distribution of fiber parameters from  $\mu$ -CT: orientation  $\phi$ , orientation  $\theta$ , and aspect ratio for (a) Specimen 1, (b) Specimen 2, and (c) Specimen 3.

Fatigue testing followed the IRT staircase protocol established in Section 3.2.4, using  $R = 0.1$ , 15 Hz, and 7,500-cycle load steps. The key addition here is the interrupted  $\mu$ -CT scanning protocol: fatigue testing was paused at three specific stages for each specimen:

- i. Before test (BT): An initial baseline scan is conducted on the pristine, uncycled specimen to characterize the defect distribution and track the initial pore and fiber descriptors prior to generating cyclic micro-damage.

- ii. Below fatigue limit (BF): Next scan executed immediately after the loading blocks are completed, capturing early-stage viscoelastic rearrangement and micro-void deformation prior to macroscopic damage localization.
- iii. Above fatigue limit (AF): Final scan executed after the staircase history entered the active damage accumulation regime but prior to ultimate failure, capturing accelerated pore-growth trajectories and micro-void coalescence pathways.

At each scheduled testing interruption, the specimen was removed from the hydraulic grips and allowed to cool to ambient temperature. Following the completed high-resolution  $\mu$ -CT scan, a low-strain monotonic tensile test was executed on the hydraulic frame to measure the exact fatigue-stage-resolved stiffness degradation prior to re-clamping and resuming the cyclic staircase blocks. This synchronized protocol enables direct correlation between local microstructural evolution and macroscopic compliance loss in the same specimen, eliminating coupon-to-coupon material variability.

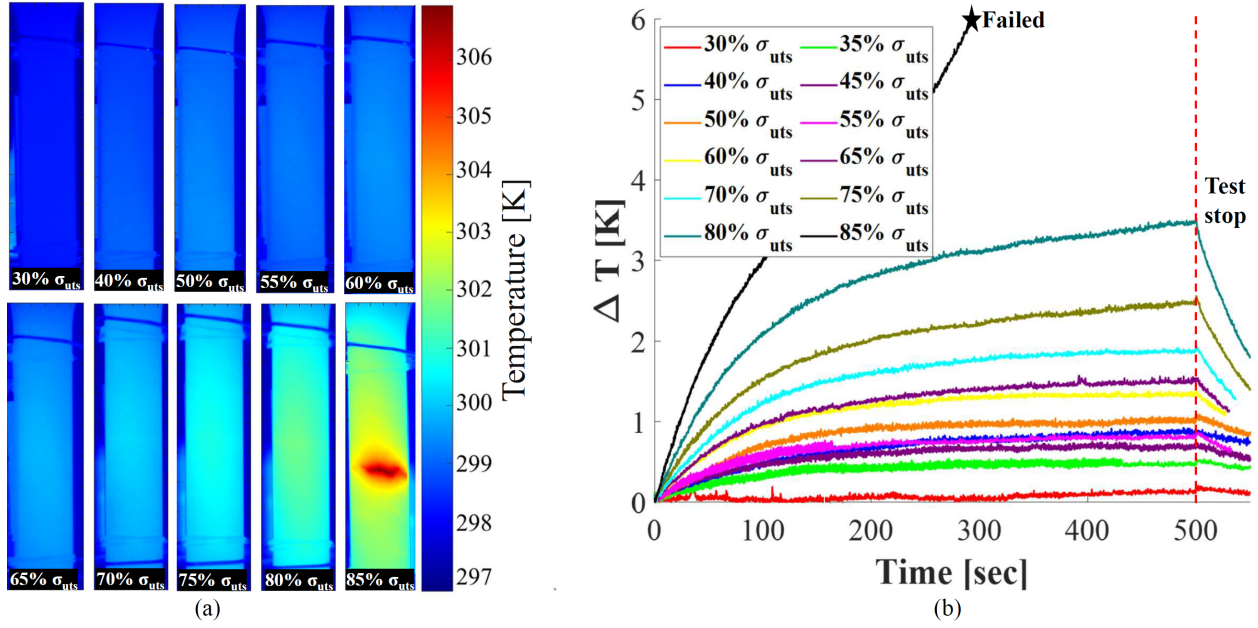
### 4.3 Porosity-Fatigue Coupling

#### 4.3.1 Effect of Initial Porosity on Fatigue Limit

Fig. 4.7a shows representative in-situ full-field thermograms for Specimen 1 at each staircase load step. The temperature evolution follows the three-phase behavior established in Chapter 3 (Section 3.3.1): up to 65%  $\sigma_{uts}$ , the temperature field remains uniform across the gauge section. Beyond this, a localized hot zone forms at the eventual failure site, progressively narrowing as  $\sigma_{max}$  increases. At 85%  $\sigma_{uts}$ , the specimen fails within 7,500 cycles without forming a Phase II plateau, indicating rapid irreversible damage growth driven by the combined effect of high applied stress and elevated porosity.

Fig. 4.8 plots  $\Delta T_{stab}$  versus  $\sigma_{max}$  for all three specimens. The bi-linear inflection point gives fatigue limits of 63.89%  $\sigma_{uts}$  (Specimen 1, 1.41% porosity), 59.15%  $\sigma_{uts}$  (Specimen 2,

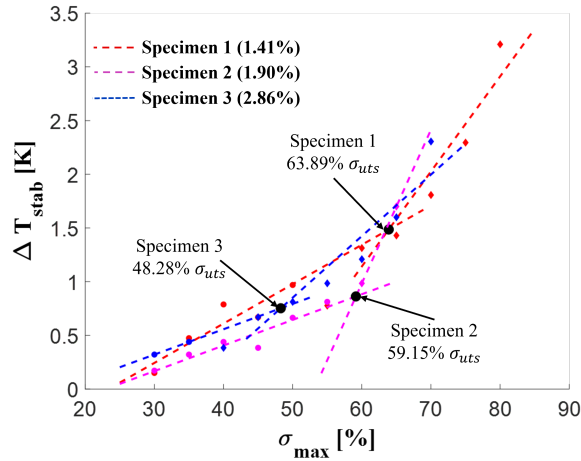




**Figure 4.7:** (a) Stabilized full-field surface temperature profiles of Specimen 1 with increasing staircase load steps; (b) maximum surface temperature evolution of Specimen 1 under staircase loading, with rest-period cooling visible between each step.

1.90% porosity), and 48.28%  $\sigma_{uts}$  (Specimen 3, 2.86% porosity). These results establish a direct, monotonic correlation between initial porosity content and fatigue limit: a 1.45% increase in initial porosity (from Specimen 1 to Specimen 3) corresponds to a 15.6 percentage-point reduction in fatigue limit (from 63.89% to 48.28%  $\sigma_{uts}$ ), reflecting an approximate 11% reduction in fatigue limit per 1.45% increase in initial porosity.

These results confirm the reliability of the IRT approach for rapid HCFS estimation across specimens with systematically varied defect content. The bilinear inflection points are computed from the spatially averaged  $\Delta T_{stab}$  within the gauge-section ROI rather than from local maxima, thereby capturing the representative macroscopic thermal response whilst averaging over microscale non-uniformities arising from porosity clustering. The close correspondence between IRT-derived HCFS values and the monotonic porosity trend (Table 4.3) confirms that  $\Delta T_{stab}$  is a reliable macroscopic indicator of fatigue endurance in specimens with varying initial void content [114].



**Figure 4.8:** HCFS limit estimation from bi-linear  $\Delta T_{\text{stab}}$  curves for all three specimens with initial porosity volume shown in brackets at 15 Hz,  $R = 0.1$ . Higher initial porosity correlates directly with a lower fatigue limit.

#### 4.3.2 Porosity Evolution Under Cyclic Loading

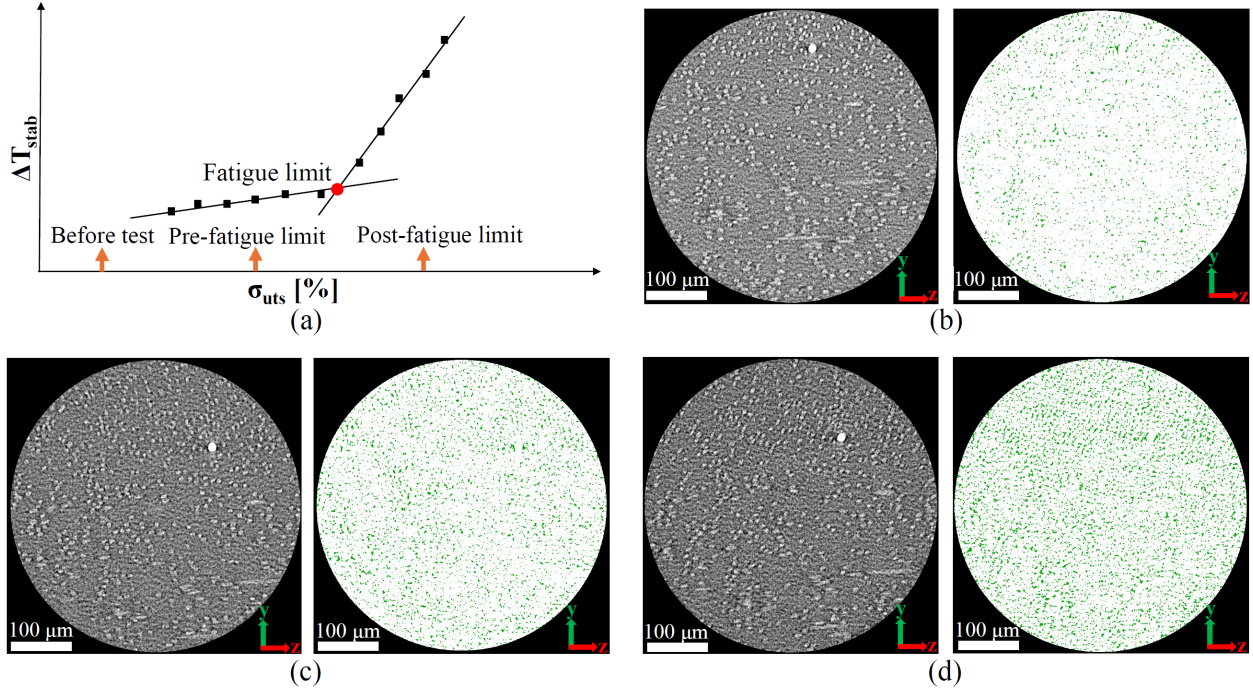
The high-resolution  $\mu$ -CT datasets generated at the scheduled testing interruptions reveal systematic, spatially localized void growth and morphological tracking across all three specimens.

##### *Pore Growth and Localization:*

Fig. 4.9 shows the three scanning stages relative to the fatigue limit bi-linear curve (Fig. 4.9a) and the corresponding 2D microstructural cross-sections in grey-scale and isolated-pore views for Specimen 1 (Fig. 4.9b–d). The number of pores increases progressively from BT to BF to AF, with the most pronounced increase occurring between BF and AF—consistent with the bilinear transition at the fatigue limit, above which irreversible damage mechanisms activate.

A comparison of grey-scale microstructure and isolated pores reveals that pore growth is spatially concentrated near fiber ends and within fiber clusters — not distributed uniformly through the matrix. This localization is mechanistically consistent: in the AM-CM process, fiber ends lack sizing after extrusion-induced chopping, producing weak fiber-matrix bonding at these locations and high stress concentrations predicted by shear-lag





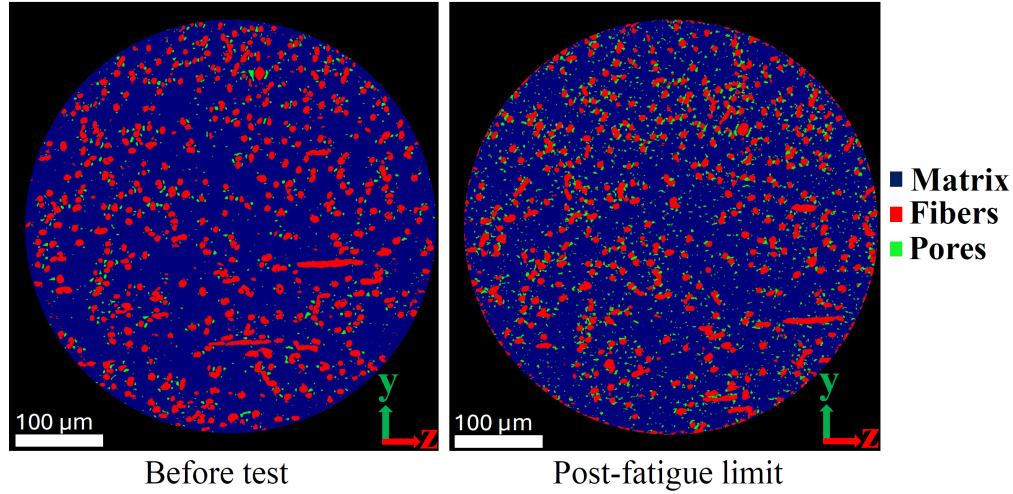
**Figure 4.9:** Interrupted  $\mu$ -CT imaging for Specimen 1: (a) three scanning stages marked on the bi-linear  $\Delta T_{stab}$  curve; 2D cross-sections in grey-scale (left) and isolated-pore views (right) at (b) before test, (c) pre-fatigue limit, and (d) post-fatigue limit.

theory [33, 115, 116]. The co-location of initial pores with these stress concentrators creates a self-reinforcing damage mechanism: pores amplify local stresses, which drive further debonding and void growth, generating new pores at adjacent fiber ends. Beyond fiber ends, new pores are also seen to nucleate in matrix-rich regions between fiber clusters, indicating that pore evolution under cyclic loading is twofold: (i) growth and coalescence at existing pores near fiber termini, and (ii) nucleation of new pores in matrix-rich zones under sustained mean stress.

Fig. 4.10 compares the BT and AF 2D cross-sections for Specimen 1, directly visualizing this progression.

#### *Quantitative Porosity Evolution Summary:*

Table 4.3 summarizes the void volume fraction evolution across all three specimens at all three fatigue stages. Void fraction increases monotonically from BT through BF to AF for all specimens, with the growth rate accelerating markedly above the fatigue limit,



**Figure 4.10:** Pore evolution during fatigue for Specimen 1: before test (left) and post-fatigue limit (right). Pore growth is concentrated near fiber ends and in fiber-cluster regions. New pores appear in matrix-rich zones above the fatigue limit.

consistent with the activation of irreversible damage mechanisms identified in Chapter 3 (Section 3.3.1). Specimen 3 (2.86% initial porosity) exhibits the most pronounced evolution: an approximately three-fold increase from BF to AF (3.57% to 11.86%), consistent with its lowest measured fatigue limit (48.28%  $\sigma_{uts}$ ). By contrast, Specimen 1, which combines the lowest initial porosity with the highest degree of fiber alignment, exhibits the slowest pore growth rate and the highest fatigue limit (63.89%  $\sigma_{uts}$ ), reinforcing the conclusion that both void content and fiber topology jointly govern fatigue endurance.

**Table 4.3:** Summary of porosity volume fraction (%) evolution and IRT-derived fatigue limits for all three specimens.

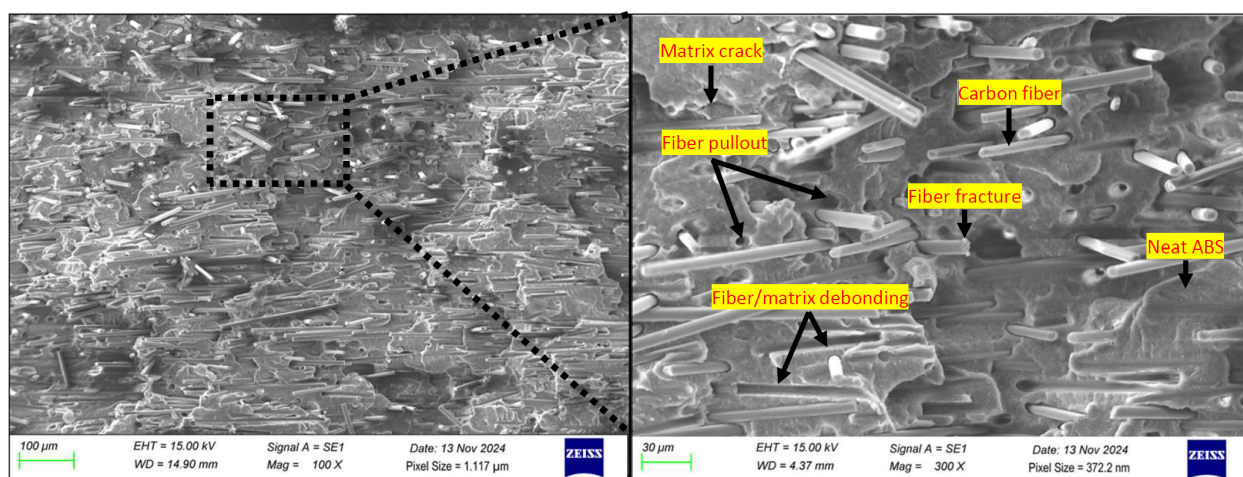
| Specimen | Before Test (%) | Below Fatigue Limit (%) | Above Fatigue Limit (%) | Fatigue Limit (% $\sigma_{uts}$ ) |
|----------|-----------------|-------------------------|-------------------------|-----------------------------------|
| 1        | $1.41 \pm 0.17$ | $2.33 \pm 0.21$         | $6.63 \pm 0.70$         | 63.89                             |
| 2        | $1.90 \pm 0.15$ | $2.56 \pm 0.18$         | $8.64 \pm 0.60$         | 59.15                             |
| 3        | $2.86 \pm 0.11$ | $3.57 \pm 0.15$         | $11.86 \pm 0.56$        | 48.28                             |

*Note on same volume reconstruction:* A mechanical fiducial marker was engraved on each specimen prior to testing, and SIFT image registration was applied during reconstruction to align the 3D volumes acquired at different fatigue stages. While sub-voxel registration errors remain possible, the achieved alignment accuracy was verified to be within one voxel ( $<0.6 \mu\text{m}$ ) based on the overlap of stationary reference features between

scans. Any residual volume-positioning uncertainty is treated as a minor contributor to the reported measurements of porosity evolution.

### 4.3.3 Failure Analysis and Fractography

Fig. 4.11 shows SEM images of a failed 20 wt.% CF-ABS Specimen 1. SEM analysis provides microstructural confirmation of the damage mechanisms inferred from the  $\mu$ -CT pore evolution and IRT thermal response.



**Figure 4.11:** SEM image of the failed 20 wt.% CF-ABS Specimen 1, showing fiber pull-out, fiber fracture, fiber/matrix debonding, matrix cracks, and regions of neat ABS matrix.

Fiber ends experience the highest local stress concentrations in SFTs and serve as the primary sites for damage initiation [106, 108], consistent with the  $\mu$ -CT evidence of preferential pore nucleation at fiber termini (Section 4.3.2). The fractographic analysis confirms that fiber–matrix interfacial debonding is the predominant damage mode, consistent with the Phase II–III thermographic signatures observed in Chapter 3 (Section 3.3.1). Additional damage features observed across the fracture surfaces include fiber pull-out, fiber fracture, and matrix cracking, with the relative prevalence of each depending on local fiber alignment and stress state. The absence of surface sizing on the chopped fiber ends — a direct consequence of the AM-CM extrusion process — provides minimal chemical adhesion to the ABS matrix, rendering interfacial debonding the energetically

preferential crack propagation path. These fractographic observations are consistent with the fatigue-induced pore localization patterns established in Section 4.3.2, completing the mechanistic picture: pores nucleate at fiber ends → debonding propagates along the fiber-matrix interface → fiber pull-out and eventual fracture complete failure.

#### **4.3.4 Effective Property Estimation via Numerical Homogenization**

With complete, fatigue-stage-resolved definitions of the AM-SFT microstructure, the key modeling question is: how accurately can the effective stiffness degradation observed experimentally be predicted from the evolving  $\mu$ -CT microstructural descriptors alone? This section answers this question using 3D RUCs with periodic boundary conditions (PBCs), populated via the Octree algorithm and subjected to numerical homogenization in ABAQUS (ver. 2020) with Python scripting (ver. 2.7.15).

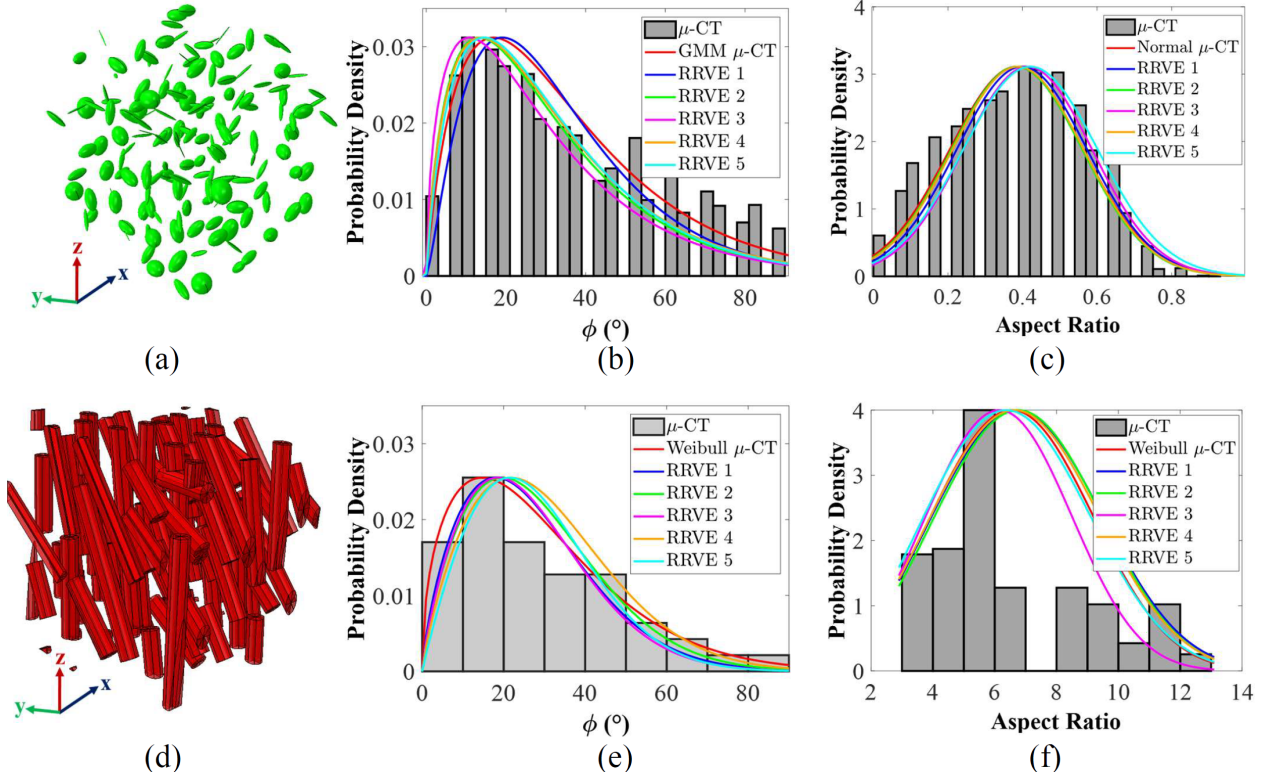
##### *RUC Generation via Octree Algorithm:*

Fiber and pore placements within each 3D-RUC are governed by the PDF distributions fitted to  $\mu$ -CT data (Tables 4.1 and 4.2) for each specimen and fatigue stage. The Octree algorithm facilitates efficient spatial packing by recursively subdividing the simulation domain into hierarchical cubic sub-regions, allowing localized adjustments to fiber and pore placements without intersections [117–120]. The algorithm works as follows: as the domain approaches its capacity for a given fiber or pore count, it is subdivided into eight smaller subdomains; the placement of the next inclusion is validated for intersections within its assigned subdomain; this recursive subdivision continues until the target fiber or pore volume fraction is achieved. Multiple RUC realizations (Fig. 4.12) confirm the repeatability of this approach across statistically equivalent microstructures.

##### *Two-Step Homogenization Procedure:*

A two-step homogenization procedure is employed to isolate the effect of porosity on matrix stiffness from the effect of fiber topology on composite stiffness (Fig. 4.13).





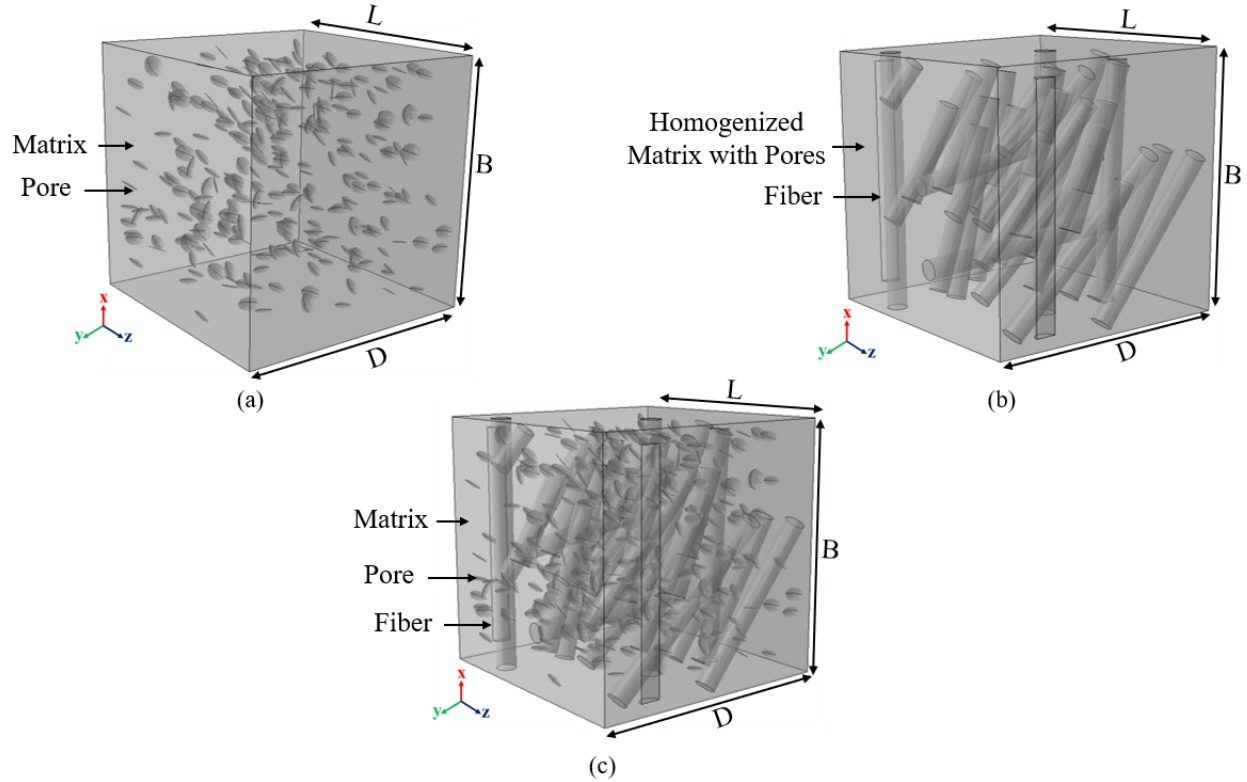
**Figure 4.12:** Multiple RUC realizations from the Octree algorithm: (a) pore distribution with orientation  $\phi$ , (b) aspect ratio, (c) fiber distribution with orientation  $\phi$ , (d) aspect ratio. Fitted PDFs overlay experimental  $\mu$ -CT data, confirming statistical equivalence of RUC realizations.

#### Step 1 — Porous matrix homogenization:

A matrix-only RUC containing  $\mu$ -CT-resolved pores distributed according to the measured PVD, PAD, and POD is numerically homogenized under prescribed macroscopic strains (three normal and three shear). The volume-averaged stress response yields an effective porous-matrix stiffness tensor  $C_m^{\text{eff}}$  that reflects the porosity level at each fatigue stage.

#### Step 2 — Composite homogenization:

A two-phase fiber-matrix RUC is constructed in which fibers (with transversely isotropic properties from Table 5.1) are embedded in the  $C_m^{\text{eff}}$  porous matrix from Step 1. Homogenization of this RUC under the same six loading cases yields the effective composite



**Figure 4.13:** Two-step micromechanical homogenization procedure: Step 1 homogenizes a porous matrix RUC to obtain an effective porous matrix stiffness tensor  $C_m^{\text{eff}}$ ; Step 2 uses  $C_m^{\text{eff}}$  as the matrix phase in a fiber-matrix RUC to predict the composite effective properties.

stiffness tensor, incorporating both the porosity effect (through  $C_m^{\text{eff}}$ ) and the fiber architecture effect (through the fiber volume fraction, orientation, and aspect ratio). Constituent elastic properties are listed in Table 5.1.

**Table 4.4:** Elastic properties of the 20 wt.% CF-ABS constituents used in micromechanical homogenization.

| Constituent  | $E_{11}$ (GPa) | $E_{22}$ (GPa) | $E_{33}$ (GPa) | $G_{12}$ (GPa) | $G_{13}$ (GPa) | $G_{23}$ (GPa) | $\nu_{12}$ | $\nu_{13}$ | $\nu_{23}$ |
|--------------|----------------|----------------|----------------|----------------|----------------|----------------|------------|------------|------------|
| Carbon fiber | 230            | 14             | 14             | 9              | 9              | 5              | 0.25       | 0.25       | 0.30       |
| ABS matrix   | 1.47           | 1.47           | 1.47           | 0.43           | 0.43           | 0.43           | 0.35       | 0.35       | 0.35       |

#### *Boundary Conditions and Homogenization:*

PBCs are imposed on the 3D-RUC via multi-point constraints relating the displacements of corresponding nodes on opposing boundary faces to the applied macroscopic strain components. This ensures that the unit cell is periodic and eliminates artificial stiffening effects arising from rigid boundary conditions. Quadratic tetrahedral elements

(C3D10R) with matched nodes on opposing faces, obtained via node-copy meshing, were used. Mesh sensitivity analysis confirmed convergence at an element size of half the fiber diameter. The RUC was subjected to applied normal and shear strains of 1% in six independent loading cases. Volume-averaged stresses and strains from Finite Element Analysis (FEA) post-processing yield the full effective stiffness tensor via:

$$\bar{\sigma}_{ij} = \frac{1}{V} \sum_{e=1}^{N_e} \sum_{k=1}^{N_{\text{int}}} \sigma_{ij}^{k,e} V^{k,e} \quad (4.1)$$

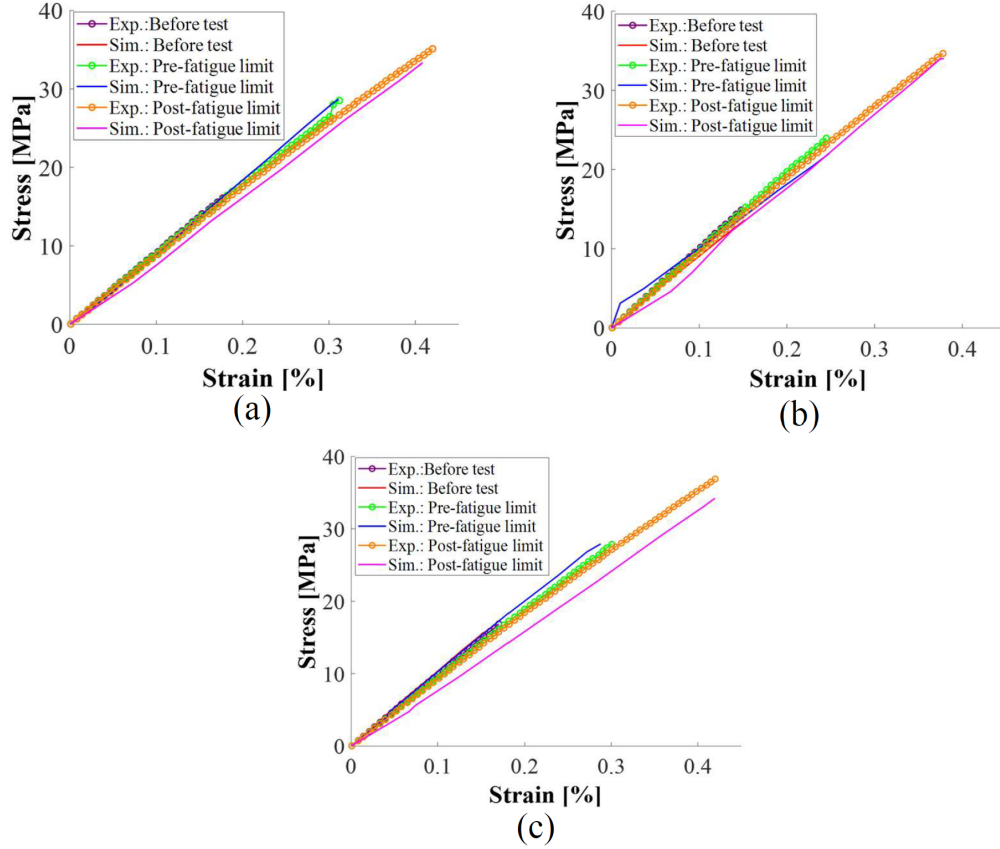
Full details of the PBC formulation are provided in Appendix C.1.

#### *Simulation Results and Validation:*

Fig. 4.14 compares the predicted effective axial stiffness from the 3D-RUC model against experimental interrupted tensile data for all three specimens at all three fatigue stages.

The model captures the progressive stiffness reduction across all three stages for all specimens with good quantitative agreement. As porosity increases from BT to AF, the porous matrix stiffness  $C_m^{\text{eff}}$  decreases, and this reduction is faithfully propagated through the two-step procedure to the composite level. The primary source of discrepancy between simulation and experiment is the current assumption of linear-elastic matrix behavior: the model does not account for progressive matrix damage (micro-cracking, plastic yielding) that accumulates at high stress levels, causing the simulation to slightly overestimate stiffness near the post-fatigue limit stage. Future work will incorporate the CDM damage model developed in Chapter 6 to address this limitation.

These results confirm that  $\mu$ -CT-derived microstructural descriptors — FLD, FOD, PVD, PAD, and POD — at each fatigue stage are sufficient to predict stage-resolved stiffness degradation without direct experimental stiffness measurement at every damage state. This finding directly motivates the surrogate modeling framework of Chapter 5, in which the computationally intensive repeated FE homogenization performed here is replaced by



**Figure 4.14:** Comparison of simulation (Sim.) and experimental (Exp.) stress–strain responses for (a) Specimen 1, (b) Specimen 2, and (c) Specimen 3, at before test (BT), below-fatigue limit (BF), and above-fatigue limit (AF) stages.

a GNN–LSTM surrogate trained on the  $\mu$ -CT-informed RUC simulations generated in this chapter, enabling microstructure-to-property prediction at a fraction of the FE computational cost.

#### 4.4 Conclusions

This chapter presented a systematic experimental and computational investigation of the role of process-induced porosity in governing the fatigue behavior of 20 wt.% CF-ABS AM-CM SFTs. The following key findings emerge:

1. *Porosity directly controls the fatigue limit:* Across three specimens spanning initial porosity levels of 1.41% to 2.86%, the IRT-derived HCFS decreased from 63.89%



to 48.28%  $\sigma_{\text{uts}}$ , corresponding to a reduction of approximately 11% in HCFS per unit percentage-point increase in initial void content. IRT effectively captured this porosity-fatigue limit correlation using a single specimen per porosity level, reinforcing the efficiency of the IRT approach established in Chapter 3.

2. *Pore evolution is spatially localized and stage-dependent:* Interrupted  $\mu$ -CT scanning at three fatigue stages revealed that pore growth is concentrated near fiber ends and within fiber clusters, consistent with shear-lag-driven stress concentrations at unsized fiber termini. Below the fatigue limit, porosity growth is modest (e.g., 1.41% to 2.33% for Specimen 1); above the fatigue limit, growth accelerates sharply (2.33% to 6.63%), with a  $\approx 3\times$  increase for the highest-porosity specimen. New pore nucleation in matrix-rich regions above the fatigue limit indicates a dual pore evolution mechanism: fiber-end-driven growth and matrix-fatigue-driven nucleation.
3. *Two-step FE homogenization accurately predicts stiffness degradation:* The  $\mu$ -CT-informed two-step homogenization (porous matrix RUC followed by fiber-matrix RUC) predicted stiffness degradation across all three fatigue stages and specimens in good agreement with experimental data, with residual discrepancies attributable to the absence of matrix damage in the current linear-elastic formulation.
4. *The microstructural dataset from this chapter is the direct input for Chapter 5:* The fatigue-stage-resolved FLD, FOD, PVD, PAD, and POD descriptors generated here form the  $\mu$ -CT input to the GNN-LSTM surrogate model developed in Chapter 5. The finding that  $\mu$ -CT descriptors alone suffice to predict stiffness degradation validates the surrogate approach and establishes the physical basis for replacing repeated FE homogenization with a data-driven, topology-preserving surrogate.

Collectively, these results establish a quantitative process–defect–performance relationship for AM-CM SFTs: manufacturing-induced void content, determined by panel

location and process parameters, governs both the initial HCFS and the rate of three-dimensional microstructural degradation under cyclic loading. Process optimization strategies targeting residual porosity reduction — particularly in fiber-end-adjacent matrix regions — represent the most direct route to improved fatigue endurance in these materials, with IRT providing a non-destructive diagnostic for initial void content at sub- $\mu$ -CT timescales. The fatigue-stage-resolved microstructural descriptors generated in this chapter serve as direct input to the GNN–LSTM surrogate framework in Chapter 5.

## Chapter 5

### Microstructure-Informed Constitutive Prediction via GNN–LSTM

#### 5.1 Introduction

Chapter 4 showed that the quasi-static response of AM-CM SFTs is governed by fatigue-stage-resolved microstructural topology rather than bulk porosity alone, and that FE homogenization of  $\mu$ -CT-resolved RUCs predicts this degradation accurately. This does not scale: each topologically distinct Voronoi cell requires an independent nonlinear FE simulation, and realistic specimens contain hundreds to thousands of cells, making coupon-scale multiscale analysis intractable for parametric studies or digital-twin applications.

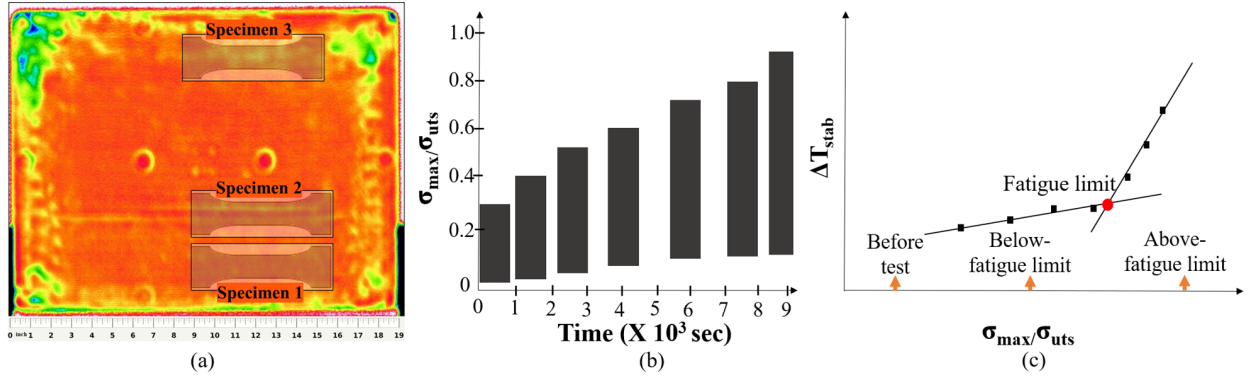
This chapter addresses Gap 4 (Section 1.2) with a data-driven surrogate that learns the mapping from  $\mu$ -CT-resolved fiber topology to each Voronoi cell's nonlinear response, preserving fiber–fiber interactions that mean-field homogenization cannot capture [88–90]. A hybrid GNN–LSTM is trained on FE homogenization data from the Chapter 4 microstructures: fibers are graph nodes with physics-informed edges encoding shear-lag load transfer, while the LSTM captures path-dependent plasticity and damage evolution; individual cell predictions are then assembled to recover coupon-scale behavior.

#### 5.2 Materials and Methods

##### 5.2.1 Materials, Specimens, and Experimental Data

The material system (20 wt.% CF-ABS, AM-CM process at ORNL), specimen fabrication,  $\mu$ -CT characterization, and interrupted fatigue protocol are identical to those described in Chapter 4 (Sections 4.2.1–4.2.3). The same three specimens (Panel B), representing

initial porosity levels of 1.41%, 1.90%, and 2.86%, were used.  $\mu$ -CT scans acquired at the three interrupted fatigue stages (BT; BF; AF) provide the fiber centerline coordinates, fiber volume fractions, and pore morphology distributions that serve as inputs to the multiscale framework described here. Figure 5.1 summarizes the specimen selection strategy and interrupted fatigue protocol for reference.

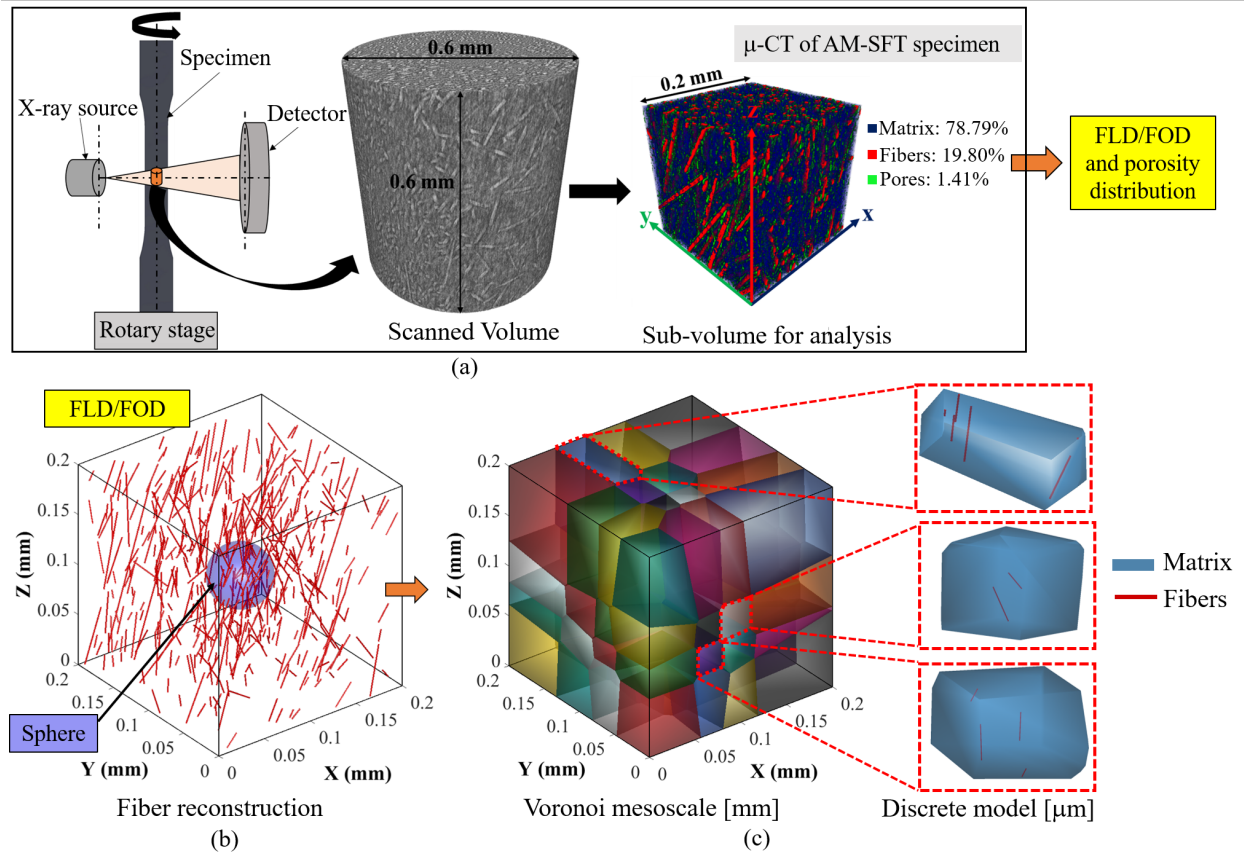


**Figure 5.1:** Specimen selection strategy and interrupted fatigue protocol (reproduced from Chapter 4). (a) Ultrasonic C-scan attenuation map of the AM–CM panel used to select three specimens with distinct porosity levels. (b) Stepwise cyclic loading protocol with periodic interruptions for  $\mu$ -CT scanning and quasi-static tensile testing. (c) Three scanning stages: BT, BF, and AF.

By repeatedly performing  $\mu$ -CT scanning and quasi-static tensile testing on the same specimen at each stage, a direct correlation is established between evolving microstructural features and mechanical property degradation, while eliminating specimen-to-specimen variability. The quasi-static stress–strain responses at each stage serve as the validation target for the coupon-scale predictions of this chapter.

## 5.2.2 Microstructure-Resolved Multiscale Framework

Figure 5.2 presents an overview of the multiscale framework. To capture fiber interaction physics while maintaining computational tractability at the coupon scale, direct discrete-cell nonlinear FE homogenization is replaced by a physics-informed GNN–LSTM surrogate that learns the mapping from local fiber interaction topology to the strain-dependent nonlinear stress response. The following subsections describe each component of the framework in sequence. Later sections describe each of these aspects in detail.



**Figure 5.2:** Microstructure reconstruction and mesoscale discretization workflow. (a)  $\mu$ -CT imaging of an AM-CM SFT specimen yields 3D-volumetric data segmented into carbon fiber, ABS matrix, and pore phases, from which fiber length, orientation, and clustering statistics are extracted within 0.2 mm sub-volumes. (b) A moving sphere traverses the reconstructed volume, grouping fibers whose centerlines intersect each sphere into localized interaction neighborhoods; representative points (centroids of fiber-sphere assemblies) serve as seeds for spatial partitioning. (c) Voronoi tessellation of the mesoscale cell produces a set of non-overlapping polyhedral cells, each representing a mechanically distinct fiber-interaction neighborhood for subsequent FE homogenization or surrogate evaluation (adapted from [4]).

### Extracting Fiber Features from $\mu$ -CT:

The volumetric data from high-resolution  $\mu$ -CT scans were segmented into three phases: carbon fibers, ABS matrix, and pores, as shown in Figure 5.2a. Fiber centerlines were then extracted from the segmented sub-volume (Figure 5.2b), preserving key geometric features governing mechanical response, including fiber lengths, orientation, clustering, and spatial distribution. In short-fiber thermoplastics, stress transfer is governed by shear-lag mechanisms, making the relative spatial arrangement of fibers critical. In

particular, regions of high fiber density (clusters) and low fiber density (resin-rich zones) exhibit fundamentally different load transfer characteristics and damage evolution. Accurately preserving these spatial heterogeneities is therefore essential for any physically meaningful microstructural representation.

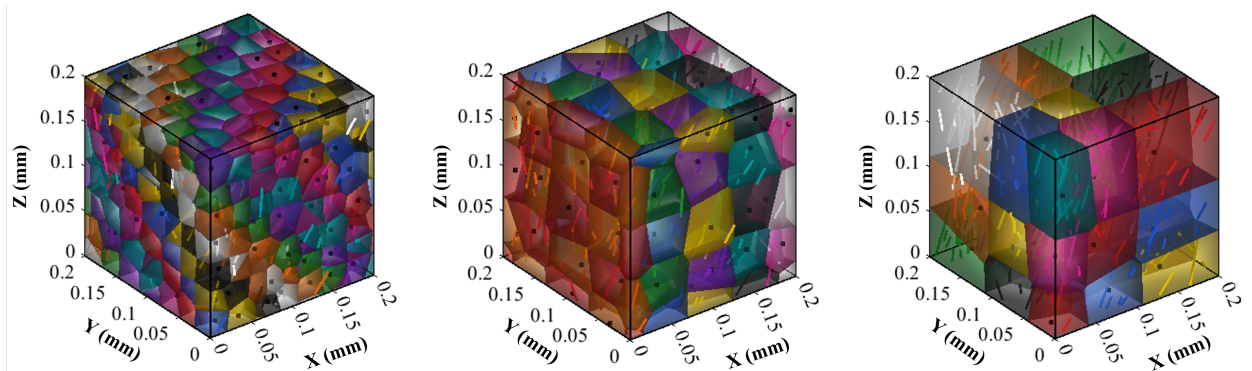
To capture these localized interactions, a moving-sphere sampling procedure is employed (Figure 5.2b). A sphere of radius  $R_s$  traverses the reconstructed volume on a regular three-dimensional Cartesian grid with uniform spacing equal to  $R_s$  in all three directions, and fibers whose centerlines intersect the sphere are grouped into local neighborhoods. The radius  $R_s$  thus defines an interaction length scale: a smaller  $R_s$  captures highly localized fiber interactions, while a larger  $R_s$  yields coarser neighborhoods that average over multiple clusters and matrix-rich regions. Moreover,  $R_s$  is selected as a global parameter based on the mean fiber length  $l_{f,mean}$  obtained from the  $\mu$ -CT data. Specifically,  $R_s \gtrsim l_{f,mean}$  ensures that individual fibers are sufficiently resolved within each sampled neighborhood and that shear-lag-based load transfer along the fiber length is not artificially truncated.

As the sphere traverses the microstructure, the chosen radius  $R_s$  generates a set of overlapping neighborhoods that capture local fiber interactions. Due to this overlap, individual fibers may be included in multiple neighborhoods, ensuring continuity of interaction information across adjacent regions. Each neighborhood is associated with a representative point, defined as the centroid of the combined set comprising the moving sphere center and the centroids of all fibers contained within the sphere. These representative points provide a discrete sampling of the microstructure and form the basis for subsequent spatial partitioning. A visualization of the moving-sphere traversal across a representative microstructure is available at GitHub (<https://github.com/AMPL-Gururaja>).

### **Voronoi Tessellation of the Mesoscale Domain:**

The representative points obtained from the moving-sphere sampling procedure serve as seeds to construct a Voronoi tessellation of the mesoscale domain. Voronoi tessellation

is preferred over alternative discretization methods, such as regular grids,  $k$ -means clustering, or Octree decomposition, because it preserves the intrinsic structural consistency of the underlying fiber distribution. First, because the seeds are derived directly from the fiber sampling process, the resulting cells are inherently topology-adaptive: fiber-dense regions naturally produce smaller cells, while matrix-rich regions yield larger cells, eliminating the need for user-defined mesh scales. Second, the tessellation provides a complete, non-overlapping partition of the domain, ensuring volumetric integrity during homogenization. Consequently, the mesoscale domain is decomposed into a set of non-overlapping polyhedral cells ( $\Omega_c$ ) that collectively span the entire domain (Figure 5.2c). Third, the equidistant nature of Voronoi boundaries defines a geometrically consistent local neighborhood. This geometry is directly controlled by the sampling sphere radius ( $R_s$ ), which dictates the minimum spacing between seeds, thereby influencing the spatial distribution and local fiber volume fraction. For instance, a larger sampling radius ( $R_s = 180 \mu\text{m}$ ) results in a coarser partition with fewer cells compared to a more refined sampling at  $R_s = 60 \mu\text{m}$  (see Figure 5.3). The Python implementation of the moving-sphere sampling and Voronoi tessellation described here is publicly available at GitHub (<https://github.com/AMPL-Gururaja>). The repository includes scripts for sphere traversal, seed generation, Voronoi cell construction, STL export, and fiber volume fraction computation for each discrete cell.



**Figure 5.3:** Dependence of Voronoi cell morphology on the moving-sphere sampling radius  $R_s$ , illustrated for three representative values:  $R_s = 60 \mu\text{m}$  (left),  $R_s = 120 \mu\text{m}$  (center), and  $R_s = 180 \mu\text{m}$  (right). As  $R_s$  increases, the number of seed points decreases, and individual cells grow larger.

### Discrete-Cell Finite-Element Homogenization:

Each discrete Voronoi cell  $\Omega_c$  is treated as a RUC with PBCs over which effective properties are evaluated using FE simulations. All FE simulations were performed using the commercially available software Abaqus 2022. Automated Python scripting was employed to generate equivalent cuboidal RUCs from the irregular Voronoi polyhedra through the following mapping procedure.

First, the bounding box of each Voronoi cell is computed from its vertex coordinates, and an equivalent cuboid is constructed such that its volume matches the Voronoi cell volume. Second, the fiber centerline coordinates extracted from  $\mu$ -CT—specifically the start and end points of each fiber segment clipped to the Voronoi cell—are directly transferred into the cuboidal RUC coordinate system by applying a rigid translation that maps the Voronoi centroid to the cuboid centroid, preserving the absolute fiber orientations and inter-fiber spacing. This mapping ensures two key microstructural properties are preserved: (i) the fiber volume fraction within the Voronoi cell, and (ii) the fiber orientation distribution within the cell.

The fibers and matrix were modeled using three-dimensional tetrahedral elements (C3D4), with PBCs applied on face, edge, and vertex pairs of the cuboidal RUC following the implementation detailed in our prior work [4, 121, 122]. To extract the effective response of the RUC, six independent macroscopic strain cases (three normal and three shear) are applied sequentially in the form of far-field displacement fields. For each loading configuration, the stress and strain fields within the RUC are obtained from finite element simulations. The effective (homogenized) stress response is determined through volume averaging of the local fields at integration points using Equation 5.1:

$$\bar{\sigma} = \frac{1}{V} \sum_{e=1}^{N_e} \sum_{g=1}^{N_{\text{int}}} \sigma^{g,e} V^{g,e} \quad (5.1)$$



where  $\bar{\sigma}$  is the homogenized second-order stress tensor,  $N_e$  is the total number of elements,  $N_{\text{int}}$  is the number of integration points per element (i.e. 1 in this case),  $\sigma^{g,e}$  is the stress tensor at the  $g$ -th integration point in the  $e$ -th element,  $V^{g,e}$  is the volume (weight) of the  $g$ -th integration point in the  $e$ -th element, and  $V$  is the total volume of the RUC.

The Voronoi cell-level effective response is represented by a strain-dependent constitutive operator (tangent stiffness evolution)  $\mathbb{C}(\bar{\epsilon})$  and the corresponding stress–strain curve. Mesh convergence studies were conducted until the change in homogenized Young’s modulus between successive refinements fell below 2%. A converged mesh element size of  $0.5 \mu\text{m}$  was used in the remainder of the study. The effective stress–strain response obtained from FE homogenization of each discrete Voronoi cell is subsequently assembled across the full mesoscale Voronoi tessellation through volume-weighted averaging to predict the coupon-scale mechanical response, as described in detail in Section 5.2.4.

### Constitutive Modeling of Constituents:

Carbon fibers are modeled as orthotropic linear-elastic solids using the properties listed in Table 5.1. Under the investigated quasi-static loading regime, post-mortem SEM analysis reveals no evidence of fiber fracture [4]; stiffness degradation is therefore attributed primarily to matrix-driven degradation mechanisms, and fiber damage has not been accounted for in the current analysis. Additionally, the fiber-matrix interface is assumed to be perfectly bonded.

**Table 5.1:** Elastic properties of the carbon fiber and ABS matrix constituents used in the 20 wt.% CF-ABS discrete-cell models.

| Constituent               | $E_{11}$<br>(GPa) | $E_{22}$<br>(GPa) | $E_{33}$<br>(GPa) | $G_{12}$<br>(GPa) | $G_{13}$<br>(GPa) | $G_{23}$<br>(GPa) | $\nu_{12}$ | $\nu_{13}$ | $\nu_{23}$ |
|---------------------------|-------------------|-------------------|-------------------|-------------------|-------------------|-------------------|------------|------------|------------|
| Carbon fiber <sup>a</sup> | 230               | 14                | 14                | 9                 | 9                 | 5                 | 0.25       | 0.25       | 0.30       |
| ABS matrix <sup>b</sup>   | 2.31              | 2.31              | 2.31              | 0.86              | 0.86              | 0.86              | 0.35       | 0.35       | 0.35       |

<sup>a</sup> Carbon fiber properties adopted from literature [123].

<sup>b</sup> ABS matrix elastic modulus and Poisson’s ratio are determined experimentally.

The baseline elastic properties of the ABS matrix phase were assumed to be isotropic and were experimentally determined in this study by quasi-static uniaxial tensile testing in accordance with ASTM D638 Type I at 2 mm/min. Standalone neat ABS specimens were manufactured using the same processing conditions as the composite matrix phase. Testing was performed at room temperature under a displacement-controlled loading rate to isolate the baseline elastic modulus ( $E = 2.31$  GPa) and Poisson's ratio ( $\nu = 0.35$ ), which are assigned as the initial undamaged properties in Table 5.1.

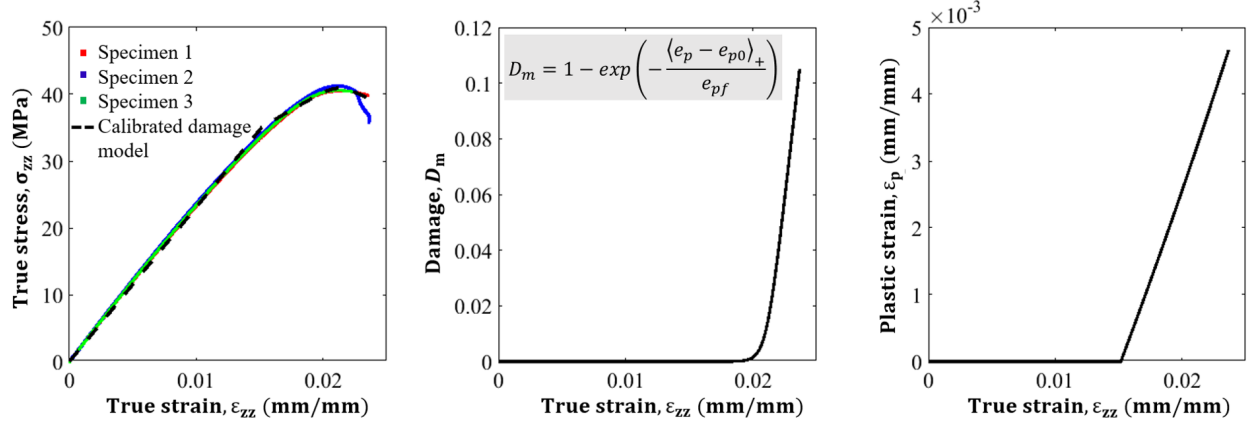
### **Matrix damage:**

The ABS matrix was modeled as an isotropic elastoplastic material with progressive damage to capture the experimentally observed nonlinearity, near-peak softening, and stiffness degradation. All damage model calibrations were performed using true stress–true strain data to ensure consistency under finite deformation. The initial elastic modulus  $E$  was obtained via linear regression within the small-strain regime. The global yield stress  $\sigma_Y$  was defined using the experimentally measured 0.2% offset criterion, averaged across 3 specimens.

Plastic hardening was represented using a two-term Voce law [124, 125]:

$$\sigma_y(e_p) = \sigma_Y + R_1 (1 - e^{-b_1 e_p}) + R_2 (1 - e^{-b_2 e_p}), \quad (5.2)$$

where  $e_p$  is the plastic strain and  $R_1, b_1, R_2, b_2$  are global hardening parameters identified by fitting the true stress–strain response up to peak stress while enforcing consistency with the prescribed yield stress (see Figure 5.4a). The two-term form was adopted because ABS, as an amorphous thermoplastic, exhibits a characteristic saturating hardening response in which the hardening rate declines progressively with plastic strain [67]; a single exponential term is insufficient to simultaneously capture both the early nonlinear hardening and the near-peak plateau, whereas the two-term superposition provides the required flexibility without additional physical assumptions. Progressive stiffness degra-



**Figure 5.4:** Calibration of the ABS matrix elastoplastic damage constitutive model. (a) Comparison of the calibrated two-term Voce plasticity plus exponential damage model against true stress ( $\sigma_{11}$ )–true strain ( $\epsilon_{11}$ ) curves from three specimens, demonstrating excellent agreement through the elastic, nonlinear hardening, and post-peak softening regimes. (b) Evolution of the scalar damage variable  $D_m$  with applied true strain ( $\epsilon_{11}$ ), showing damage initiation near peak stress followed by progressive softening. (c) Equivalent plastic strain ( $\epsilon_p$ ) at the onset of damage initiation (matrix failure index), illustrating the threshold beyond which crack-band-regularized softening is activated.

dation observed near and beyond peak stress was captured using a phenomenological scalar CDM framework. Within this framework, the scalar damage variable  $D_m \in [0, 1)$  acts uniformly on the undamaged elastic stiffness tensor  $\mathbb{C}_m$ , so that all normal and shear stiffness components are degraded by the same factor  $(1 - D_m)$ . The nominal Cauchy stress is therefore:

$$\boldsymbol{\sigma}_m = (1 - D_m) \mathbb{C}_m : \boldsymbol{\epsilon}_m \quad (5.3)$$

This isotropic stiffness degradation representation is consistent with established CDM formulations for thermoplastic matrices [67].

Damage initiates once  $e_p \geq e_{p0}$  and evolves according to an exponential softening law (see Figure 5.4b and Figure 5.4c):

$$D_m = 1 - \exp\left(-\frac{\langle e_p - e_{p0} \rangle_+}{e_{pf}}\right), \quad (5.4)$$

where the Macaulay bracket  $\langle \cdot \rangle_+$  ensures damage activates only when  $e_p > e_{p0}$ . The damage initiation strain  $e_{p0}$  and the characteristic softening strain  $e_{pf}$  were both treated as

phenomenological parameters identified directly from the post-peak true stress–strain data of each specimen. The complete set of calibrated parameters is summarized in Table 5.2.

**Table 5.2:** Calibrated ABS elastoplastic and damage parameters identified from true stress–strain data. Global plasticity parameters are common across all specimens; damage parameters are specimen-specific owing to differing porosity levels.

| Parameter                       | Symbol     | Value       |
|---------------------------------|------------|-------------|
| Elastic modulus                 | $E$        | 2311.29 MPa |
| 0.2% offset yield stress        | $\sigma_Y$ | 35.05 MPa   |
| Voce parameter                  | $R_1$      | 13.37 MPa   |
| Voce parameter                  | $b_1$      | 72.89       |
| Voce parameter                  | $R_2$      | 17.44 MPa   |
| Voce parameter                  | $b_2$      | 72.73       |
| Damage initiation strain        | $e_{p0}$   | 0.0032      |
| Characteristic softening strain | $e_{pf}$   | 0.013       |

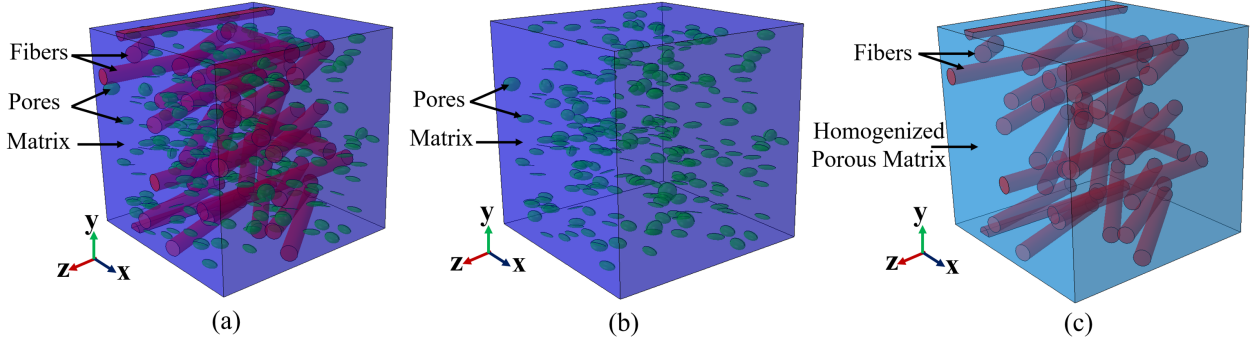
### Effective Matrix Stiffness Incorporating Porosity:

A two-step homogenization strategy was employed to incorporate the effect of porosity on the matrix’s effective stiffness (Figure 5.5). First, a matrix-only RUC containing  $\mu$ -CT-resolved pores was numerically homogenized (similar to the procedure described in 4.3.4) to obtain an effective porous-matrix stiffness tensor  $C_m^{\text{eff}}$ . Second, this matrix stiffness tensor was assigned to all fiber-matrix RUC models. This procedure isolated pore-induced matrix degradation while allowing the fiber topology to vary spatially between cells [126].

### 5.2.3 Surrogate Modeling Framework

A surrogate constitutive framework is introduced to efficiently approximate the non-linear, history-dependent homogenized response of each discrete Voronoi cell. For each Voronoi cell  $\Omega_c$ , the nonlinear finite-element homogenization defines a path-dependent constitutive operator in which the homogenized stress at pseudo-time  $t$  depends on the entire applied macroscopic strain history up to  $t$ :

$$\bar{\sigma}^{(\Omega_c)}(t) = \mathcal{H}_{\mathcal{T}_{\Omega_c}}(\{\bar{\varepsilon}(s)\}_{s \leq t}), \quad (5.5)$$



**Figure 5.5:** Two-step micromechanical homogenization procedure for incorporating matrix porosity effects. (a) Microstructure of SFTs consisting of carbon fibers and ABS matrix with micro-porosity, as reconstructed from  $\mu$ -CT imaging. (a) Step 1: a matrix-only RUC with  $\mu$ -CT-resolved pore morphology is homogenized under prescribed macroscopic strains to obtain the effective porous-matrix stiffness tensor  $C_m^{\text{eff}}$  ("Homogenized porous matrix"), (b) Step 2:  $C_m^{\text{eff}}$  is assigned to all fiber-matrix RUC used in the discrete-cell FE simulations ("Homogenized SFTs"), yielding fatigue-stage-resolved constitutive data that reflect measured porosity levels without explicitly meshing pores in every cell.

where  $\{\bar{\epsilon}(s)\}_{s \leq t}$  denotes the macroscopic strain history up to time  $t$ , and  $\mathcal{H}_{\mathcal{T}_{\Omega_c}}$  is a constitutive operator parameterized by the local fiber-interaction topology  $\mathcal{T}_{\Omega_c}$ , comprising fiber geometry, spacing, clustering, and orientation, within  $\Omega_c$ . The explicit dependence on strain history reflects the path-dependent nature of the response, which arises from evolving internal variables (accumulated plastic strain  $e_p$  and scalar damage  $D_m$ ) in the elastoplastic-damage matrix described in Section 5.2.2. The operator is therefore not reducible to a single-valued function of current strain, and any surrogate intended to replace it must inherit this history-dependent structure. As the number of discrete cells in a mesoscale assembly grew to the order of  $10^2$ – $10^3$ , repeated evaluation of  $\mathcal{H}_{\mathcal{T}_{\Omega_c}}$  through high-fidelity nonlinear FE simulations became computationally prohibitive. A surrogate operator  $\hat{\mathcal{H}}_{\mathcal{T}_{\Omega_c}}$  is therefore constructed such that

$$\hat{\sigma}^{(\Omega_c)}(t) = \hat{\mathcal{H}}_{\mathcal{T}_{\Omega_c}}(\{\bar{\epsilon}(s)\}_{s \leq t}) \approx \mathcal{H}_{\mathcal{T}_{\Omega_c}}(\{\bar{\epsilon}(s)\}_{s \leq t}). \quad (5.6)$$

The surrogate was trained on FE-generated stress–strain trajectories that satisfy equilibrium, the Hill–Mandel macro-homogeneity condition, and the two-term Voce isotropic-hardening

elastoplastic-damage constitutive law calibrated for the ABS matrix phase (Section 5.2.2). The construction of  $\hat{\mathcal{H}}_{\mathcal{T}_{\Omega_c}}$  was decomposed into two complementary components that mirror the structure of classical history-dependent constitutive models: (i) a GNN that encodes the topology  $\mathcal{T}_{\Omega_c}$  into a fixed-dimensional descriptor capturing the cell's stiffness potential and matrix-mediated load-transfer pathways, and (ii) a LSTM network that propagates the strain history through learned hidden- and cell-state vectors that serve as surrogate internal variables encoding accumulated plasticity and damage. The GNN therefore parametrizes the topology argument of  $\hat{\mathcal{H}}$ , while the LSTM parametrizes the history argument. These components are described in Sections 5.2.3 and 5.2.3, respectively, and combined into the integrated architecture in Section 5.2.3.

### Encoding Fiber Interactions via GNN:

Each discrete Voronoi domain  $\Omega_c$  was represented as an undirected weighted graph  $\mathcal{G}_{\Omega_c} = (\mathcal{V}_{\Omega_c}, \mathcal{E}_{\Omega_c}, \mathcal{X}_{\Omega_c})$ , where  $\mathcal{V}_{\Omega_c}$  is the set of nodes representing individual fibers within the cell,  $\mathcal{E}_{\Omega_c}$  is the set of weighted edges encoding shear-lag-mediated load-transfer pathways between fiber pairs, and  $\mathcal{X}_{\Omega_c} \in \mathbb{R}^{N_f \times 8}$  is the node-feature matrix whose rows store per-fiber geometric attributes, with  $N_f = |\mathcal{V}_{\Omega_c}|$  denoting the number of fibers in the cell. The microstructural input to the GNN for each fiber node  $n$  consists of its three-dimensional start and end coordinates,  $\mathbf{x}_n^{(s)}, \mathbf{x}_n^{(e)} \in \mathbb{R}^3$ , extracted directly from  $\mu$ -CT, together with the cell-level fiber volume fraction  $V_{f,\Omega_c}$  obtained from phase segmentation of the reconstructed volume (Figure 5.2). From these primitives, the fiber length  $l_n = \|\mathbf{x}_n^{(e)} - \mathbf{x}_n^{(s)}\|$ , orientation vector  $\mathbf{t}_n = (\mathbf{x}_n^{(e)} - \mathbf{x}_n^{(s)})/l_n$ , and per-fiber volume-fraction contribution  $V_{f,n} = V_{f,\Omega_c} l_n / \sum_k l_k$  were computed for each Voronoi cell. To accelerate learning, an 8-dimensional feature vector is defined per fiber:

$$\mathbf{x}_n = [l_n, V_{f,n}, \mathbf{x}_n^{(s)}, \mathbf{x}_n^{(e)}] \in \mathbb{R}^8 \quad (5.7)$$

Figure 5.6 depicts the graph representation for a discrete Voronoi cell. Here, each fiber node  $n$  is represented using two descriptors: (i) the local fiber volume-fraction contribution  $V_{f,n}$  and (ii) the spatial endpoint coordinates  $\mathbf{x}_n^{(s)}$  and  $\mathbf{x}_n^{(e)}$ , which together encode the fiber length and orientation. The edges of  $\mathcal{G}_{\Omega_c}$  are assigned weights  $w_{pq}$  that quantify the load-transfer efficiency between fiber pairs (see Figure 5.6).

**A note about edge weights:** As previously mentioned, the edge weights capture the load-transfer efficiency between adjacent fiber pairs via matrix-mediated shear. In short-fiber composites, axial stress is transferred between adjacent fiber ends through interfacial shear stress transfer that occurs over a characteristic shear transfer length  $L_c$ . A neighboring fiber at end-to-end separation  $d_{pq}$  therefore experiences a shear stress whose magnitude is proportional to  $\exp(-d_{pq}/L_c)$ : fiber pairs within  $L_c$  interact strongly, while pairs separated by distances much greater than  $L_c$  are effectively mechanically decoupled.  $L_c$  was computed from Nairn's (1997) shear-lag formulation [95–100], which extended the classical Cox result to account for the geometric confinement of the matrix between neighboring fibers:

$$L_c = r_f \sqrt{\frac{E_{11}^f \ln(R/r_f)}{2\pi G_{12}^m}} \quad (5.8)$$

where  $r_f$  is the fiber radius,  $E_{11}^f$  is the fiber axial Young's modulus (Table 1),  $G_{12}^m$  is the matrix in-plane shear modulus (Table 1), and  $R = r_f \sqrt{\pi/(2\sqrt{3} V_{f,\Omega_c})}$  is the mean matrix cylinder radius determined by local fiber packing geometry within the Voronoi cell.

The pairwise interaction weight between fibers  $p$  and  $q$  was defined as:

$$w_{pq} = \exp\left(-\frac{d_{pq}}{L_c}\right) (0.90 |\mathbf{t}_p \cdot \mathbf{t}_q| + 0.10) \quad (5.9)$$

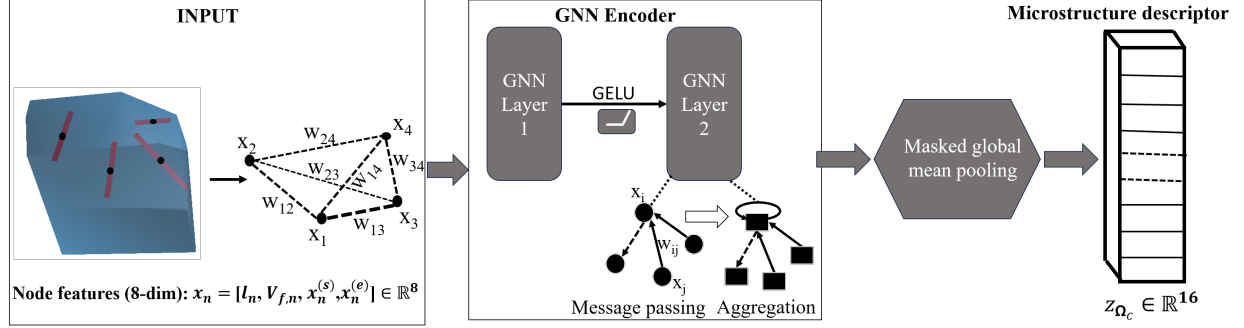
where  $d_{pq}$  was the minimum segment-to-segment distance between fibers  $p$  and  $q$ , and  $\mathbf{t}_p$ ,  $\mathbf{t}_q$  are their unit direction vectors. The exponential term encodes the attenuation of the shear-mediated stress field with fiber–fiber separation: as fiber ends move apart, the

driving stress available to transfer load into a neighboring fiber diminishes exponentially over the length  $L_c$ .

The orientation-dependent edge weight is defined as  $(0.90|\mathbf{t}_p \cdot \mathbf{t}_q| + 0.10)$ , capturing both axial and residual interaction mechanisms. The dominant term (0.90) represents shear-lag-driven axial coupling, which scales with the cosine of the inter-fiber angle. It is strongest for parallel fibers, while highly misaligned fibers contribute minimally to axial stress redistribution. The constant term (0.10) accounts for a residual, orientation-independent interaction arising from transverse stress concentration due to fiber–matrix elastic stiffness mismatch, ensuring nonzero coupling even for orthogonal fibers. The 0.90/0.10 split was determined from the normalized peak interfacial shear stress ratio obtained in the two-fiber interaction finite element simulations (Appendix D). These simulations show that the peak interfacial shear stress for orthogonal ( $\phi = 90^\circ$ ) fibers dropped to approximately 10% (ranging between 8–22% depending on the inter-fiber gap distance) of the fully aligned ( $\phi = 0^\circ$ ) baseline configuration. This baseline residual ratio served as the basis for using 0.10, while the remaining normalized load-bearing capacity (0.90) was allocated to the orientation-dependent cosine term.

The edge weight function operates strictly at the pairwise level. Higher-order multi-fiber interaction effects—such as load redistribution within fiber clusters and cooperative load sharing—are not explicitly encoded in the edge weights but emerge through neighborhood aggregation in the GNN message-passing operation (Equation (5.10)). The graph is undirected  $w_{pq} = w_{qp}$  and complete: every pair of fibers within a Voronoi cell is connected. A lower bound of  $10^{-6}$  was imposed on edge weights to maintain numerical stability of the degree-normalized aggregation in Equation (5.10), without altering the graph topology. The parametric finite-element study (Appendix D) further confirmed that both the cosine-dependent axial coupling and the orientation-independent residual are physically operative for fiber geometries and spacings consistent with  $\mu$ -CT observations.





**Figure 5.6:** Graph construction and GNN encoding for a Voronoi cell. **Left:** Fibers are represented as graph nodes, with node features given by local volume fraction  $V_{fiber, \Omega_c}$  and spatial endpoints  $\mathbf{x}_n^{(s)}$ ,  $\mathbf{x}_n^{(e)}$ . Fiber–fiber interactions were modeled as weighted edges ( $w_{pq}$ ), computed from geometric proximity and directional alignment using a shear-lag-informed weight function (Equation 5.9). **Center:** The graph is processed through two stacked graph convolutional layers, where message passing and neighborhood aggregation update node embeddings to reflect local load redistribution. **Right:** Masked global mean pooling aggregates the final node embeddings into a compact 16-dimensional region-level microstructural descriptor  $z_{\Omega_c} \in \mathbb{R}^{16}$ , representing the combined effect of fiber geometry and interaction topology on the Voronoi cell’s effective response.

### Graph convolutional network (GCN) layer formulation:

Node features were first projected from the 8-dimensional input space to a 64-dimensional embedding space via a linear layer with GELU activation. Two stacked graph convolutional layers then updated node embeddings through degree-normalized weighted aggregation with residual connections:

$$\mathbf{h}_n^{(l+1)} = \mathbf{h}_n^{(l)} + \text{Dropout} \left( \text{LN} \left( \text{GELU} \left( \sum_{m \in \mathcal{N}(n)} \frac{w_{nm}}{\sqrt{\hat{d}_n \hat{d}_m}} \mathbf{W}^{(l)} \mathbf{h}_m^{(l)} \right) \right) \right) \quad (5.10)$$

where  $\mathbf{h}_m^{(l)}$  is the embedding of neighboring fiber node  $m$  at layer  $l$ ,  $w_{nm}$  is the edge weight from Equation 5.9,  $\hat{d}_n = 1 + \sum_j w_{nj}$  is the weighted node degree with self-loop,  $\mathbf{W}^{(l)}$  is the trainable weight matrix at layer  $l$ , LN denotes layer normalization, and the residual connection  $\mathbf{h}_n^{(l)}$  stabilized gradient flow across layers. The degree normalization factor  $1/\sqrt{\hat{d}_n \hat{d}_m}$  prevents embedding magnitudes from scaling with local fiber connectivity, ensuring that fibers in dense clusters were not artificially amplified relative to isolated fibers.

From a mechanical standpoint, this message-passing operation approximated multi-fiber load redistribution within the fiber network: edge weights encoded pairwise shear-mediated stress-transfer efficiency, neighborhood aggregation represented multi-fiber load sharing among all neighboring fibers, and stacked layers iteratively propagated this redistribution across the interaction network—analogous to FE solver iterations.

After two message-passing layers, masked global mean pooling aggregated active node embeddings into a 64-dimensional graph-level representation, which was projected by a linear layer to a compact 16-dimensional microstructural descriptor:

$$z_{\Omega_c} = \mathbf{W}_{\text{pool}} \left( \frac{1}{N_f} \sum_{n=1}^{N_f} \mathbf{h}_n^{(2)} \right) \in \mathbb{R}^{16} \quad (5.11)$$

This embedding served as a compact, fixed-length representation of the cell's effective stiffness potential and interaction topology, capturing the combined influence of fiber geometry, spatial distribution, volume fraction, and interaction network structure on the cell's effective mechanical response. Because  $z_{\Omega_c}$  was derived exclusively from quantities computable from  $\mu$ -CT fiber coordinates and  $V_{f,\Omega_c}$ , the GNN required no microstructural inputs beyond standard reconstruction outputs.

### **Modeling History-Dependent Nonlinear Evolution via LSTM:**

The homogenized stress response of each cell was a history-dependent trajectory that reflected progressive accumulation of matrix plastic strain  $e_p$  and scalar damage  $D_m$  under monotonic loading. Because these internal variables evolved with loading history, the stress at any increment depended not only on the current strain but on the entire prior deformation path. A feedforward network that treats each strain increment independently could not enforce this temporal consistency. A LSTM network was therefore employed to process the loading history as a sequence, maintaining hidden state vectors  $\mathbf{h}_t \in \mathbb{R}^{128}$  and cell state vectors  $\mathbf{c}_t \in \mathbb{R}^{128}$  as surrogate internal state variables implicitly encoding accumulated plasticity and damage without explicitly tracking them.

LSTM input features: The LSTM input at each strain increment  $t$  was a 21-dimensional feature vector concatenated from two categories of inputs:

$$\mathbf{q}_t = \underbrace{\left[ \frac{\varepsilon_t}{\varepsilon_{\text{pk}}}, \left( \frac{\varepsilon_t}{\varepsilon_{\text{pk}}} \right)^2, \left( \frac{\varepsilon_t}{\varepsilon_{\text{pk}}} \right)^3, \ln \left( 1 + \frac{\varepsilon_t}{\varepsilon_{\text{pk}}} \right), V_{f,\Omega_c} \right]}_{5 \text{ loading-side features}} \parallel \underbrace{z_{\Omega_c}}_{16 \text{ D topology}} \quad (5.12)$$

These input vector maintains a fixed size of 21 dimensions across all strain increments rather than growing with the sequence length. The history of prior deformation is captured entirely through the step-by-step updates of the fixed-dimensional internal state. The first category comprised five loading-side features derived analytically from the applied scalar strain  $\varepsilon_t$  and the fiber coordinate inputs used by the GNN. The polynomial and logarithmic strain features, motivated by the hyperelastic model, enriched the nonlinear strain representation, enabling the LSTM to distinguish between the linear elastic, nonlinear hardening, and near-peak softening regimes without requiring an explicit constitutive form. Normalizing strain by  $\varepsilon_{\text{pk}}$  mapped the stress peak of every cell to a universal reference strain of 1.0, enabling the LSTM to learn a shape that was subsequently amplitude-rescaled. The cell-level volume fraction  $V_{f,\Omega_c}$  directly conveyed the available reinforcement content.

The LSTM hidden and cell state vectors evolved as:

$$(\mathbf{h}_t, \mathbf{c}_t) = \text{LSTM}(\mathbf{q}_t, \mathbf{h}_{t-1}, \mathbf{c}_{t-1}) \quad (5.13)$$

with two stacked layers (hidden dimension 128, inter-layer dropout 0.25). The hidden and cell states serve as surrogate internal variables implicitly encoding accumulated plastic strain and damage history at each loading increment. The GNN component performed geometric and topological encoding of the fiber interaction network, while the LSTM modeled the path-dependent evolution of the constitutive response — a separation that mirrors classical constitutive modeling, in which microstructural descriptors govern stiffness capacity while evolution laws govern nonlinear progression.

### Integrated GNN–LSTM Architecture:

The final surrogate mapping from fiber interaction topology to normalized stress trajectory was:

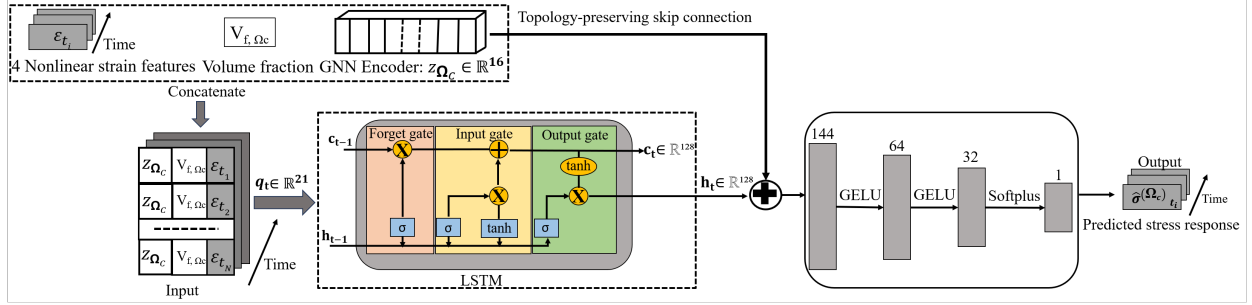
$$\hat{\sigma}_t^{(\Omega_c)} = \text{Softplus}\left(\mathcal{F}_{\text{out}}\left(\left[\mathbf{h}_t ; z_{\Omega_c}\right]\right)\right), \quad \mathbf{h}_t = \mathcal{F}_{\text{LSTM}}(\mathbf{q}_t, \mathbf{h}_{t-1}, \mathbf{c}_{t-1}), \quad z_{\Omega_c} = \mathcal{F}_{\text{GNN}}(\mathcal{G}_{\Omega_c}) \quad (5.14)$$

where  $\mathcal{F}_{\text{GNN}}(\mathcal{G}_{\Omega_c})$  denoted the GNN encoder operating on the fiber interaction graph  $\mathcal{G}_{\Omega_c}$  of cell  $\Omega_c$ , and  $\mathcal{F}_{\text{out}}$  was a three-layer residual output network. Figure 5.7 illustrates the complete architecture.

The output network received a skip-connected input formed by concatenating the LSTM hidden state  $\mathbf{h}_t \in \mathbb{R}^{128}$  with the GNN embedding  $z_{\Omega_c} \in \mathbb{R}^{16}$  at every strain increment, producing a 144-dimensional input to a three-layer MLP ( $144 \rightarrow 64 \rightarrow 32 \rightarrow 1$ , GELU activations). The skip connection ensured that the GNN-encoded topology signal—which carried direct information about the cell’s peak stress potential through its fiber arrangement—remained accessible at every prediction step, regardless of the LSTM hidden state depth. Without this connection, the GNN amplitude signal would need to propagate through all LSTM gates over potentially 100 or more time steps, risking attenuation due to gate saturation. A Softplus nonlinearity, defined as  $f(x) = \ln(1 + e^x)$ , at the network output enforced the physical constraint that predicted stress remained strictly non-negative throughout the trajectory.

To recover stress in physical units, the surrogate output was trained against FE-computed stress trajectories, normalized by the cell-level peak stress, with the peak stress predicted independently from the GNN embedding via a post hoc regression model trained on the same FE dataset. This architecture enforced a physically meaningful factorization: the GNN captured topology-dependent stiffness potential from the fiber interaction structure; the LSTM captured the path-dependent evolution of the constitutive response.

The peak stress amplitude was predicted using a Random Forest regressor (300 trees, MultiOutputRegressor) trained post-hoc on the frozen GNN embedding  $z_{\Omega_c}$  concatenated with the cell-level volume fraction  $V_{f,\Omega_c}$ , using the same 500-cell dataset and 70–15–15 train–validation–test split. Although the GNN auxiliary head also predicted peak stress during joint training, it exhibited a degradation in generalization on unseen cells due to its coupling with the evolving LSTM gradients during end-to-end optimization. The post-hoc Random Forest, applied to frozen embeddings after GNN–LSTM convergence, provided more robust amplitude generalization without requiring additional finite-element simulations, achieving a coefficient of determination  $R^2 = 0.98$  on the held-out test set for peak stress prediction compared with the discrete FE model.



**Figure 5.7:** Integrated GNN–LSTM architecture for physics-informed, history-dependent stress–strain prediction. The GNN microstructure encoder (left) processes the fiber interaction graph  $\mathcal{G}_{\Omega_c}$  to produce a fixed 16-dimensional cell embedding  $z_{\Omega_c} \in \mathbb{R}^{16}$ . At each strain increment  $t$ , this embedding is concatenated with four nonlinear strain features and the cell-level volume fraction  $V_{f,\Omega_c}$  to form the 21-dimensional input vector  $q_t \in \mathbb{R}^{21}$ , which is fed sequentially into a two-layer LSTM (hidden dimension 128). The LSTM hidden state  $h_t \in \mathbb{R}^{128}$  evolves as a surrogate set of internal state variables encoding accumulated plasticity and damage history. A skip connection concatenates  $z_{\Omega_c}$  directly with  $h_t$ , producing a 144-dimensional input to a three-layer output MLP ( $144 \rightarrow 64 \rightarrow 32 \rightarrow 1$ , Softplus), which yields the normalized predicted stress  $\hat{\sigma}_t^{(\Omega_c)}$  at each increment.

## Physics-Informed Regularization

Composite loss function: To ensure physically plausible surrogate predictions, a composite loss function was used alongside additional structural training constraints. Model

parameters were optimized by minimizing:

$$\mathcal{L} = \mathcal{L}_{\text{Huber}} + 0.05 \mathcal{L}_{\text{mono}} + 0.001 \mathcal{L}_{\text{smooth}} + 0.02 \mathcal{L}_{\text{zero}} + 0.3 \mathcal{L}_{\text{aux}} + 0.5 \mathcal{L}_{\text{peak}} \quad (5.15)$$

The scalar scaling coefficients were assigned to each loss component (0.05, 0.001, 0.02, 0.3, and 0.5) and function as regularization hyperparameters. These constants were determined empirically via a grid search on the validation subset to ensure stable convergence during joint training, balancing trajectory-tracking accuracy with physical admissibility constraints (e.g., preventing non-physical oscillations without over-penalizing post-yield softening). The primary term  $\mathcal{L}_{\text{Huber}}$  was a strain-weighted Huber loss ( $\delta = 0.1$ ) computed exclusively over real, non-padded data points:

$$\mathcal{L}_{\text{Huber}} = \frac{\sum_t w_t \mathcal{H}_\delta(\hat{\sigma}_t - \sigma_t^{\text{FE}})}{\sum_t w_t} \quad (5.16)$$

where  $\hat{\sigma}_t$  denotes the surrogate-predicted normalized stress at strain increment  $t$ ,  $\sigma_t^{\text{FE}}$  represents the corresponding high-fidelity FE homogenization target stress, and  $w_t$  is the strain-dependent tracking weight matrix. The tracking weights are defined explicitly as:

$$w_t = 1 + 3 \left[ \text{clip} \left( \frac{\varepsilon_t / \varepsilon_{\text{pk}} - 0.8}{0.8}, 0, 1 \right) \right]^2 \quad (5.17)$$

where  $\varepsilon_t$  is the applied macroscopic strain at step  $t$ , and  $\varepsilon_{\text{pk}}$  is the localized cell-level strain corresponding to the peak stress point. The term  $\text{clip}(x, a, b)$  represents a standard mathematical bounding operation defined to constrain the scaling window strictly between  $a$  and  $b$ .

This custom weighting scheme is engineered to prioritize tracking accuracy along highly nonlinear paths. It assigns a tracking penalty up to  $4\times$  higher to data points approaching and exceeding the stress peak ( $\varepsilon_t / \varepsilon_{\text{pk}} \geq 0.8$ ), where accurate prediction of the onset and progression of nonlinear matrix softening is most mechanically significant. The Huber

loss component  $\mathcal{H}_\delta$  is intentionally employed in preference to a standard mean-squared error framework to reduce gradient sensitivity to extreme outlier stress fluctuations arising from highly localized damage events in individual cells, while retaining stable quadratic penalization for minor prediction errors.

Pre-peak monotonicity: Stress increments prior to the peak were regularized to prevent non-physical oscillations:

$$\mathcal{L}_{\text{mono}} = \frac{1}{t_{\text{pk}} - 1} \sum_{t=1}^{t_{\text{pk}}-1} \text{GELU}(\hat{\sigma}_{t-1} - \hat{\sigma}_t) \quad (5.18)$$

where  $t_{\text{pk}}$  was the index of the true stress peak identified from the FE data for each cell. The post-peak regime was explicitly excluded from this constraint, consistent with the experimentally observed and FE-computed post-peak softening behavior of the ABS matrix following peak stress.

Smoothness: Second-order differences of the predicted stress trajectory were penalized to suppress artificial stiffness fluctuations:

$$\mathcal{L}_{\text{smooth}} = \frac{1}{T-2} \sum_{t=1}^{T-2} (\hat{\sigma}_{t+1} - 2\hat{\sigma}_t + \hat{\sigma}_{t-1})^2 \quad (5.19)$$

where  $T$  represents the total sequence length (total number of strain increments) in the complete loading history.

Elastic consistency: The predicted normalized stress at the first strain increment was penalized to enforce physically correct onset from zero stress:

$$\mathcal{L}_{\text{zero}} = \hat{\sigma}_0^2 \quad (5.20)$$

where  $\hat{\sigma}_0$  is the surrogate-predicted normalized stress at the initial strain increment ( $t = 0$ ), ensuring that the predicted stress trajectory originates strictly from a state of zero stress.

Auxiliary physics supervision: The auxiliary loss  $\mathcal{L}_{\text{aux}}$  penalized deviation of the GNN auxiliary head predictions  $[\tilde{E}, \tilde{\sigma}_{\text{pk}}, \tilde{\epsilon}_{\text{pk}}, \tilde{\delta}]$  from their normalized FE-computed targets, ensuring that the 16-dimensional cell embedding encoded mechanically interpretable information initial modulus, peak stress, peak strain, and post-peak softening rate throughout training rather than converging to a representation that satisfied the trajectory loss without physical meaning.

Peak stress penalty: The term:

$$\mathcal{L}_{\text{peak}} = \left\| \hat{t}_{\text{pk}} - t_{\text{pk}}^{\text{FE}} \right\|^2 \quad (5.21)$$

applied concentrated penalization at the exact peak stress point, improving prediction accuracy at the mechanically critical transition between hardening and softening regimes independently of the weighted Huber loss.

Optimizer and training schedule: The GNN and LSTM were trained jointly end-to-end using the AdamW optimizer (initial learning rate  $5 \times 10^{-4}$ , weight decay  $2 \times 10^{-4}$ ) [127] with gradient norm clipping to 1.0 to prevent unrealistically high gradients during early training epochs. A ReduceLROnPlateau learning rate scheduler [128] halved the learning rate when the validation loss plateaued for 15 consecutive epochs, with a minimum learning rate of  $10^{-6}$ . Training ran for up to 800 epochs; early stopping was applied based on validation loss, with a patience of 57 epochs, to prevent overfitting. The complete set of training hyperparameters is summarized in Appendix E.

Error Propagation and Stability: Small-cell-level prediction errors with the GNN-LSTM surrogate did not lead to any observed instabilities in the coupon-scale simulations. Because the coupon-level response was obtained by volume averaging over many discrete cells, surrogate approximation errors were statistically mitigated through the averaging operation itself. Robust macroscopic predictions were therefore achievable even in the presence of small cell-level surrogate approximation errors, with the principal sources of



coupon-scale discrepancy attributable to structural idealizations in the Voronoi representation rather than to surrogate approximation errors.

#### 5.2.4 Mesoscale Assembly and Coupon-Scale Prediction

Having obtained the effective stress–strain response of each discrete Voronoi cell—either through direct FE homogenization (Section 4.3.4) or through the GNN-LSTM surrogate (Section 5.2.3)—the collection of cell responses defines a heterogeneous mesoscale constitutive field over the reconstructed volume. The coupon-scale response was obtained by assembling the Voronoi cell responses through volume-weighted averaging, consistent with the Hill–Mandel homogenization principle:

$$\langle \sigma \rangle = \frac{1}{V_{\text{coupon}}} \sum_{\Psi_c} V_{\Psi_c} \langle \sigma \rangle^{(\Psi_c)} \quad (5.22)$$

where  $\langle \sigma \rangle$  is the macroscopic second-order stress tensor of the coupon,  $V_{\text{coupon}}$  is the total volume of the coupon,  $\Psi_c$  denotes the  $c$ -th mesoscale Voronoi cell within the reconstructed assembly,  $V_{\Psi_c}$  is the volume of that corresponding cell, and  $\langle \sigma \rangle^{(\Psi_c)}$  is the homogenized second-order stress tensor predicted by the trained GNN-LSTM surrogate predictions under the applied macroscopic strain tensor  $\epsilon$ .

Because the macroscopic response is obtained by aggregation over many cells, moderate cell-level surrogate errors are naturally stabilized through averaging. This enables robust coupon-scale prediction while preserving sensitivity to the spatial distribution of fiber interaction topology.

### 5.3 Results and Discussion

#### 5.3.1 Microstructural Evolution under Cyclic Loading

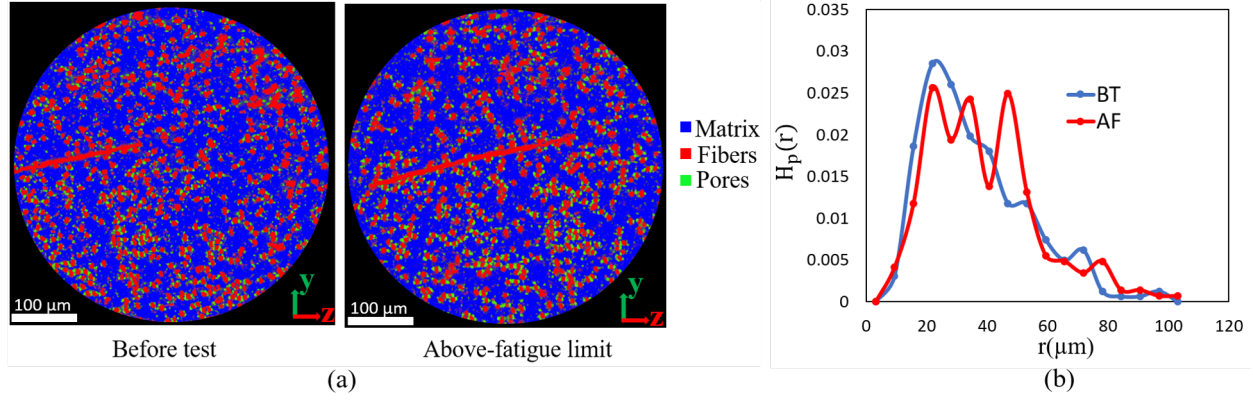
$\mu$ -CT analysis revealed that pore nucleation and growth were highly localized. Cyclic loading induced measurable shifts in ensemble-level microstructural descriptors, with pores

forming preferentially in (i) fiber-end neighborhoods and (ii) clustered fiber regions where local matrix ligaments are thin (Figure 5.8a). These locations coincide with regions of elevated shear and normal stress concentration as predicted by shear-lag theory and inter-fiber load-transfer mechanics. The preferential localization of porosity near fiber termini provided direct experimental evidence that stress-transfer discontinuities at fiber ends serve as primary damage-initiation sites.

The nearest-neighbor probability density  $H_p(r)$  provides complementary quantitative evidence of progressive fiber-cluster dispersion accompanying pore growth (Figure 5.8b). Before testing,  $H_p(r)$  exhibited a single dominant peak near  $r \approx 20\text{--}22\ \mu\text{m}$ , consistent with tight fiber clustering inherited from the manufacturing process. Above the fatigue limit, however, a secondary peak emerged near  $r \approx 45\text{--}47\ \mu\text{m}$ , producing a distinct bimodal distribution that signifies a clear signature of cluster dilation.

While fiber rotation is geometrically constrained within a pristine, continuous polymer matrix, this observable shift in the FOD is a direct structural consequence of severe, localized matrix failure that accumulates during cyclic loading. As fatigue cycles progress, a massive threefold increase in localized matrix porosity occurred preferentially within the thin matrix ligaments separating dense fiber clusters and around stress-concentrating fiber ends (see Table 5.3). This progressive micro-voiding, debonding, and matrix degradation effectively dismantled the local geometric constraints holding the fibers rigid. Under macroscopic tensile strain, the fibers adjacent to these expanding void networks are physically tilted and reallocated into the newly vacated micro-volumes. This localized rearrangement and shifting of the fiber network under cyclic loading directly aligns with experimental observations of damage-induced microstructural evolution reported in the literature [129, 130].

The extracted descriptors revealed a gradual yet systematic microstructural evolution under fatigue loading. Figure 5.9 shows shifts in orientation distributions and aspect-ratio

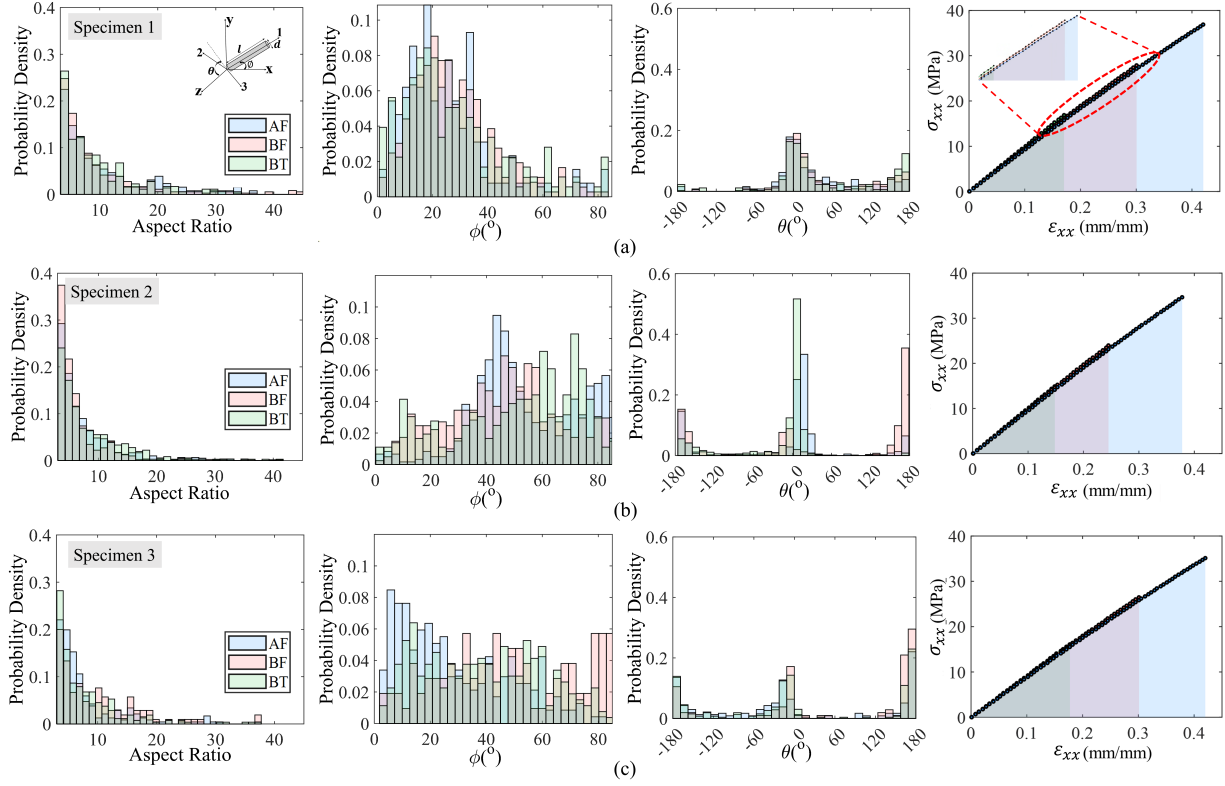


**Figure 5.8:** Fatigue-driven microstructural damage in 20 wt.% CF-ABS, fabricated via AM-CM at ORNL, was characterized using  $\mu$ -CT. (a) Representative cross-sectional images at two damage states are shown: prior to fatigue loading (Before test) and after exceeding the fatigue limit (Above-fatigue limit). Post-fatigue scans reveal pronounced localized pore nucleation and growth, predominantly near fiber termini and within fiber-clustering regions, indicating stress-concentration-mediated damage initiation and propagation. (b) Nearest-neighbor probability density  $H_p(r)$  tracked longitudinally for a representative sample (Specimen 2) for the Before test (BT) and Above fatigue limit (AF) stages, indicating progressive cluster dilation driven by pore growth within the inter-fiber zones, resulting in a dispersed sub-population of fibers with substantially increased nearest-neighbor distances.

**Table 5.3:** Porosity volume fraction (%) evolution under cyclic loading. Values represent the mean  $\pm$  standard deviation (adopted from [4]).

| Specimen | Before test     | Below fatigue limit | Above fatigue limit |
|----------|-----------------|---------------------|---------------------|
| 1        | $1.41 \pm 0.17$ | $2.33 \pm 0.21$     | $6.63 \pm 0.70$     |
| 2        | $1.90 \pm 0.15$ | $2.56 \pm 0.18$     | $8.64 \pm 0.60$     |
| 3        | $2.86 \pm 0.11$ | $3.57 \pm 0.15$     | $11.86 \pm 0.56$    |

statistics, indicative of microstructural rearrangement and spatial reallocation of fiber-interaction neighborhoods under cyclic loading. Consistent with these observations, the porosity volume fraction increased progressively under cyclic loading for all three specimens (Table 5.3). The presence of pores reduces the effective load-bearing capacity of the matrix and modifies the local stress state within the composite. The increase is particularly pronounced for specimens loaded above the fatigue limit, where porosity growth exceeded the initial (pre-fatigue) state by threefold. Although these changes were moderate at the ensemble level, their spatial localization significantly amplifies the progression of localized damage.



**Figure 5.9:** Statistical characterization of fiber morphology and its correlation with mechanical response across fatigue stages. **Left:** Histograms of measured fiber aspect ratios at each fatigue stage (BT, BF, AF), revealing quantifiable shifts in fiber length distribution under cyclic loading. **Center:** Histograms of the in-plane fiber orientation angle  $\phi$  measured from the x-axis and angle  $\theta$  in the y-z plane. **Right:** Experimentally measured axial stress-strain responses in the fiber-dominated direction: BT, BF, and AF. Rows correspond to Specimen 1 (top), Specimen 2 (middle), and Specimen 3 (bottom), which span three distinct initial porosity levels.

When correlated with the macroscale mechanical response (Figure 5.9), the progressive increase in porosity and localized damage accumulation corresponded to only marginal reductions in the longitudinal elastic stiffness and a subtle, early onset of axial nonlinear deformation. This highly stable axial behavior is consistent with the fiber-dominated nature of short-fiber architectures, where the longitudinal modulus is governed primarily by the high-stiffness reinforcement phase and remains relatively insensitive to low-to-moderate variations in matrix void content within the 1%–6% range. However, as fatigue-induced

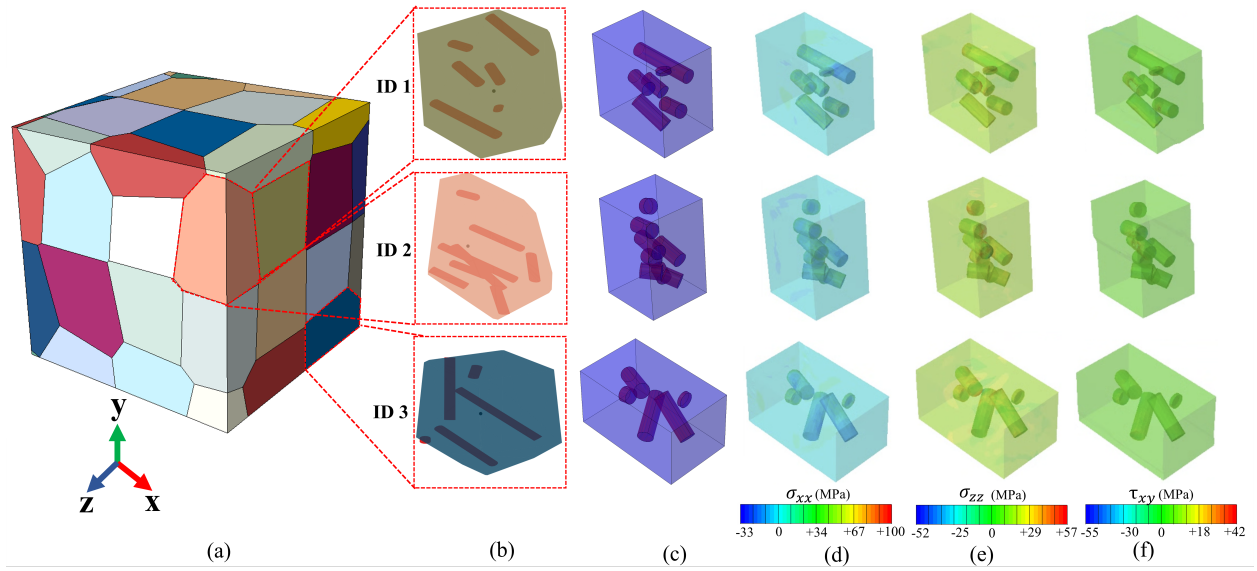
porosity grows, it severely disrupts matrix continuity and degrades matrix-mediated shear-lag load transfer between adjacent fibers. Consequently, while the axial modulus experiences minor degradation, this microstructural breakdown exerts a far more pronounced influence on the matrix- and interface-dominated mechanical properties, specifically the transverse normal and shear responses where voids act as localized stress concentrators [95]. Importantly, this distinct sensitivity establishes that the severity of anisotropic stiffness loss is dictated by the local topology of the fiber network and inter-fiber matrix ligaments rather than a uniform volumetric loss of load-bearing material [4, 126].

Taken together, these experimental observations establish a clear, path-dependent microstructure–property relationship. The localized geometric heterogeneity within the material defines the initial fiber interaction topology; cyclic loading systematically modifies this topology through localized porosity growth and microstructural rearrangement, and the evolved topology ultimately governs the subsequent quasi-static mechanical response. These experimentally characterized features form the direct physical basis for the mesoscale interaction-based modeling framework utilized in the following section.

### 5.3.2 Microstructure-Dependent Stiffness from Finite Element Homogenization

Figure 5.10 presents the local stress distributions for three discrete Voronoi cells subjected to identical far-field loading conditions. As shown in Figure 5.10a–c, these Voronoi cells were selected to represent contrasting microstructural topologies, varying significantly in their local fiber volume fractions, spatial alignments, clustering, and inter-fiber spacing. When subjected to simulated loading, these distinct microstructural descriptors produced markedly different mechanical responses, as reflected in the localized stress-field heterogeneity across panels Figure 5.10d–f and quantified by the macroscopic stress–strain trajectories in Figure 5.11.

Under axial loading along the x-axis ( $\sigma_{xx}$ ), cells containing clusters of nearly aligned fibers (such as ID 1) exhibited pronounced stress localization along the fiber axes. This



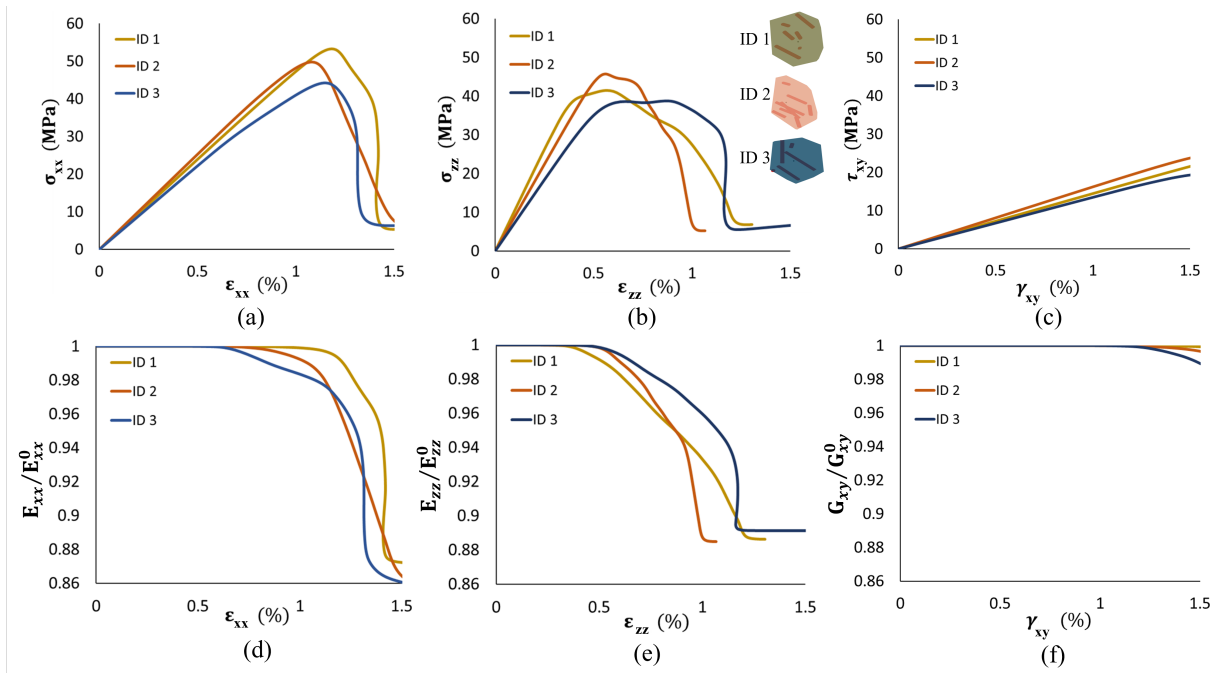
**Figure 5.10:** Discrete-cell multiscale modeling framework. (a) Mesoscale Voronoi tessellation of the reconstructed AM-CM microstructure. (b) Three representative polyhedral discrete cells (ID 1, ID 2, ID 3) depicting different fiber topologies. (c) Equivalent RUC FE models with explicitly resolved fiber geometries embedded in a homogenized porous matrix. (d–f) Representative local stress fields under: fiber-aligned normal loading in the x-direction (left), transverse loading in the z-direction (center), and axial shear in the x-y plane (right). Color scales are independently normalized per loading case to highlight intra-cell stress distribution patterns.

pattern indicates highly efficient load transfer via axial fiber stretching, yielding a correspondingly high effective longitudinal stiffness. Conversely, cells characterized by dispersed or obliquely oriented fibers (such as ID 3) exhibited more diffuse stress fields, in which a significantly larger fraction of the applied far-field load was carried by the surrounding thermoplastic matrix rather than the reinforcement phase. Because the continuous polymer matrix is substantially more compliant than the carbon fibers, these matrix-dominated cells exhibit an earlier onset of localized plastic deformation. The resulting variation in initial axial stiffness among the three representative cells examined here reaches approximately 8%–12%, highlighting the exceptional sensitivity of macroscale load-transfer efficiency to localized fiber topology.

Under in-plane shear loading ( $\tau_{xy}$ ), the stress concentrations arose predominantly within the thin matrix ligaments separating adjacent fibers rather than within the fibers themselves. This shifts the structural burden, indicating that shear transfer across the

microstructural domain was controlled primarily by matrix-mediated interactions rather than direct fiber reinforcement. Consequently, the axial shear stiffness was more strongly governed by local inter-fiber spacing and matrix continuity than by absolute fiber orientation—a mechanistic distinction with critical implications for the anisotropic damage evolution observed at later, highly cycled fatigue stages.

The cell-level stress–strain responses shown in Figure 5.11a–c further illustrate the influence of local fiber topology on the resulting nonlinear constitutive behavior. Cells whose fibers were preferentially aligned with the primary loading axis exhibited both a higher initial elastic modulus and a more gradual transition to nonlinear softening. This observation is consistent with classical shear-lag theory, where the axial stress-transfer capacity and structural reinforcement efficiency scale directly with fiber orientation and aspect ratio. In contrast, cells with fewer load-aligned fibers exhibited lower initial stiffness and an accelerated onset of matrix-dominated nonlinearity.



**Figure 5.11:** Nonlinear mechanical responses for the chosen discrete cells (ID 1, ID 2, ID 3). **Top row:** predicted stress–strain curves under (a) fiber-aligned normal loading ( $\sigma_{xx}$ – $\epsilon_{xx}$ ), (b) transverse normal loading ( $\sigma_{zz}$ – $\epsilon_{zz}$ ), and (c) axial shear loading ( $\tau_{xy}$ – $\gamma_{xy}$ ). **Bottom row:** corresponding normalized tangent stiffness degradation expressed as (d)  $E_{xx}/E_{xx}^0$ , (e)  $E_{zz}/E_{zz}^0$ , and (f)  $G_{xy}/G_{xy}^0$  as functions of applied strain.

The normalized tangent stiffness degradation curves in Figure 5.11d–f (where  $E_{ij}/E_{ij}^0$  denotes the ratio of instantaneous to initial undamaged stiffness) reveal three mechanistically significant trends. First, cells with well-connected fiber networks maintained their stiffness over a broader strain range, as load redistribution through multiple fiber–fiber interaction pathways remains operative even as matrix damage progresses. Second, cells characterized by sparse or poorly connected fiber networks exhibited earlier stiffness reduction, consistent with an accelerated transition from fiber- to matrix-dominated load-bearing. Third, axial shear stiffness degraded more gradually than normal stiffness, reflecting the comparatively stable matrix-controlled shear transfer mechanism.

These observations bear close resemblance to connectivity-driven stiffness transitions in disordered fiber networks, where the density and topology of load-bearing links dictate the onset and rate of stiffness loss. In the present context, locally connected fiber clusters enable load redistribution via redundant pathways, thereby delaying macroscopic stiffness degradation, whereas sparsely connected or resin-rich cells offer limited redundancy and fail earlier via matrix plasticity and void growth. These results establish that local fiber-network connectivity—rather than volume fraction alone—governs the nonlinear evolution of stiffness in AM-CM SFTs, and that the developed graph-based surrogate modeling framework accurately captures this physical mechanism.

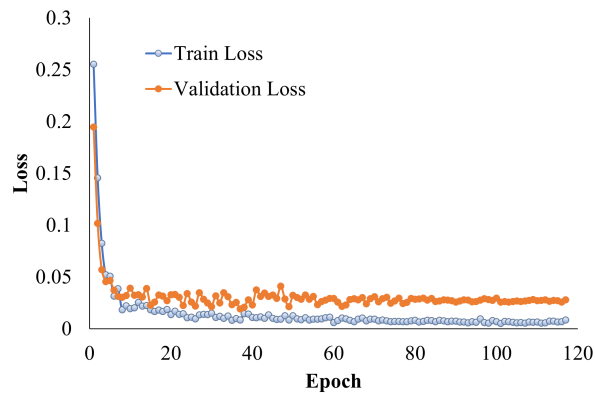
### 5.3.3 Surrogate Prediction of Cell-Level Constitutive Behavior

Direct nonlinear FE homogenization of every discrete cell is computationally prohibitive for mesoscale assemblies comprising hundreds to thousands of Voronoi cells. To enable efficient evaluation of cell-level constitutive behavior while preserving sensitivity to microstructural topology, the hybrid GNN-LSTM surrogate model described in Section 5.2.3 was trained on FE-generated stress–strain curves. The training dataset comprised stress–strain curves from 500 discrete Voronoi cells extracted from the  $\mu$ -CT microstructure, each evaluated under six independent loading cases (three normal and three shear),

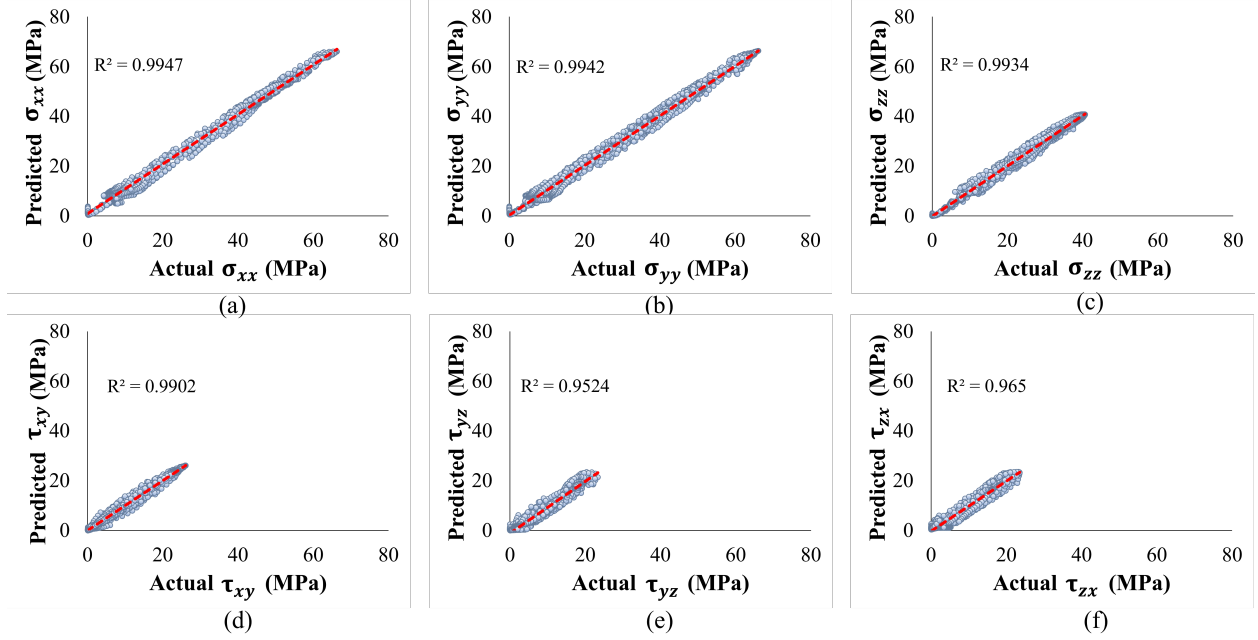


capturing a wide range of local fiber volume fractions, fiber orientations, and clustering configurations inherent to the AM-CM microstructure. The resulting dataset was partitioned using a stratified random shuffle (seed 42) into training (70%), validation (15%), and testing (15%).

*Training convergence:* The training history (Figure 5.12) exhibited two characteristic phases. A rapid initial reduction in loss was associated with the surrogate learning the topology-dependent elastic stiffness signatures encoded in the GNN embedding, as well as the peak stress predictions from the auxiliary head and the Random Forest regressor. This was followed by a more gradual convergence phase in which the LSTM captured the path-dependent plasticity and post-peak softening behavior governing the nonlinear damage regime. The strain-weighted Huber loss, which assigned up to  $4\times$  higher weight near and beyond the stress peak, directed the majority of the learning capacity toward accurate representation of the mechanically critical nonlinear regime. The absence of divergence between training and validation loss throughout both phases confirmed stable generalization without overfitting, supporting the adequacy of the 500-cell dataset for the microstructural variability encountered. Early stopping was triggered at convergence, well within the 800-epoch maximum.



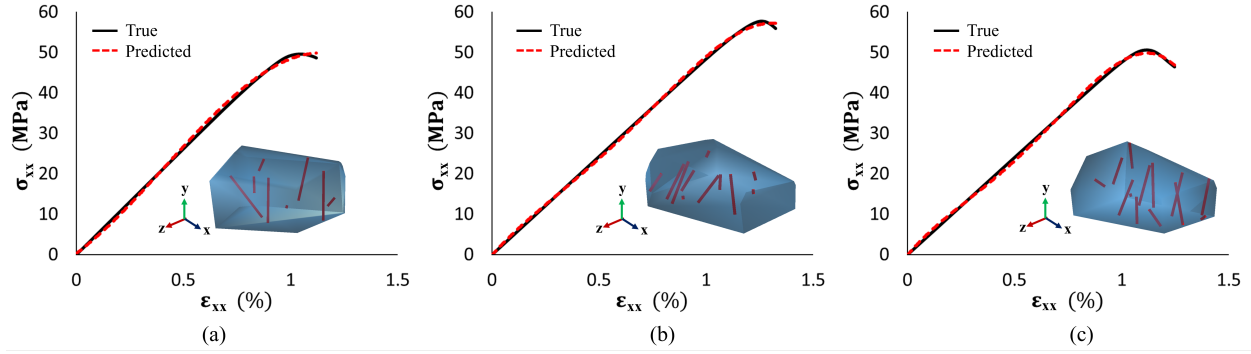
**Figure 5.12:** Training and validation loss histories demonstrating convergence of the GNN–LSTM surrogate for discrete-cell homogenization under normal loading in the fiber-dominated direction ( $\sigma_{xx}$ )



**Figure 5.13:** Parity plots comparing the high-fidelity FE homogenization benchmarks against the predictions generated by the hybrid GNN–LSTM surrogate framework. Individual coefficient of determination ( $R^2$ ) values are reported across the six independent stress components: (a) fiber-dominated normal  $\sigma_{xx}$ , (b) transverse width normal  $\sigma_{yy}$ , (c) thickness normal  $\sigma_{zz}$ , (d) transverse shear  $\tau_{xy}$ , (e) axial shear  $\tau_{yz}$ , and (f) axial shear  $\tau_{zx}$ .

*Predictive accuracy:* A parity plot (Figure 5.13a–f) demonstrated near-perfect agreement between surrogate-predicted and FE-computed stresses across the full stress range. This level of accuracy confirmed that the learned graph representation encoded physically meaningful microstructural information, capturing the topology-to-response mapping across the full diversity of fiber arrangements present in the  $\mu$ -CT microstructure—aligned fiber clusters, mixed-orientation neighborhoods, and resin-rich regions—rather than relying on globally averaged descriptors that would obscure topology-driven variability.

Representative comparisons between FE simulations and surrogate predictions across a range of fiber topologies are presented in Figure 5.14. The surrogate reproduced both the initial elastic stiffness and the post-yield nonlinear regime with high fidelity for cells characterized by aligned fiber clusters, mixed-orientation neighborhoods, and resin-rich regions, achieving  $R^2 = 0.99$ . Because all cells shared identical constituent material parameters, the variability in predicted response arose exclusively from differences in the



**Figure 5.14:** Representative comparison between nonlinear FE homogenization results (True) and GNN–LSTM surrogate predictions (Predicted) for three discrete Voronoi cells subjected to fiber-dominated normal loading. Each panel corresponds to a cell with a distinct local fiber topology: an aligned fiber cluster (a), a mixed-orientation neighborhood (b), and a resin-rich region (c).

local fiber topology encoded by the GNN—fiber count, spatial arrangement, orientation, distribution, and pairwise interaction strengths captured through the shear-lag edge weights. This confirmed that the surrogate learned a topology-sensitive constitutive mapping rather than a globally averaged response, and that the GNN embedding  $z_{\Omega_c}$  successfully encoded the mechanically distinguishing features of each cell’s fiber network.

Computational efficiency: The trained surrogate predicted the complete normalized stress–strain trajectory of an individual cell in under one second on a single CPU, with subsequent de-normalization via the Random Forest peak-stress prediction adding negligible computational cost. The total per-cell prediction time therefore remained under one second, compared with several minutes required for the equivalent nonlinear FE homogenization running on 5 CPUs in Abaqus 2022. This reduction in computational cost, by more than two orders of magnitude, enabled efficient evaluation of hundreds to thousands of discrete cells within a mesoscale Voronoi assembly and rendered the proposed multiscale framework tractable for fatigue-stage-resolved analyses across multiple specimens and damage states. Furthermore, unlike FE homogenization where cells are coupled through boundary conditions, surrogate evaluation of individual Voronoi cells is completely independent once the macroscopic strain is localized to each cell, meaning all cells could in principle be evaluated simultaneously in a parallelized implementation, with the theoretical

speedup scaling linearly with the number of available processors—an advantage that was not exploited in the present single-CPU implementation but represents a promising avenue for near-real-time coupon-scale predictions in future HPC deployments.

#### **5.3.4 Mesoscale Homogenization and Coupon-Scale Validation**

The ultimate purpose of the proposed multiscale framework is to establish a quantitative, predictive link between experimentally observed microstructural degradation and macroscopic mechanical response. To evaluate this capability, mesoscale Voronoi assemblies were constructed directly from  $\mu$ -CT reconstructions of fatigue-tested specimens. Three specimens, each representing a distinct interrupted fatigue stage (Section 2.3), were selected to capture progressive damage states ranging from nominally undamaged to near-failure.

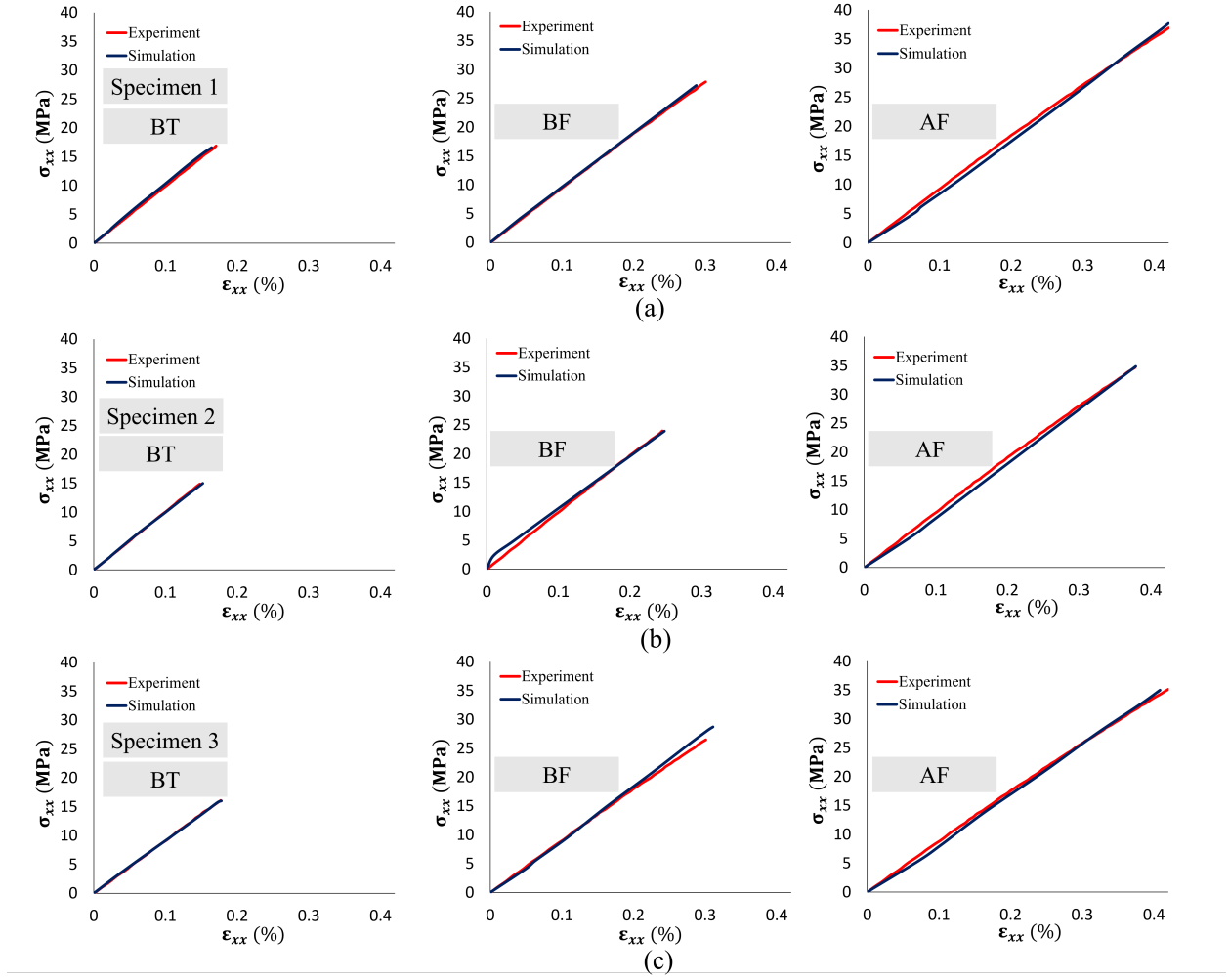
For each specimen and fatigue stage, the fiber centerline coordinates and cell-level volume fractions extracted from the  $\mu$ -CT reconstruction were passed directly to the GNN-LSTM surrogate to predict cell-level constitutive responses, which were assembled into the coupon-scale response. No constitutive parameters were recalibrated at the coupon scale between fatigue stages; all observed changes in the predicted macroscopic response arose solely from the microstructure-informed constitutive update propagated through the LSTM component of the surrogate, in which the cell parameters are uniformly applied across all time points.

At each fatigue stage, the homogenization procedure incorporated  $\mu$ -CT-measured porosity through the two-step porous-matrix model described in Section 5.2.2, which reduced the effective matrix stiffness assigned to all Voronoi cells. The GNN-LSTM then predicted the normalized stress trajectory for each cell based on its  $\mu$ -CT fiber topology, and the Random Forest predicted the corresponding peak stress amplitude from the GNN embedding and local volume fraction. As fatigue damage advanced, increasing porosity reduced the porous-matrix stiffness, loss of fiber connectivity, and cluster dispersion were

directly captured in lower GNN edge weights and reduced topology embeddings, and the Random Forest consequently predicted lower peak stresses for damaged cells, collectively degrading the assembled coupon response in a manner driven entirely by the evolving  $\mu$ -CT microstructure rather than by any manually adjusted parameter.

As illustrated in Appendix F, the full six-mode constitutive response is first obtained for each discrete Voronoi cell—either through FE homogenization or the GNN-LSTM surrogate and these cell-level responses are then assembled through volume-weighted averaging at the mesoscale Voronoi assembly level to produce the final coupon-scale response. Figure 5.15 shows the longitudinal mesoscale stress–strain response comparison with experimental monotonic tensile measurements. With increasing fatigue damage, both experiments and simulations showed a systematic reduction in elastic modulus and an earlier onset of nonlinear deformation. These trends were reproduced by the multiscale model without any coupon-scale recalibration, confirming that the observed macroscopic degradation was captured entirely through the microstructure-informed constitutive update propagated from  $\mu$ -CT observations through the surrogate.

The model reproduced the progressive softening of the stress–strain response across the three fatigue conditions. Quantitatively, predicted elastic moduli agreed with experimental measurements within 5–7% across all three specimens and fatigue stages, confirming that the surrogate captured the correct sensitivity to microstructural degradation across the full range of damage studied, as shown in Figure 5.15. The discrepancies between simulation and experiment were attributed primarily to physical mechanisms not represented in the current constitutive framework, rather than to surrogate approximation error. The matrix model captures elastoplastic damage and porosity-induced stiffness reduction, but does not explicitly resolve fiber-matrix interfacial debonding or discrete matrix cracking. Both become increasingly active at advanced stages of fatigue, causing further loss of stiffness in highly damaged regions. The surrogate itself contributed negligibly to this error, as confirmed by comparing coupon-scale predictions from the GNN-LSTM surrogate with



**Figure 5.15:** Comparison of experimentally measured and multiscale-predicted stress–strain responses obtained from the hybrid FE-surrogate framework, in which GNN-LSTM surrogate predictions of discrete Voronoi cell constitutive responses are assembled through mesoscale periodic boundary conditions and volume-weighted averaging to predict the coupon-scale response, for all three specimens at each fatigue stage (BT, BF, AF). Top (a), middle (b), and bottom (c) panels correspond to Specimen 1, Specimen 2, and Specimen 3, respectively.

those obtained from direct FE homogenization of the same Voronoi assemblies. These agree closely across all fatigue stages, isolating the source of the experiment-simulation gap to the constitutive model rather than to the surrogate model.

Taken together, these results demonstrated that the proposed FE-Voronoi-GNN framework successfully propagated microstructural information across three length scales—from the explicitly resolved fiber level through the topology-sensitive surrogate to the macroscopic coupon response—using only  $\mu$ -CT fiber coordinates and volume fractions as inputs, with no specialized characterization beyond standard reconstruction. By directly linking manufacturing-induced and fatigue-driven microstructural evolution to measurable changes in mechanical performance, the framework provided a physically grounded and computationally efficient basis for assessing the structural condition and remaining fatigue life of AM-CM short-fiber thermoplastic composite components.

It is worth noting that while a mean-field RVE approach using average microstructural descriptors may yield comparable elastic modulus predictions at the coupon scale, the present framework offers capabilities that such an approach fundamentally cannot provide: (i) spatially resolved identification of mechanically weak cells governed by local fiber clustering and sparse connectivity, (ii) direct propagation of fatigue-stage-specific microstructural evolution without constitutive recalibration, and (iii) capture of topology-driven variability in nonlinear damage evolution that is entirely lost under mean-field averaging.

## **5.4 Conclusions and Future Work**

This chapter established a microstructure-resolved, multiscale surrogate modeling framework to predict the nonlinear quasi-static mechanical response of SFT composites manufactured via AM-CM. By combining interaction-topology-based discrete FE homogenization with a physics-informed GNN–LSTM surrogate, the framework provides a computationally efficient and physically interpretable pathway for linking local fiber interaction topology to macroscopic structural performance.

The key findings are summarized below.

1. *Microstructure-controlled mechanics in discrete cells:* High-resolution  $\mu$ -CT reconstructions demonstrate that the AM-CM microstructure can be decomposed into localized Voronoi cells representing neighborhoods of interacting fibers. Even when global fiber volume fraction and constituent properties remain unchanged, these cells exhibit substantial variability in stiffness and nonlinear response arising solely from differences in fiber clustering, alignment, and spacing. The mechanical behavior of SFTs is therefore governed not only by volume fraction but also by the topology of local fiber interaction networks that control load-transfer pathways between fibers and matrix. Nonlinear FE homogenization showed that cells containing aligned or highly connected fiber clusters sustained load primarily through axial fiber stretching, yielding higher stiffness and delayed degradation, whereas cells with dispersed or sparsely connected configurations relied more on matrix-mediated load transfer, producing earlier nonlinear deformation and accelerated stiffness reduction.
2. *Physics-informed surrogate modeling:* A hybrid GNN-LSTM architecture was developed and trained to approximate the nonlinear constitutive response of discrete cells. The surrogate required 3D fiber centerline endpoints and cell-level volume fractions as inputs, both of which are available directly from standard  $\mu$ -CT reconstruction. By representing the fiber interaction network as a graph with physics-informed edge weights that encode both axial shear-lag coupling and the orientation-independent transverse stress-concentration mechanism, as confirmed by parametric two-fiber FEA, the GNN captured topology-dependent stiffness. The LSTM learned the path-dependent normalized constitutive evolution; a skip connection from the GNN embedding to the output MLP ensured that topology-encoded amplitude information directly modulated stress predictions at each loading increment, thereby preventing attenuation of the GNN signal due to LSTM gate saturation. This two-stage prediction pipeline reproduced FE-predicted stress–strain responses with  $R^2 \approx 0.98$  on de-normalized



physical stress trajectories while reducing per-cell evaluation time by more than two orders of magnitude, enabling efficient evaluation of hundreds to thousands of Voronoi cells within a mesoscale assembly.

3. *Multiscale propagation of microstructural degradation:* When integrated within mesoscale Voronoi assemblies derived directly from  $\mu$ -CT reconstructions at each fatigue stage, the surrogate-enabled framework accurately predicted coupon-level tensile responses across multiple damage states and three specimens without recalibrating any constitutive parameters. Predicted elastic moduli agreed with experiment within 5–7%, and area under the stress–strain curve within 10%, confirming that microstructure-driven degradation mechanisms were correctly propagated across scales by the surrogate alone, without any recalibration to the evolving  $\mu$ -CT microstructure.

Collectively, these results demonstrate that the quasi-static mechanical response of AM-CM SFTs is fundamentally governed by the topology of local fiber interaction networks rather than by global microstructural averages alone. The FE–Voronoi–GNN–LSTM framework established here provides a physically grounded, topology-sensitive bridge between  $\mu$ -CT-resolved microstructural evolution and macroscopic mechanical performance, deployable on any dataset from which fiber centrelines and volume fractions can be extracted. Extending this framework to cyclic fatigue loading — where cell-level stiffness evolves not only with fiber topology but also with loading frequency, stress ratio, and cumulative cyclic history — requires fundamental augmentation of the surrogate input space and constitutes the subject of Chapter 6.

## Chapter 6

### Life Prediction of Additively Manufactured Composites via Surrogate modeling

#### 6.1 Introduction

Chapter 5 remains confined to quasi-static loading; extending it to fatigue requires the effective stiffness of each Voronoi cell to evolve cycle by cycle with microstructure, loading frequency, stress ratio, peak stress, and cumulative loading history — effects a quasi-static formulation cannot capture by simply varying a cycle-count parameter.

This chapter addresses that gap with a three-phase isotropic CDM constitutive model for the ABS matrix, implemented within a Mori–Tanaka micromechanical framework [131, 132] as a sequentially coupled thermomechanical UMAT/UMATHT subroutine in Abaqus: the mechanical (UMAT) and thermal (UMATHT) solutions are updated in series within each increment, with the mechanical state driving the thermal update and the resulting temperature feeding back at the next increment. The formulation incorporates viscoelasticity, isotropic stiffness degradation, and a cycle-jump acceleration algorithm, producing a high-fidelity dataset intended as the training target for a future ML surrogate [82].

#### 6.2 Material System and Computational Framework

The CF-ABS material system, AM-CM fabrication process, specimen geometry,  $\mu$ -CT imaging procedure, and interrupted fatigue test program are identical to those described in Chapters 3 and 4 and are not reproduced here. Three specimens (Panel A) underwent constant-amplitude fatigue testing at 60%, 65%, and 70%  $\sigma_{UTS}$ , and specimen 2 (Panel B), with an initial porosity level of 1.90%, underwent an interrupted staircase fatigue test.

These datasets are used to calibrate and validate the damage model and later serve as coupon-scale validation targets.

The microstructure-resolved framework from Chapter 5 — fiber interaction extraction, Voronoi tessellation, discrete-cell FE homogenization with PBCs, and two-step porous-matrix homogenization is adopted without modification. The sole change is the constitutive model assigned to each Voronoi cell. Instead of the monotonic matrix model used in Chapter 5, this chapter employs a cycle-resolved, sequentially coupled thermomechanical fatigue damage model implemented as an Abaqus UMAT/UMATHT subroutine. This model generates the cycle-dependent stiffness trajectory  $\mathbf{C}^{(\Psi_c)}(N; f, R, \sigma_{\max})$  for each discrete cell  $\Psi_c$ , capturing frequency-dependent viscoelastic self-heating, a matrix damage variable driven by the total thermodynamic strain-energy release rate, and load-history-dependent stiffness accumulation over thousands of cycles. The coupon-level response is then assembled through volume-weighted averaging of all cell contributions (Section 6.3.6, Eq. 6.34).

### 6.3 Coupled Thermomechanical Fatigue Damage Model

Calibrating a matrix-scale fatigue damage law from composite-level experimental data requires three linked operations: (i) recovering an RVE-averaged matrix damage evolution  $D_m(N)$  from the measured composite stiffness degradation, (ii) fitting the parameters of a CDM law to the recovered  $D_m(N)$ , and (iii) deploying the calibrated law at each Gauss point of the Voronoi-cell finite-element simulation. This section develops the three operations in that order.

#### 6.3.1 Experimental Calibration Data

Composite-level fatigue data were acquired on the MTS servo-hydraulic frame described in Chapter 3, instrumented with (i) an axial extensometer sampling the secant

modulus every cycle, and (ii) a cooled IRT camera mapping surface temperature (Figure 6.1a). Three specimens were tested at 60%, 65%, and 70%  $\sigma_{UTS}$  ( $R = 0.1$ ,  $f = 15$  Hz) until failure. From the recorded secant modulus  $E_c(N)$ , the composite damage index,  $D_c$  is defined as

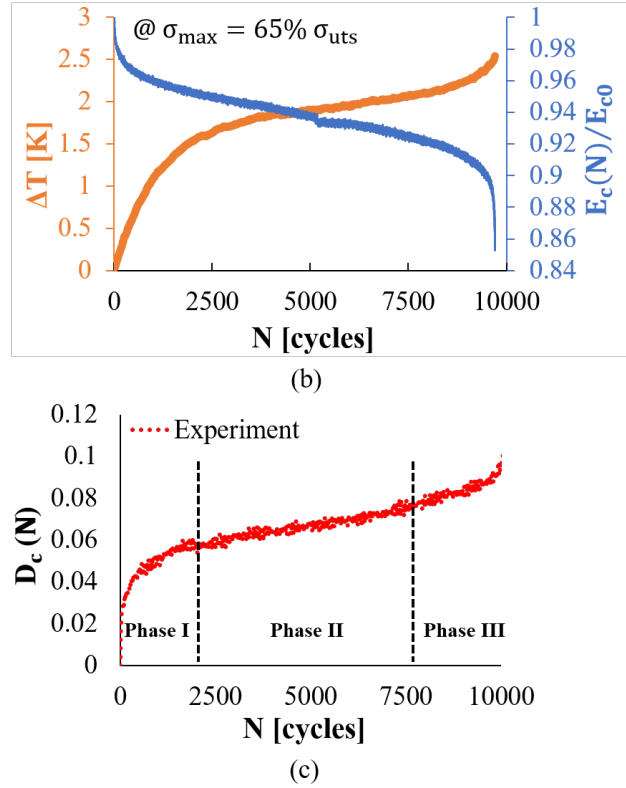
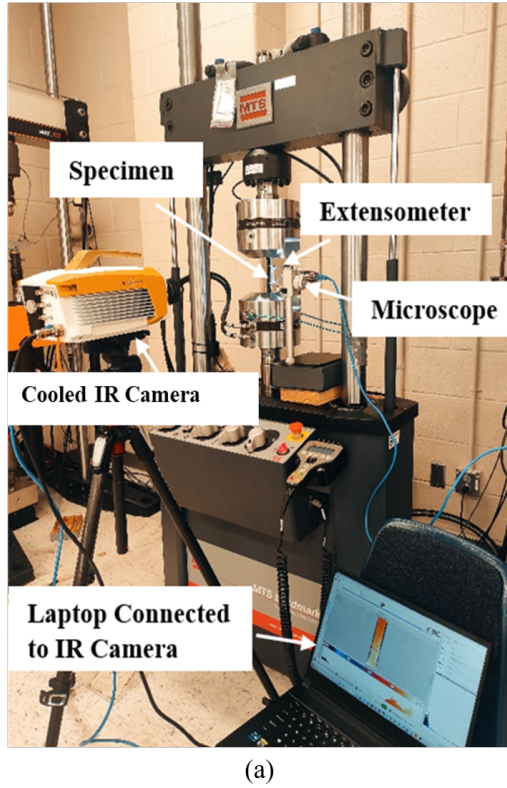
$$D_c(N) = 1 - \frac{E_c(N)}{E_{c0}}, \quad (6.1)$$

where  $E_{c0} = E_c(N=1)$  is the specimen-specific pristine axial modulus of AM-CM SFT measured at the start of each fatigue test. Figure 6.1b shows the simultaneous evolution of the surface temperature rise  $\Delta T(N)$  and the normalized modulus  $E_c(N)/E_{c0}$  for  $\sigma_{max} = 65\% \sigma_{uts}$ ; the two signals are inversely correlated, consistent with progressive matrix damage increasing local viscous dissipation while reducing effective stiffness. Figure 6.1c shows the corresponding  $D_c$  exhibiting the three characteristic fatigue phases — rapid Phase I nucleation, extended steady-state Phase II plateau, and Phase III runaway that must be reproduced by the constitutive fatigue damage model.

Because the extensometer measures the composite stiffness degradation rather than the matrix degradation, the CDM parameters cannot be fitted directly to  $D_c(N)$ : the composite response includes both the matrix stiffness loss and the (undamaged) fiber reinforcement. An inverse micromechanical operation is therefore required to recover the RVE-averaged matrix damage  $D_m(N)$  that would, under the CF-ABS microstructure, produce the observed composite degradation. Following this, the Mori–Tanaka models are developed next.

### 6.3.2 Mori–Tanaka Homogenization Framework

The micromechanical operator  $\mathcal{F}_{MT}$  computes the effective composite stiffness  $C_c$  from the constituent stiffnesses, the fiber volume fraction  $V_f$ , and the  $\mu$ -CT-measured fiber length and orientation distributions. An Eshelby–Mori–Tanaka formulation with full aspect-ratio and orientation averaging is adopted because the short carbon fibers in the AM-CM



**Figure 6.1:** Experimental setup and constant-amplitude fatigue data used for calibration. **(a)** MTS servo-hydraulic fatigue frame with extensometer, cooled IRT camera, and optical microscope. **(b)** Simultaneous evolution of surface temperature rise  $\Delta T$  (orange, left axis) and normalized stiffness  $E/E_0$  (blue, right axis) at 65%  $\sigma_{UTS}$  ( $R=0.1$ ,  $f=15$  Hz). **(c)**  $D_c$  at the same loading condition exhibiting the three characteristic fatigue phases.

microstructure exhibit both a broad aspect-ratio distribution (FOD and FLD recovered from the  $\mu$ -CT).

Constituent stiffness tensors:

The ABS matrix is treated as an isotropic material,

$$C_{ijkl}^m = \lambda_m \delta_{ij} \delta_{kl} + \mu_m (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}), \quad (6.2)$$

with Lamé constants  $\lambda_m = E_m \nu_m / [(1 + \nu_m)(1 - 2\nu_m)]$  and  $\mu_m = E_m / [2(1 + \nu_m)]$ .

The carbon fiber is treated as transversely isotropic, with its axis of material symmetry coincident with the local fiber axis (local  $x_3$ ; see coordinate-system definition below). The fiber compliance is

$$S^f = \begin{bmatrix} 1/E_{22} & -\nu_{23}/E_{22} & -\nu_{12}/E_{11} & 0 & 0 & 0 \\ -\nu_{23}/E_{22} & 1/E_{22} & -\nu_{12}/E_{11} & 0 & 0 & 0 \\ -\nu_{12}/E_{11} & -\nu_{12}/E_{11} & 1/E_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/G_{12} & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/G_{12} & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/G_{23} \end{bmatrix}, \quad (6.3)$$

with  $C_{ijkl}^f$  obtained by inverting Eq. 6.3 and mapping the resulting  $6 \times 6$  stiffness back to the minor-symmetric fourth-order tensor. Equation 6.3 is presented in Voigt notation, the form in which fiber datasheet properties are reported; it is converted to the fourth-order tensor  $C_{ijkl}^f$  before use in the tensor operations of Eqs. 6.4–6.10. Property values used in the calibration are taken from Section 5.2.2.

Local fiber coordinate system:

Each fiber is idealized as a prolate spheroid of aspect ratio  $\alpha = l/d_f$ , with  $d_f = 8 \mu\text{m}$  the nominal fiber diameter. All quantities in this subsection up to and including Eq. 6.7 (the Eshelby tensor, the transversely isotropic fiber stiffness, and the dilute concentration

tensor) are evaluated in a local fiber frame in which the fiber axis is aligned with  $x_3$ ; the transverse directions  $x_1, x_2$  are arbitrary within the fiber's transverse isotropy plane. This local frame is rotated into the shared global (specimen) frame in the orientation-averaging step (Eq. 6.8), via the rotation  $\mathbf{R}(\phi, \theta)$  defined below.

Eshelby tensor for a prolate spheroidal fiber:

Under the assumption of a uniform equivalent eigenstrain, the Eshelby tensor  $\mathbf{S}(\alpha, \nu_m)$  maps the eigenstrain to the strain inside the inhomogeneity and is given in closed form [131–137]. Note that  $\mathbf{S}$  depends only on the matrix Poisson ratio  $\nu_m$  and the inclusion aspect ratio  $\alpha$  – it is independent of the fiber's own stiffness, which enters separately in Eq. 6.7. The non-zero components involve the geometric integral

$$g(\alpha) = \frac{\alpha}{(\alpha^2 - 1)^{3/2}} \left[ \alpha \sqrt{\alpha^2 - 1} - \cosh^{-1} \alpha \right], \quad (6.4)$$

which recovers the sphere limit as  $\alpha \rightarrow 1$  and the continuous-fiber limit ( $S_{3333} \rightarrow 0$ ,  $S_{1111} \rightarrow (5 - 4\nu_m)/[8(1 - \nu_m)]$ ) as  $\alpha \rightarrow \infty$ . The geometric integral  $g(\alpha)$  enters the non-zero Eshelby tensor components directly,

$$S_{3333} = \frac{1}{1 - \nu_m} \left[ 1 - 2\nu_m - (1 - \nu_m)g(\alpha) \right] \frac{\alpha^2}{\alpha^2 - 1}, \quad (6.5)$$

$$S_{1111} = \frac{3}{8(1 - \nu_m)} \frac{\alpha^2}{\alpha^2 - 1} + \frac{1}{4(1 - \nu_m)} \left[ 1 - 2\nu_m - \frac{9}{4(\alpha^2 - 1)} \right] g(\alpha), \quad (6.6)$$

with the remaining components ( $S_{1122}$ ,  $S_{2233}$ ,  $S_{1212}$ , etc.) following the same closed-form structure in  $\alpha$ ,  $\nu_m$ , and  $g(\alpha)$  [131–133].

Dilute strain concentration tensor:

In the local fiber frame, the Eshelby equivalent-inclusion method gives the dilute (single-inhomogeneity) strain concentration tensor

$$\mathbf{A}^{\text{dil}}(\alpha) = \left[ \mathbf{I} + \mathbf{S} : \mathbf{C}_m^{-1} : (\mathbf{C}_f - \mathbf{C}_m) \right]^{-1}, \quad (6.7)$$

where  $\mathbf{I}$  is the symmetric fourth-order identity and  $(:)$  denotes double contraction. A general fourth-order tensor without symmetry has  $9 \times 9 = 81$  independent components; inverting Eq. 6.7 in this naive representation is ill-conditioned because minor symmetry makes several rows and columns linearly dependent. The inversion is instead performed via the Mandel  $6 \times 6$  representation, which removes this redundancy and is well-conditioned.

Aspect-ratio and orientation averaging:

The  $\mu$ -CT-derived FLD and FOD, with the joint orientation distribution function, factorize as  $p(\phi, \theta) = p_\phi(\phi) p_\theta(\theta)$ , assuming statistical independence between fiber inclination  $\phi$  and in-plane rotation  $\theta$ . Each orientation defines a rotation matrix  $\mathbf{R}(\phi, \theta)$  whose third column aligns with the fiber axis. For a given aspect-ratio class  $\alpha_a$  and orientation bin  $(\phi_i, \theta_j)$  – together denoted phase  $r = (\alpha_a, \phi_i, \theta_j)$  – the fourth-order rotation gives the rotated dilute concentration tensor

$$A'_{ijkl}(\alpha_a, \phi_i, \theta_j) = R_{ip} R_{jq} R_{kr} R_{ls} A^{\text{dil}}_{pqrs}(\alpha_a). \quad (6.8)$$

$\mathbf{A}'$  is retained per phase and carried forward unweighted into the Mori–Tanaka closure below, where the weights  $w_a p_\phi(\phi_i) p_\theta(\theta_j)$  are applied instead.

Mori–Tanaka closure and effective stiffness:

Each phase  $r = (\alpha_a, \phi_i, \theta_j)$  is closed self-consistently against its own rotated dilute tensor, and the population average over aspect ratio and orientation is taken outside the closure [131, 138, 139]. The weight  $w_a$  is the population fraction of fibers in aspect-ratio bin  $a$ , obtained by discretizing the  $\mu$ -CT-measured fiber length distribution into  $N_\alpha$  bins with  $\sum_{a=1}^{N_\alpha} w_a = 1$ :

$$\mathbf{A}^{\text{MT}} = \sum_{a=1}^{N_\alpha} \sum_i \sum_j w_a p_\phi(\phi_i) p_\theta(\theta_j) \left\{ \mathbf{A}'(\alpha_a, \phi_i, \theta_j) : \left[ (1-V_f) \mathbf{I} + V_f \mathbf{A}'(\alpha_a, \phi_i, \theta_j) \right]^{-1} \right\}. \quad (6.9)$$



Because the carbon fiber is transversely isotropic, its stiffness tensor is defined in the local fiber-aligned frame, so its global-frame components are orientation-dependent: the rotated fiber stiffness for phase  $r$  is  $\mathbf{C}_{f,r} = \mathbf{R}(\phi_i, \theta_j) \star \mathbf{C}_f^{\text{local}}$ , where  $(\star)$  denotes the same fourth-order rotation as Eq. 6.8,  $(C_{f,r})_{ijkl} = R_{ip}R_{jq}R_{kr}R_{ls}(C_f^{\text{local}})_{pqrs}$ , applied here to  $\mathbf{C}_f$  instead of  $\mathbf{A}^{\text{dil}}$ . The effective (pristine) composite stiffness therefore follows the same phase-resolved structure as Eq. 6.9 — i.e., computed per discretized aspect-ratio/orientation subclass  $r = (\alpha_a, \phi_i, \theta_j)$  and only summed afterward — rather than contracting a single  $\mathbf{C}_f$  against a single  $\mathbf{A}^{\text{MT}}$ :

$$\mathbf{C}_c = \mathbf{C}_m + V_f \sum_{a=1}^{N_\alpha} \sum_i \sum_j w_a p_\phi(\phi_i) p_\theta(\theta_j) (\mathbf{C}_{f,r} - \mathbf{C}_m) : \mathbf{A}_r^{\text{MT}}, \quad (6.10)$$

where  $\mathbf{A}_r^{\text{MT}}$  denotes the term inside the braces of Eq. 6.9 for phase  $r$ , prior to summation. Eq. 6.10 is symmetrised as  $C_{ijkl} \leftarrow \frac{1}{2}(C_{ijkl} + C_{klij})$  to enforce major symmetry. The axial Young's modulus is extracted from the compliance  $\bar{\mathbf{S}} = \mathbf{C}_c^{-1}$  as  $E_c = 1/\bar{S}_{1111}$ .

The fiber volume fraction  $V_f$  is used for all subsequent evaluations of the operator  $\mathcal{F}_{\text{MT}}$ , both for the inverse-MT extraction of  $D_m(N)$  and for the cell-scale stiffness update inside the UMAT (Section 6.3.3).

For notational compactness, the entire operator defined by Eqs. 6.2–6.10 is henceforth denoted

$$\mathbf{C}_c = \mathcal{F}_{\text{MT}}(\mathbf{C}_m, \mathbf{C}_f, V_f, \{w_a, \alpha_a\}, p_\phi, p_\theta). \quad (6.11)$$

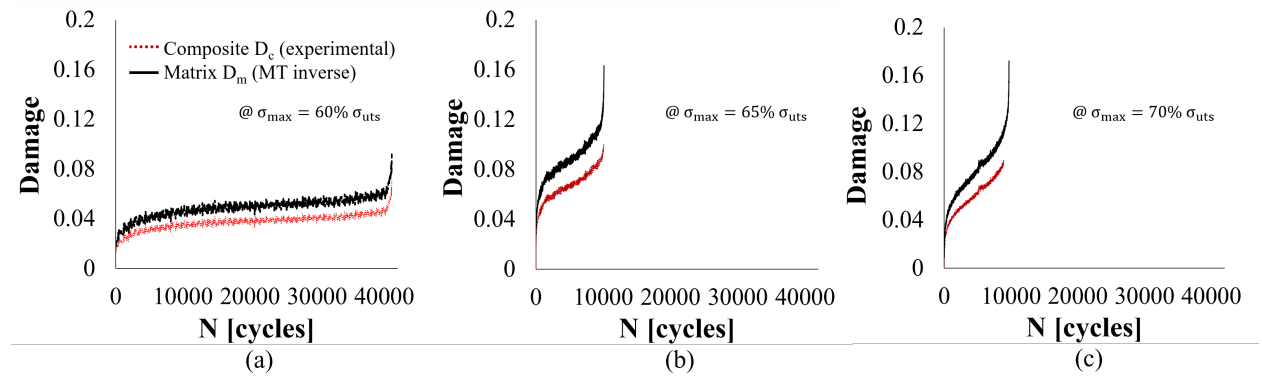
With  $\mathcal{F}_{\text{MT}}$  calibrated, matrix damage is recovered from measured composite damage by pointwise inversion. Under the assumption that the carbon fibers remain elastic throughout the fatigue history ( $D_f = 0$ ), Eq. 6.11 specializes to

$$E_c(N) = \mathcal{F}_{\text{MT}}(E_m^0(1 - D_m(N)), \nu_m, \mathbf{C}_f, V_f, \{w_a, \alpha_a\}, p_\phi, p_\theta), \quad (6.12)$$

where the matrix damage acts only through a scalar reduction of  $E_m$ ;  $\nu_m$  is held fixed under damage, so the reduced matrix stiffness at any point in the fatigue history is recovered directly from  $C_m(N)$  as  $E_m(N) = E_m^0(1 - D_m(N))$  and  $\nu_m(N) = \nu_m$ . This is the pair of scalars subsequently passed to the UMAT/UMATHT subroutine (Section 6.3.3).

For each  $D_m$ , Eq. 6.12 is evaluated to produce a corresponding composite modulus  $E_c(D_m)$  and thus a composite damage  $D_c(D_m) = 1 - E_c(D_m)/E_c^0$ . The resulting map  $D_m \mapsto D_c$  is monotonic and single-valued under the CF-ABS microstructure. Second, the measured trajectory  $D_c(N)$  is inverted, cycle by cycle, using monotone piecewise cubic interpolation to yield  $D_m(N)$ .

Figure 6.2 shows the recovered  $D_m(N)$  against the measured  $D_c(N)$  for the three constant-amplitude stress levels. Two features are noteworthy. First,  $D_m(N) > D_c(N)$  holds throughout every stress level, quantifying the fiber-shielding effect: the undamaged fibers continue to carry load, so a significantly larger matrix stiffness loss is required to produce the observed composite degradation. Second, the amplification  $D_m/D_c$  increases monotonically with applied stress, reflecting stronger contributions from Phase II and Phase III at higher energy release rates.



**Figure 6.2:** Inverse Mori–Tanaka extraction of RVE-averaged matrix damage  $D_m(N)$  from experimentally measured composite damage  $D_c(N)$ . Red dotted curves: experimentally derived  $D_c(N) = 1 - E(N)/E_0$ . Black solid curves: recovered  $D_m(N)$  from pointwise inversion of the calibrated Mori–Tanaka relation (Eq. 6.12). The amplification  $D_m/D_c$  increases with stress, reflecting stronger contributions from Phase II and Phase III at higher energy release rates.

Note that, at this stage,  $D_m(N)$  is recovered as a single RVE-averaged history calibrated against the volume-averaged  $\mu$ -CT fiber distribution and is applied uniformly at every Gauss point and every Voronoi cell in the UMAT (Section 6.3.3).

The pointwise stiffness-degradation inversion approach used here follows the general CDM framework established for fatigue stiffness degradation in fiber-reinforced composites [140–143].

### 6.3.3 Constitutive and Damage Evolution Law for the Matrix Phase

With  $\mathcal{F}_{\text{MT}}$  calibrated and the RVE-averaged matrix damage history  $D_m(N)$  recovered by inversion, the remaining task is to specify how  $D_m$  enters the matrix constitutive response and how it evolves with cycle count. The isotropic scalar damage law developed in this subsection is the physical core of the fatigue model. Together with the viscoelastic and thermo-mechanics introduced in Sections 6.3.4–6.3.6, it constitutes the full set of physics that the UMAT/UMATHHT subroutine of Section 6.3.7 evaluates at every Gauss point.

#### Constitutive Framework: Isotropic Damaged Matrix:

The ABS matrix is intrinsically isotropic, and the  $D_m$  extracted from the axial composite modulus is a scalar quantity. In other words,  $D_m \in [0, D_F]$  degrades the matrix Young's modulus and shear modulus by the same factor,

$$E_m(N) = E_m^0 (1 - D_m(N)), \quad G_m(N) = G_m^0 (1 - D_m(N)), \quad (6.13)$$

while the Poisson ratio  $\nu_m$  is preserved. When  $D_m$  reaches the failure threshold  $D_F$ , the modulus is clamped at  $0.01 C_m^0$  to prevent singularities while still representing local physical failure.

The total strain at the end of each increment is decomposed as

$$\epsilon_{\text{tot}} = \epsilon_{\text{el}} + \epsilon_{\text{ve}} + \epsilon_{\text{th}}, \quad (6.14)$$

where  $\varepsilon_{\text{th}}$  is a kinematic thermal strain, and  $\varepsilon_{\text{ve}}$  is the viscoelastic strain. The  $\varepsilon_{\text{ve}}$  is updated using a recursive three-term Prony series, with its amplitudes and relaxation rates fitted to DMA master curves for the ABS matrix (see Appendix A). For each of the six strain components ( $j = 1, \dots, 6$ ) and each Maxwell branch ( $i = 1, 2, 3$ ), the branch strain advances as

$$\varepsilon_{ij}^{\text{ve}}(t) = e^{-p_i \Delta t} \varepsilon_{ij}^{\text{ve}}(t^-) + (1 - e^{-p_i \Delta t}) \varepsilon_{ij}^{\text{el}}(t), \quad (6.15)$$

where  $p_i$  is the  $i$ -th relaxation rate. The total viscoelastic strain is  $\varepsilon_{ij}^{\text{ve}} = \sum_{i=1}^3 \varepsilon_{ij}^{\text{ve}}$ , and the elastic driving strain is  $\varepsilon_{\text{el}} = \varepsilon_{\text{tot}} - \varepsilon_{\text{ve}} - \varepsilon_{\text{th}}$ . The viscoelastic update (Eq. 6.15) assumes linear viscoelasticity: the Prony coefficients are fixed, strain- and stress-independent material constants, valid because the matrix remains deep in its glassy state throughout the small-strain fatigue loading considered in this chapter. The viscous energy dissipated per unit volume during the increment is evaluated by the trapezoidal rule

$$\Delta W_{\text{ve}} = \frac{1}{2} \sum_{i=1}^3 \sum_{j=1}^6 (\sigma_{ij,\text{old}}^{\text{ve}} + \sigma_{ij,\text{new}}^{\text{ve}}) \Delta \varepsilon_{ij}^{\text{ve}}, \quad (6.16)$$

with the branch stress  $\sigma_{ij}^{\text{ve}} = d_i \bar{E}_j^0 \varepsilon_{ij}^{\text{ve}}$ , where  $d_i$  is the Prony amplitude of branch  $i$  and  $\bar{E}_j^0$  the pristine long-term modulus for the  $j$ -th strain component.

The Prony branches are deliberately left undamaged by  $D_m$ : the relaxation spectrum is a property of the undamaged ABS polymer network (measured independently by DMA on pristine coupons). Only the driving elastic stiffness  $C_c(D_m)$  that acts on  $\varepsilon_{\text{el}}$  is degraded

The cell-scale tangent stiffness at cycle  $N$  is finally obtained by homogenization with the current degraded matrix tensor  $C_m$ .

#### Damage Evolution: Modal Driving Force and Scalar Law:

Damage growth is driven by the thermodynamic energy release rate, defined as the negative partial derivative of the Helmholtz free energy density with respect to the damage variable.

Although the matrix damage is scalar and isotropic, the damage driving force for the whole composite is not. At each representative matrix Gauss point, it experiences a multi-axial elastic strain state  $\varepsilon_{\text{el}}$  arising from the interaction between the applied cell boundary traction and the embedded fibers. Even under nominally uniaxial coupon loading, the fibers constrain lateral matrix deformation and impose compressive, transverse, and shear components on the local matrix strain. The elastic strain energy density therefore admits a natural decomposition into contributions from each stiffness mode of the homogenized cell:

$$Y_{11} = \frac{E_{11}}{2\Xi} \varepsilon_{1,\text{el}} \left( \varepsilon_{1,\text{el}} + \nu_{21} \varepsilon_{2,\text{el}} + \nu_{31} \varepsilon_{3,\text{el}} \right), \quad (6.17)$$

$$Y_{22} = \frac{E_{22}}{2\Xi} \varepsilon_{2,\text{el}} \left( \varepsilon_{2,\text{el}} + \nu_{12} \varepsilon_{1,\text{el}} + \nu_{32} \varepsilon_{3,\text{el}} \right), \quad (6.18)$$

$$Y_{33} = \frac{E_{33}}{2\Xi} \varepsilon_{3,\text{el}} \left( \varepsilon_{3,\text{el}} + \nu_{13} \varepsilon_{1,\text{el}} + \nu_{23} \varepsilon_{2,\text{el}} \right), \quad (6.19)$$

$$Y_{12} = \frac{1}{2} G_{12} \varepsilon_{4,\text{el}}^2, \quad (6.20)$$

$$Y_{13} = \frac{1}{2} G_{13} \varepsilon_{5,\text{el}}^2, \quad (6.21)$$

$$Y_{23} = \frac{1}{2} G_{23} \varepsilon_{6,\text{el}}^2, \quad (6.22)$$

where  $\Xi = 1 - \nu_{12}\nu_{21} - \nu_{23}\nu_{32} - \nu_{13}\nu_{31} - 2\nu_{21}\nu_{32}\nu_{13}$  is the engineering-constants denominator of the homogenized Voigt stiffness matrix.  $Y_{11}$  is the strain energy per unit damage that would be released by a stiffness loss in the axial (fiber-aligned) mode,  $Y_{22}$  and  $Y_{33}$  the two transverse normal counterparts, and  $Y_{12}$ ,  $Y_{13}$ ,  $Y_{23}$  the three shear counterparts.

A tension-only activation criterion is applied to the normal modes via the Macaulay bracket  $\langle x \rangle \equiv \max(x, 0)$  (defined in Eq. 6.24):  $Y_{11}$ ,  $Y_{22}$ , and  $Y_{33}$  are set to zero whenever the corresponding normal strain is compressive, preventing spurious damage under compression-dominated loading.

#### Assembly of the scalar equivalent driving force:

The six modal contributions combine into a single equivalent strain energy release rate

that is thermodynamically conjugate to the scalar  $D_m$ :

$$Y_{\text{eq}} = Y_{11} + Y_{22} + Y_{33} + Y_{12} + Y_{13} + Y_{23}. \quad (6.23)$$

Equation 6.23 is the complete elastic strain energy density in the matrix, summed over all six independent stiffness modes. Because  $D_m$  degrades all stiffness components uniformly (Eq. 6.13), damage growth must be driven by the total strain energy rather than by any single modal component.

Three-phase evolution law:

The cycle counter is advanced as  $N_t = N_{t-1} + f\Delta t$ . The cycle-by-cycle growth rate of the scalar matrix damage follows a three-phase evolution law [144–147]:

$$\frac{dD_m}{dN} = \frac{\Gamma \langle Y_{\text{eq}} - Y^{\text{th}} \rangle^Q + \Lambda Y_{\text{eq}} e^{-\Delta N}}{(1 - D_m/D_F)^{K_{\text{tert}}}}, \quad \langle x \rangle \equiv \max(x, 0), \quad (6.24)$$

where  $\Gamma, \Lambda, \Delta, Q, Y^{\text{th}}, K_{\text{tert}}, D_F$  are seven fixed, stress-level-independent constants and the Macaulay bracket  $\langle \cdot \rangle$  enforces that the Phase-II power-law term is identically zero whenever  $Y_{\text{eq}} < Y^{\text{th}}$  — without this gate,  $(Y_{\text{eq}} - Y^{\text{th}})^Q$  is undefined for non-integer  $Q$  whenever the base is negative. In the numerical implementation, the Phase-III denominator is additionally floored at  $(1 - D_m/D_F) \geq 0.01$  to prevent a singularity as  $D_m \rightarrow D_F$  [148, 149]; the clamp is inactive over the range of  $D_m$  reached in all calibration and validation runs. The calibrated parameters are used without modification in all subsequent Voronoi-cell simulations.

The three physically distinct phases are as follows. **Phase I** (early transient): the exponentially decaying numerator term  $\Lambda Y_{\text{eq}} e^{-\Delta N}$  captures rapid microcrack nucleation at fiber termini and pre-existing voids immediately after loading commences. **Phase II** (steady-state propagation): once  $Y_{\text{eq}}$  exceeds the endurance threshold  $Y^{\text{th}}$ , damage accumulates through the power-law term  $\Gamma \langle Y_{\text{eq}} - Y^{\text{th}} \rangle^Q$  at a stable rate until  $D_m$  approaches  $D_F$ . **Phase III** (failure): as  $D_m \rightarrow D_F$ , the denominator  $(1 - D_m/D_F)^{K_{\text{tert}}}$  vanishes, reproducing the runaway stiffness loss observed in the final fatigue stage.

The damage variable is advanced by an explicit forward-Euler step over the cycle increment  $\Delta N = f\Delta t$ :

$$D_m^{(N)} = D_m^{(N_0)} + \frac{dD_m}{dN} \Delta N, \quad D_m^{(N)} \in [D_m^{(N_0)}, D_F]. \quad (6.25)$$

### 6.3.4 Cycle-Jump Acceleration

Direct cycle-by-cycle integration over tens of thousands of cycles is computationally prohibitive at the mesoscale. A cycle-jump scheme [150–152] advances the damage state by  $\Delta N_{\text{jump}}$  cycles in a single increment whenever damage evolves slowly. At each converged mechanical increment, the algorithm executes:

1. *Baseline update*: A standard forward-Euler step (Eq. 6.25) yields  $D_m^{\text{new}}$ .
2. *Jump-eligibility check*: The local rate of change is evaluated,

$$\Delta D^{\max} = \max_t |D_{m,t} - D_{m,t-1}|, \quad (6.26)$$

and a jump is permitted only if (i)  $N > N_{\text{cyc,min}}$  (here 1,500 cycles), this  $N_{\text{cyc,min}}$  is considered so that there will be some data points to show phase I and (ii)  $\Delta D^{\max} < \delta_{\text{tol}}$  (here 0.001), confirming that the Gauss point is in stable Phase-II propagation.

3. *Jump execution*: The cycle counter advances by  $\Delta N_{\text{jump}}$  (here 100 cycles) chosen to accelerate the simulation by 100 cycles each time if  $\Delta D^{\max} < \delta_{\text{tol}}$ ,

$$N^* = N + \Delta N_{\text{jump}}, \quad (6.27)$$

the damage rate is re-evaluated at  $N^*$ , and a second forward-Euler step yields

$$D_m^{(N^*)} = D_m^{(N)} + \left. \frac{dD_m}{dN} \right|_{N^*} \Delta N_{\text{jump}}. \quad (6.28)$$

4. *No-jump path*: If either eligibility condition fails, the baseline update is committed, and single-increment integration continues.

This adaptive strategy reduces wall-clock time by more than two orders of magnitude relative to full cycle-by-cycle integration while maintaining pointwise damage deviations below 1% (cf. Figure 6.8).

#### Heat Generation and State Variable Architecture:

The net energy per unit volume released as heat during the cycle increment combines viscoelastic and damage contributions minus the reversible elastically stored fraction:

$$\Delta W = \Delta W_{\text{ve}} + \Delta W_{\text{d}} - \Delta W_{\text{diss}}, \quad (6.29)$$

Equation 6.29 follows from a first-law energy balance over the increment: the mechanical work input each increment splits into a reversible part, stored and recovered elastically, and an irreversible part released as heat. Only the irreversible part — viscoelastic dissipation  $\Delta W_{\text{ve}}$  (Eq. 6.16, itself already the dissipated, not total, viscous work) and damage dissipation  $\Delta W_{\text{d}}$  — contributes to  $\Delta W$  in Eq. 6.29; the reversible elastic energy  $\Delta W_{\text{diss}}$  is subtracted out, not added.  $\Delta W_{\text{diss}}$  is evaluated by the same trapezoidal rule as Eq. 6.16, applied to the elastic strain increment,

$$\Delta W_{\text{diss}} = \frac{1}{2} \sum_{j=1}^6 (\sigma_{j,\text{old}}^{\text{el}} + \sigma_{j,\text{new}}^{\text{el}}) \Delta \varepsilon_j^{\text{el}}, \quad (6.30)$$

and the damage contribution is

$$\Delta W_{\text{d}} = Y_{\text{eq}} \Delta D_m. \quad (6.31)$$

Equation 6.31 is the thermodynamically consistent statement that damage growth releases strain energy at a rate proportional to the scalar driving force  $Y_{\text{eq}}$  and the scalar damage



increment  $\Delta D_m$ . The volumetric heat-generation rate returned to Abaqus via RPL [107, 153] is

$$\dot{q} = \Delta W \times f, \quad (6.32)$$

where multiplication by the loading frequency  $f$  [Hz] converts energy per cycle to power per unit volume. The adiabatic temperature increment tracked internally [141] is

$$\Delta T_{\text{adiab}} = \Delta W / (\rho c_p). \quad (6.33)$$

Equation 6.33 is a purely local, adiabatic energy balance with no spatial gradient term — it estimates the Gauss-point heat source strength for RPL, not the diffused temperature field. Spatial heat transport between Gauss points and between Voronoi cells is not present in this local balance; it is resolved separately by the coupled thermal solve described in Section 6.3.6.

To ensure quadratic convergence of the coupled Newton iteration, the subroutine also supplies the off-diagonal Jacobian terms DDSDDT, DRPLDE, and DRPLDT.

### 6.3.5 Subroutine inputs and final outputs.

The material property vector PROPS passed to the UMAT/UMATHT subroutine at the start of the analysis fully specifies the calibrated model: the seven damage-law fit constants  $\Gamma$ ,  $\Lambda$ ,  $\Delta$ ,  $Q$ ,  $Y^{\text{th}}$ ,  $K_{\text{tert}}$ , and  $D_F$  (Eq. 6.24); the porosity-inclusive matrix material properties  $E_m^0$ ,  $\nu_m$ , and  $G_m^0$  obtained from the two-step porous-matrix homogenization of the local  $\mu$ -CT porosity; the applied loading frequency  $f$ ; and the room-temperature reference state  $T_0$  at which testing was conducted, used to initialize the adiabatic temperature tracking. No other inputs are required: STATEV is initialized to zero at  $N = 0$  and evolves entirely from these five inputs through the algorithm of Section 6.3.7. The complete input-to-output

pipeline, including the outer cycle-stepping loop that drives the subroutine across the full simulated run, is summarized in Figure 6.4.

The two quantities ultimately sought from the subroutine, at every Gauss point in every Voronoi cell, are the scalar matrix damage  $D_m(N)$  and the local temperature change  $\Delta T(N)$  — STATEV indices 33 and 43, respectively. All other state variables exist only to support the cycle-by-cycle evaluation of these two quantities and are not, by themselves, outputs of interest. Once  $D_m(N)$  and  $\Delta T(N)$  are available for every cell, each discrete Voronoi cell carries forward its own damage progression, temperature history, and correspondingly degraded homogenized material property  $C_c(D_m)$  (Eq. 6.11). These discrete-scale quantities are subsequently combined via volume-weighted homogenization in Section 6.3.6 (Eq. 6.34) to recover the coupon-scale composite damage  $D_c(N)$  and temperature rise, which are directly comparable to the experimental extensometer and IRT measurements.

#### State variable architecture:

The subroutine maintains 46 scalar state variables (STATEV) per integration point, summarized in Table 6.1. Indices 1–32 store the viscoelastic strain history (total, per-branch, and elastic driving strain); index 33 stores the scalar damage variable  $D_m$ ; indices 34–39 store the six modal driving forces  $Y_{11}$ ,  $Y_{22}$ ,  $Y_{33}$ ,  $Y_{12}$ ,  $Y_{13}$ ,  $Y_{23}$ ; indices 40–41 the cycle counters; and 42–46 the increment-level energies and diagnostics.

### **6.3.6 Coupon-Level Upscaling**

Once individual cell stiffness histories  $C^{(\Psi_c)}(N)$  are computed by the UMAT/UMATHT subroutine, the coupon-scale response is obtained through volume-weighted averaging consistent with the Hill–Mandel macro-homogeneity principle [139, 154]. This averaging is a spatial, single-instant operation performed at each cycle  $N$ ; it is appropriate for stiffness because stiffness is a local state variable with no transport between cells. The stiffness

**Table 6.1:** State variable (STATEV) map for the UMAT/UMATHT subroutine.

| Index | Physical quantity                                | Symbol                   |
|-------|--------------------------------------------------|--------------------------|
| 1–6   | Total viscoelastic strain vector                 | $\varepsilon_{ij}^{ve}$  |
| 7–12  | Elastic driving strain vector                    | $\varepsilon_{ij}^{el}$  |
| 13    | Cumulative viscoelastic dissipated energy        | $W_{ve}^{\Sigma}$        |
| 14    | Cumulative viscoelastic temperature rise         | $\Delta T_{ve}^{\Sigma}$ |
| 15–32 | Per-branch viscoelastic strains ( $3 \times 6$ ) | $\varepsilon_{ij}^{ve}$  |
| 33    | Scalar matrix damage                             | $D_m$                    |
| 34    | Axial modal driving force                        | $Y_{11}$                 |
| 35    | Transverse modal driving force (axis 2)          | $Y_{22}$                 |
| 36    | Transverse modal driving force (axis 3)          | $Y_{33}$                 |
| 37    | Axial-shear modal driving force (1–2)            | $Y_{12}$                 |
| 38    | Axial-shear modal driving force (1–3)            | $Y_{13}$                 |
| 39    | Transverse-shear modal driving force (2–3)       | $Y_{23}$                 |
| 40    | Previous cycle counter                           | $N_{old}$                |
| 41    | Current cycle counter                            | $N$                      |
| 42    | Cumulative dissipated energy                     | $W_{diss}^{\Sigma}$      |
| 43    | Temperature at increment end (diagnostic)        | $T_{now}$                |
| 44    | Last jump cycle                                  | $N_{jump}$               |
| 45–46 | Adiabatic $\Delta T$ ; load-step diagnostics     | —                        |

assembly itself is

$$\mathbf{C}^{coupon}(N; f, R, \sigma_{max}) = \frac{1}{V_{coupon}} \sum_{\Psi_c} V_{\Psi_c} \mathbf{C}^{(\Psi_c)}(N; f, R, \sigma_{max}), \quad (6.34)$$

where  $V_{coupon}$  is the total reconstructed volume. The homogenized axial stiffness  $E_{xx}^{coupon}(N)$  is compared directly with experimental modulus-degradation curves in the coupon-scale validation of Section 6.4.3.

On the other hand, temperature is fundamentally different: it is governed by the transient heat conduction equation, and its coupon-scale value cannot be obtained by volume-averaging independently computed adiabatic cell temperatures (Eq. 6.33). Instead, the RPL heat source computed at each Gauss point (Eq. 6.32) drives the coupled UMATHT thermal pass, which integrates this equation over both space and time across the Voronoi mesh, producing a spatiotemporally resolved temperature field. The coupon-scale  $\Delta T(N)$  reported in Section 6.4.3 is a spatial average of this already-diffused field at each output time, not a substitute for solving diffusion.

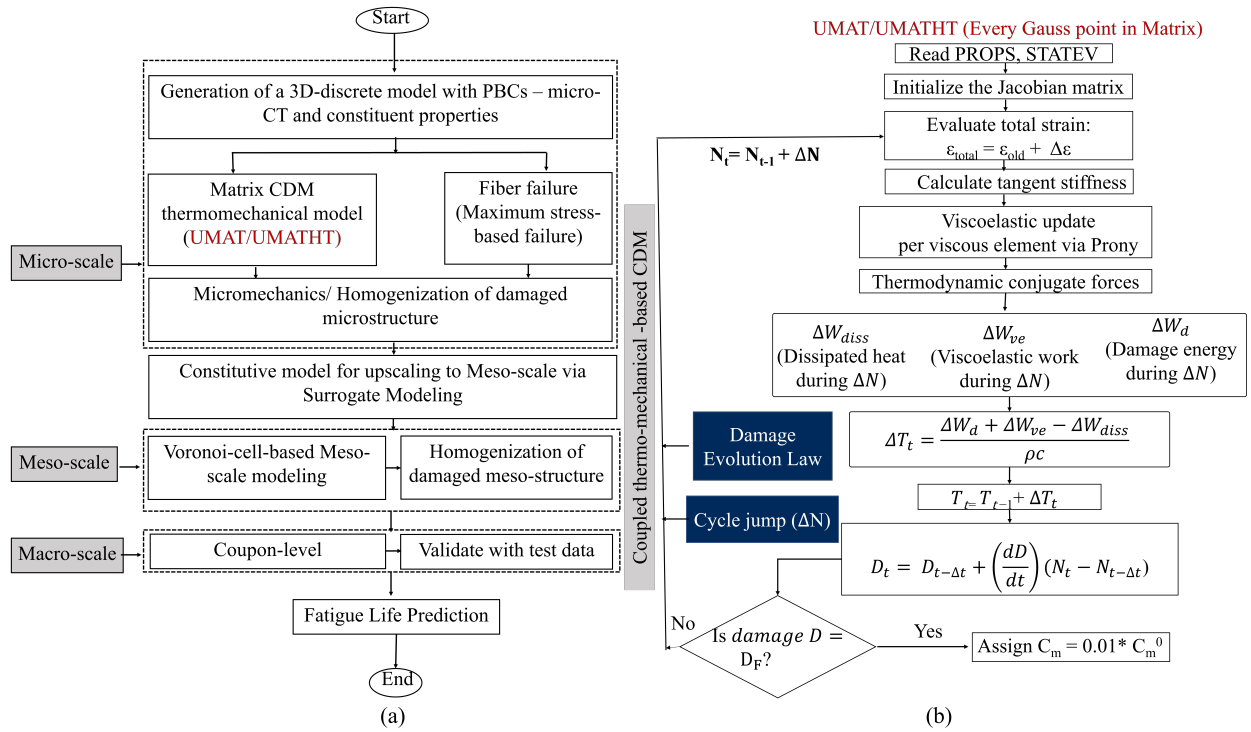
The matrix thermal diffusivity is a fixed material property and does not itself vary with loading frequency; what varies is the ratio between the rate of heat generation and the rate of diffusive transport. Since  $\dot{q} \propto f$  (Eq. 6.32) while thermal diffusivity is fixed, higher-frequency loading generates heat faster than it can diffuse across the RVE lengthscale between cycles, concentrating transient temperature rise near local dissipation hot spots (fiber termini, high- $Y_{eq}$  regions) before conduction has time to smooth the field. Lower-frequency loading allows more diffusion time per unit heat generated, producing a more spatially uniform, quasi-steady temperature distribution at a given cumulative dissipation. This distinction is consistent with the frequency-dependent self-heating trends examined experimentally in Chapter 3 (Section 2.4.2).

### 6.3.7 UMAT/UMATHT Subroutine Architecture

Sections 6.3.3–6.3.6 developed the physics evaluated at each matrix Gauss point: the damage-degraded matrix stiffness (Eq. 6.13), the Prony-series viscoelastic update (Eq. 6.15), the modal driving force  $Y_{eq}$  (Eq. 6.23), the three-phase damage evolution law (Eq. 6.24), the cycle-jump acceleration scheme (Section 6.3.4), and the RPL heat-generation rate (Eq. 6.32). This subsection closes the methodology by summarizing how these components are assembled into a single sequentially coupled Abaqus UMAT/UMATHT subroutine that executes at every Gauss point in every Voronoi cell. The multiscale linkage from  $\mu$ -CT topology, through mesoscale FE homogenization, to coupon-level prediction, together with the internal Gauss-point execution logic, is shown in Figure 6.3.

The subroutine executes the following operations at each converged Gauss-point increment (right panel of Figure 6.3), drawing on the equations and algorithms established earlier in this section:

1. *Read state*: The material property vector PROPS and the state variable vector STATEV (Table 6.1) are read, and the Jacobian (tangent stiffness) matrix is initialized.



**Figure 6.3:** Multi-scale fatigue modeling framework and UMAT/UMATHT subroutine logic. (a) Three-scale computational workflow linking  $\mu$ -CT fiber topology, via Voronoi-cell FE homogenization with periodic boundary conditions and two-step porous-matrix correction, to coupon-level fatigue life prediction. (b) Gauss-point execution flowchart of the sequentially coupled subroutine.

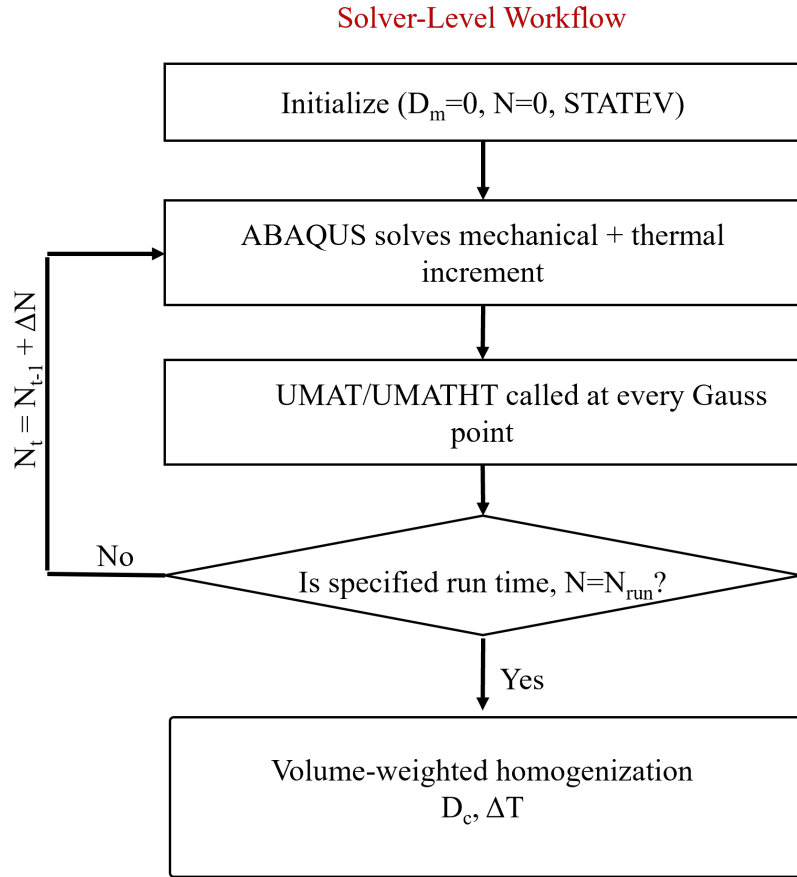
2. *Strain update*: The total strain is incremented as  $\varepsilon_{\text{tot}} = \varepsilon_{\text{tot,old}} + \Delta\varepsilon$  using the strain increment supplied by Abaqus.
3. *Tangent stiffness*: The cell tangent stiffness  $C_c(D_m)$  is assembled from the scalar damage variable  $D_m$  retrieved from STATEV (its rate depends on local microstructure), via the Mori–Tanaka operator (Eq. 6.11) applied to the degraded matrix stiffness  $C_m(D_m)$  of Eq. 6.13.
4. *Viscoelastic update*: The three Maxwell-branch viscoelastic strains are advanced via the recursive Prony relation (Eq. 6.15), and the elastic driving strain  $\varepsilon_{\text{el}}$  is extracted.
5. *Thermodynamic driving force*: The six modal energy release rates  $Y_{11}, Y_{22}, Y_{33}, Y_{12}, Y_{13}, Y_{23}$  (Eqs. 6.17–6.22) and their scalar equivalent  $Y_{\text{eq}}$  (Eq. 6.23) are evaluated from  $\varepsilon_{\text{el}}$  and the current homogenized engineering constants.
6. *Increment energies*: The viscoelastic, damage, and elastic-storage energies for the increment —  $\Delta W_{\text{ve}}, \Delta W_{\text{d}},$  and  $\Delta W_{\text{diss}}$  — are accumulated every cycle (Eqs. 6.16, 6.31).
7. *Adiabatic temperature update*: A local adiabatic increment  $\Delta T_t = (\Delta W_{\text{ve}} + \Delta W_{\text{d}} - \Delta W_{\text{diss}})/(\rho c_p)$  (Eq. 6.33) is tracked, and  $T_t = T_{t-1} + \Delta T_t$  is stored as the running temperature output.
8. *Damage update*: The scalar damage  $D_m$  is advanced by one forward-Euler step of the three-phase evolution law (Eq. 6.24) over the cycle increment  $\Delta N = f\Delta t$ :  $D_{m,t} = D_{m,t-\Delta t} + (dD_m/dN)(\Delta N)$ .
9. *Cycle-jump check*: If the eligibility conditions of Section 6.3.4 are satisfied, the cycle counter is extended by  $\Delta N_{\text{jump}}$  and the damage rate is re-integrated at the projected cycle (Eq. 6.28); otherwise the baseline update of Step 8 is committed, and single-increment integration continues.

10. *Failure clamp*: If  $D_m \geq D_F$  — the calibrated Phase-III failure damage recovered by the Mori–Tanaka inversion of Section 6.3.2 — the cell tangent stiffness is clamped at  $0.01 C_m^0$  (Eq. 6.13), preventing element inversion in the FE solver while still representing local physical failure.
11. *Heat rate return for UMATHT*: The volumetric heat-generation rate given by  $\dot{q} = \Delta W \times f$  (Eq. 6.32) is written to RPL for the coupled thermal pass.

The UMATHT pass consumes  $\dot{q}$  to advance the transient heat equation on the mesoscale block, producing the spatially resolved temperature field that is compared with the IRT measurements at the coupon surface. Across the entire fatigue life, the IRT-measured surface temperature rise remains modest ( $\Delta T \lesssim 3$  K, cf. Figure 6.1b) — well below the ABS glass-transition temperature, and low enough to produce a negligible modulus change over the fatigue history in its own right. The extracted  $D_m(N)$  therefore absorbs all stiffness degradation into a single damage variable, with no ambiguity between mechanical damage and thermal softening.

Figure 6.3b details this Gauss-point-level execution logic; Figure 6.4 now situates it within the outer solver loop that drives the subroutine across the simulated run. Following initialization ( $D_m = 0$ ,  $N = 0$ , STATEV=0 everywhere), ABAQUS solves each mechanical/thermal increment and invokes UMAT/UMATHT at every Gauss point in every Voronoi cell. The cycle counter is checked against the user-specified run length; while  $N < N_{run}$ , the counter advances ( $N_t = N_{t-1} + \Delta N$ , with  $\Delta N$  possibly extended by the cycle-jump logic of Section 6.3.4) and the loop repeats. Once  $N = N_{run}$ , the individual cell-level damage and temperature histories are assembled via volume-weighted homogenization in Section 6.3.6 (Eq. 6.34) to yield the coupon-scale outputs  $D_c(N)$  and  $\Delta T(N)$ .

With the constitutive law, damage evolution, cycle-jump algorithm, and subroutine architecture now fully specified, Section 6.4 turns to the microstructure-resolved predictions and their validation against the coupon-scale experiments.



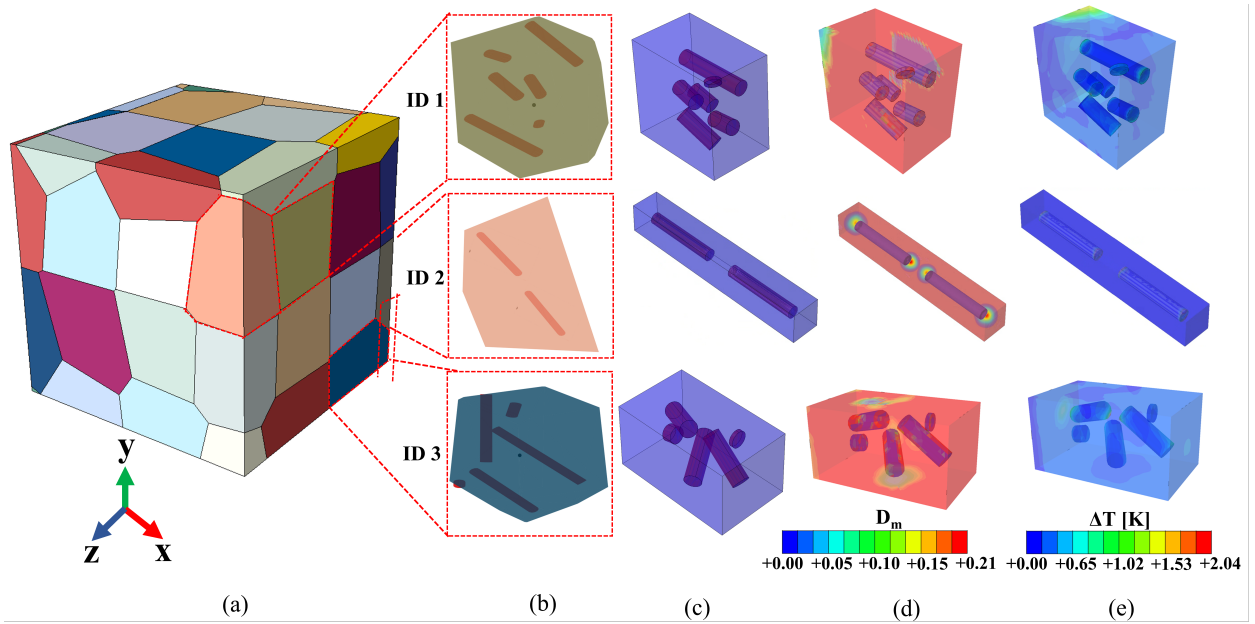
**Figure 6.4:** Solver-level workflow driving the coupled UMAT/UMATHT across the specified simulation run. Following initialization ( $D_m = 0$ ,  $N = 0$ , STATEV=0), ABAQUS solves each mechanical/thermal increment and invokes the UMAT/UMATHT subroutine at every Gauss point (Gauss-point-level physics detailed in Figure 6.3b). The cycle counter is checked against the user-specified run length  $N_F$ ; if not yet reached,  $N$  is advanced ( $N_t = N_{t-1} + \Delta N$ ) and the loop repeats. Once  $N = N_F$ , the individual cell-level histories are assembled through volume-weighted homogenization (Eq. 6.34) to yield the coupon-scale damage  $D_c$  and temperature rise  $\Delta T$ .



## 6.4 Results and Discussion

### 6.4.1 Microstructure-Driven Damage Heterogeneity and Load Sensitivity

Figure 6.5 presents the spatial fields of matrix damage  $D_m$ , temperature rise  $\Delta T$ , and effective stiffness ratio across the three representative Voronoi cells (IDs 1–3) at  $N = 10,000$  cycles under  $70\% \sigma_{UTS}$  ( $R = 0.1$ ,  $f = 15$  Hz). The three cells were selected from the  $\mu$ -CT reconstruction to span the observed range of local fiber volume fractions, spatial alignments, clustering intensity, and inter-fiber spacing. Despite identical boundary conditions and cycle counts, the three cells accumulate substantially different damage.



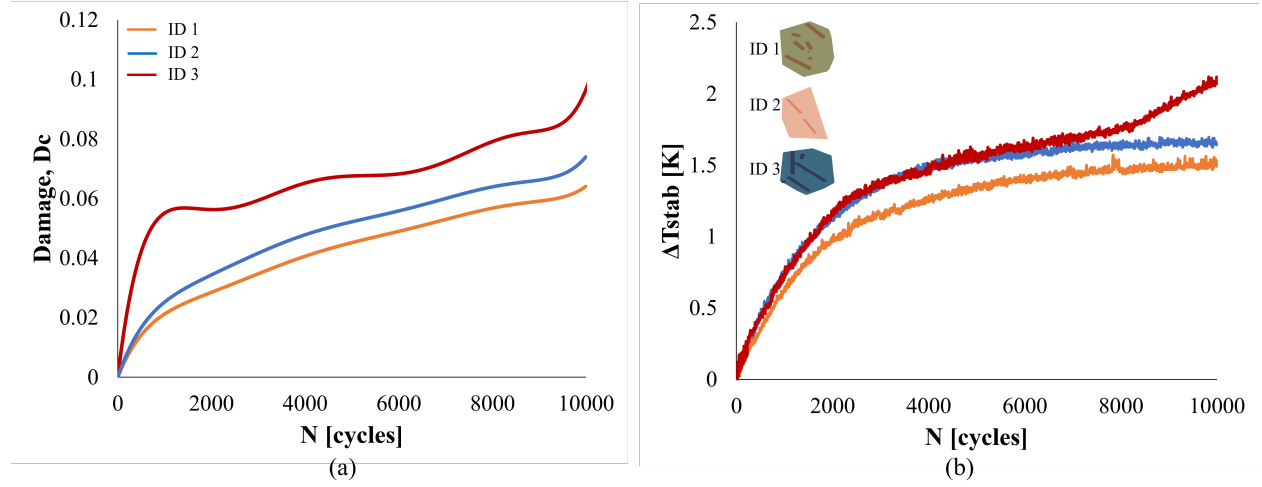
**Figure 6.5:** Microstructure-resolved fatigue response across three representative Voronoi cells (IDs 1–3) at  $N = 10,000$  cycles ( $70\% \sigma_{uts}$ ,  $R = 0.1$ ,  $f = 15$  Hz). **(a)** Voronoi-tessellated mesoscale block with periodic boundary conditions. **(b)** Cross-sectional fiber configurations for each cell, showing distinct local fiber volume fractions, spatial alignments, clustering, and inter-fiber spacing. **(c)** Equivalent RUC FE models with explicitly resolved fiber geometries embedded in a homogenized porous matrix. **(d)** Matrix damage  $D_m$  contours; damage concentrates near fiber termini and in narrow inter-fiber matrix ligaments, and is most severe in the densely packed ID 3. **(e)** Temperature rise  $\Delta T$  [K] fields; thermal hot spots co-localize with high-damage zones, confirming that thermomechanical coupling concentrates dissipation where damage is active.

ID 1 shows the least damage: with more matrix volume per fiber, the stress-concentration zones around adjacent fiber tips remain well separated, and the axial

modal contribution  $Y_{11}$  stays close to the endurance threshold for much of the loading history, keeping  $Y_{eq}$  only marginally above  $Y^{th}$ . ID 2 shows intermediate damage concentrated in thin matrix ligaments between closely spaced fibers, where the in-plane shear contribution  $Y_{12}$  dominates the composition of  $Y_{eq}$ . In ID 3, which has the densest local fiber packing, damage is both widespread and severe. Multiple neighboring fiber tips generate overlapping stress-concentration zones in the surrounding matrix; the local  $Y_{11}$  contribution at these intersections is large, and combined with elevated transverse and shear contributions, the total  $Y_{eq}$  far exceeds  $Y^{th}$ , driving rapid Phase-II growth. The high fiber density simultaneously reduces the volume of matrix available to distribute the load, thereby amplifying the mean matrix stress even before tip concentrations are considered. Denser fiber clustering therefore both raises the initial cell stiffness (through fiber reinforcement) and accelerates local matrix damage rates, causing the onset of Phase-III tertiary acceleration relative to less-dense cells. The temperature fields in column (d) mirror this ordering: the highest dissipation density is in ID 3, producing the hottest hotspots, and the thermomechanical coupling — rising  $T$  tracked as an output, no feedback into  $E_m$  — co-localizes cleanly with the damage field because  $\dot{q}$  and  $D_m$  both scale with  $Y_{eq}$ .

Figure 6.6 shows the time evolution of the homogenized damage  $D_c(N)$  and the stabilized surface temperature  $\Delta T_{stab}(N)$  for all three IDs over 10,000 cycles under the same loading conditions. Both panels confirm the topology-ordering established by the contour fields. ID 3 reaches  $D_c \approx 0.10$  and  $\Delta T_{stab} \approx 2.1$  K by  $N = 10,000$  cycles; ID 2 reaches approximately  $D_c \approx 0.07$  and  $\Delta T_{stab} \approx 1.8$  K; ID 1 remains at  $D_c \approx 0.04$  and  $\Delta T_{stab} \approx 1.2$  K. These differences arise entirely from the local fiber topology — the applied load and cycle count are identical across the three simulations — and confirm that microstructural heterogeneity governs fatigue damage accumulation as directly as the global stress amplitude. The temperature evolution parallels the damage evolution because

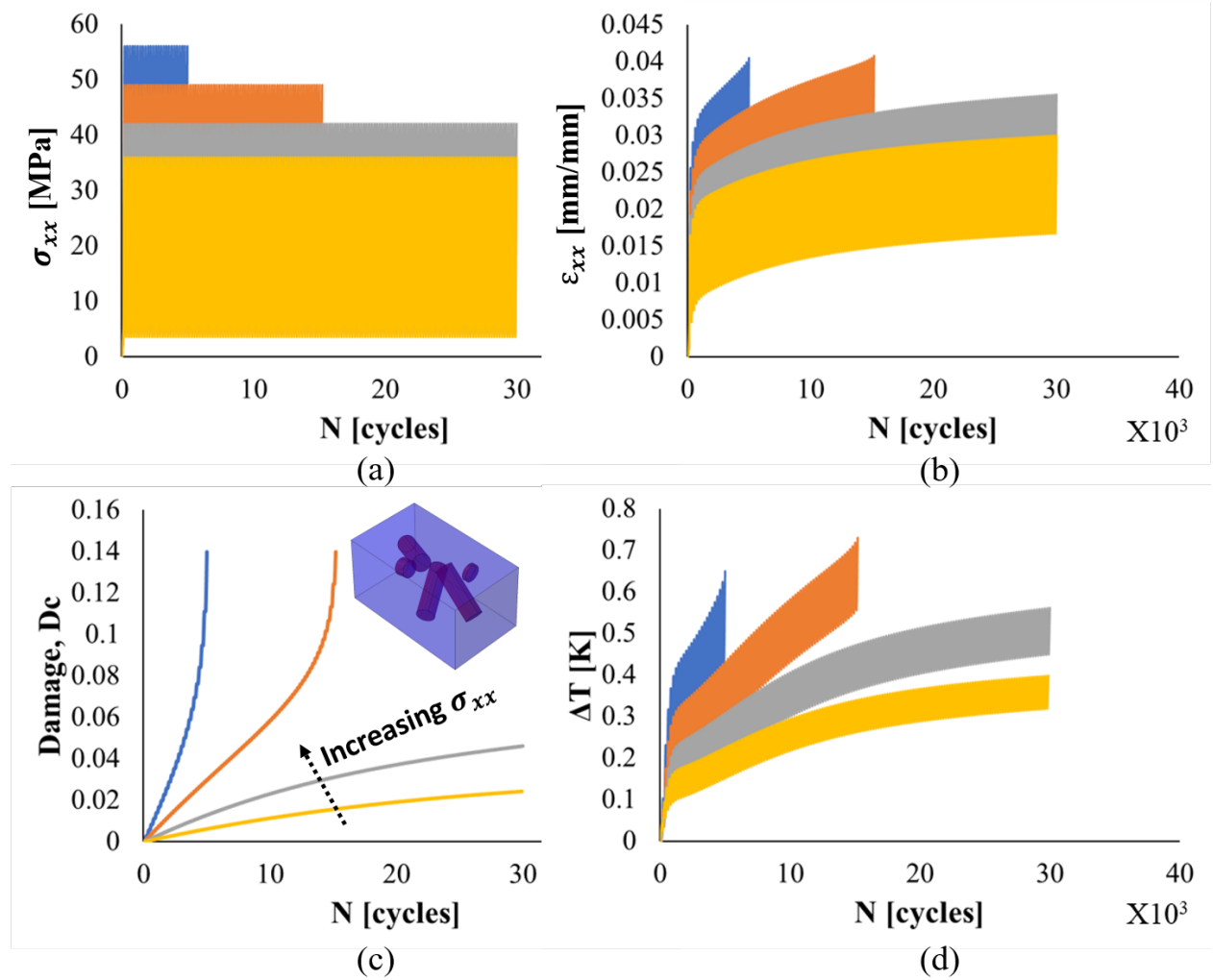
$\dot{q} = \Delta W \times f$  (Eq. 6.32) and  $\Delta W_d$  scales linearly with the local  $Y_{eq}$ , which is larger wherever more fiber ends concentrate stress into a given matrix volume.



**Figure 6.6:** Cycle-resolved fatigue response of the three representative Voronoi cells (IDs 1–3) under 70%  $\sigma_{UTS}$ ,  $R = 0.1$ ,  $f = 15$  Hz. **(a)** Composite damage  $D_c(N)$  for each cell. ID 3 accumulates damage fastest, reaching  $D_c \approx 0.10$  at  $N = 10,000$  cycles; ID 1 reaches only  $D_c \approx 0.04$  at the same cycle count. **(b)** Stabilized surface temperature rise  $\Delta T_{stab}(N)$ ; the thermal response preserves the same topology-driven ordering, since the volumetric heat-generation rate (Eq. 6.32) scales with  $Y_{eq}$ , which is amplified in fiber-dense cells. The  $\approx 2.5\times$  spread in both  $D_c$  and  $\Delta T_{stab}$  across three cells subjected to identical boundary conditions confirms that local fiber topology governs the fatigue response as directly as the global load amplitude.

The sensitivity of the fatigue response to applied stress amplitude, at fixed microstructure, is demonstrated in Figure 6.7. Four stress levels ranging from  $\approx 30\%$  to  $70\%$   $\sigma_{UTS}$  are applied to a single Voronoi cell. The applied stress history (Figure 6.7a) illustrates the four distinct load levels; the axial strain trajectories (Figure 6.7b) show progressive ratcheting driven by the Prony-series viscoelastic formulation, which amplifies strains as damage softens the effective modulus. The composite damage curves (Figure 6.7c) exhibit the load-dependent transition from Phase-I initiation through Phase-II plateau to Phase-III runaway; terminal damage values differ by more than fourfold across the stress range, and the cycles-to-failure shift by nearly two orders of magnitude between the lowest and highest levels. The surface temperature (Figure 6.7d) increases monotonically with both cycle count and stress amplitude, consistent with the frequency-scaled heat-generation law (Eq. 6.32) and with the  $Y_{eq}^{P_r}$  scaling of the effective damage-growth pre-factor (Eq. 6.24).

Taken together, Figures 6.5–6.7 establish that the three-phase CDM law reproduces the expected physical dependence on both microstructure and loading amplitude within a single, calibration-consistent constitutive framework, without stress-level or cell-specific parameter recalibration.



**Figure 6.7:** Influence of applied stress amplitude on fatigue response for a single representative Voronoi cell ( $R = 0.1$ ,  $f = 15$  Hz). Four stress levels, in order of decreasing peak stress (blue, orange, grey, yellow), are superimposed. **(a)** Applied axial stress history; higher amplitudes produce earlier Phase-III onset. **(b)** Axial strain accumulation via viscoelastic ratcheting; strains grow as damage reduces the effective stiffness. **(c)** Composite damage  $D_c(N)$ ; terminal values differ by more than fourfold across the stress range. **(d)** Surface temperature rise  $\Delta T(N)$ ; the monotonic increase with both cycle count and stress level is consistent with Eq. 6.32.

### 6.4.2 Cycle-Jump Algorithm: Efficiency and Accuracy

Figure 6.8 demonstrates the cycle-jump algorithm for a representative Voronoi cell at 70%  $\sigma_{\text{UTS}}$  ( $R = 0.1$ ,  $f = 15$  Hz). Figure 6.8 shows the matrix damage field  $D_m$  at the end of the simulation, with damage concentrated at fiber termini and in narrow inter-fiber matrix ligaments, as expected from the modal-decomposition argument of Section 6.3.3. The stress history in Figure 6.8(a) illustrates the discrete cycle-jump intervals: during stable Phase-II propagation, each eligible increment is extended by  $\Delta N_{\text{jump}} = 100$  cycles, visible as the uniform spacing in the stress sampling. The axial strain in Figure 6.8(b) accumulates in a staircase pattern corresponding to these jumps.

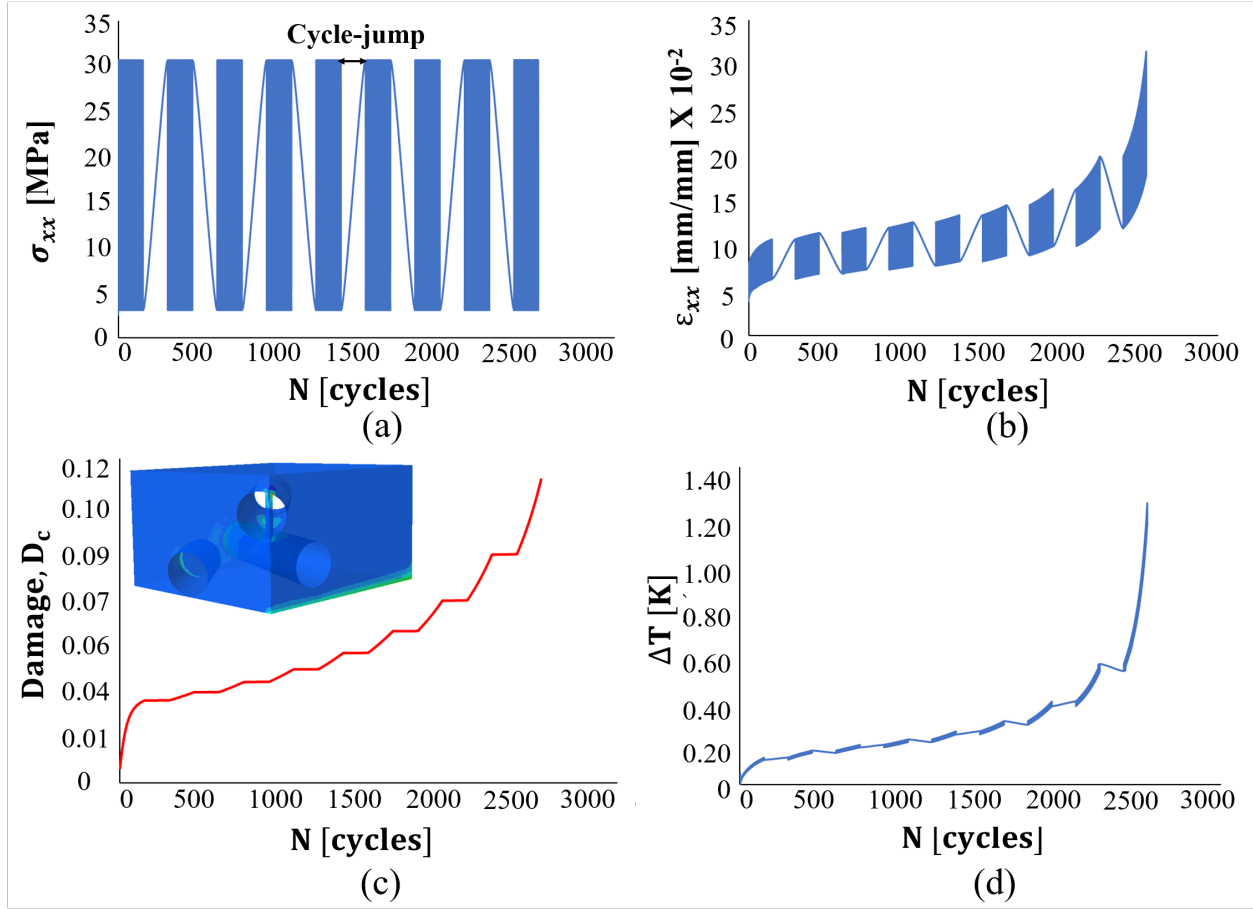
Figure 6.8(c) and (d) confirm the accuracy of the cycle-jump solution. The composite damage  $D_c(N)$  reproduces all three fatigue phases — rapid Phase-I nucleation over the first  $\sim 100$  cycles, a Phase-II propagation plateau reaching  $D_c \approx 0.04$  at  $N \approx 2,000$  cycles, and Phase-III runaway beyond that — with a maximum pointwise deviation below 1% relative to a full cycle-by-cycle reference. The nodal temperature rise  $\Delta T(N)$  co-evolves with damage dissipation and reaches approximately 1.4 K at final failure. The wall-clock time of the cycle-jump simulation was more than two orders of magnitude lower than that of the full reference, making mesoscale assembly calculations with thousands of Voronoi cells computationally tractable [150, 152].

### 6.4.3 Coupon-Scale Validation: Constant-Amplitude and Interrupted Fatigue

The multiscale framework is validated against two independent experimental datasets: CAF at three stress levels and the interrupted staircase fatigue test. Both datasets were used, at the homogeneous (non-mesoscale) level, to calibrate the CDM parameters.

#### Constant-amplitude fatigue:

Mesoscale Voronoi assemblies were constructed from the  $\mu$ -CT reconstructions of Panel B specimens. At each load level, the  $\mu$ -CT-measured porosity was propagated into

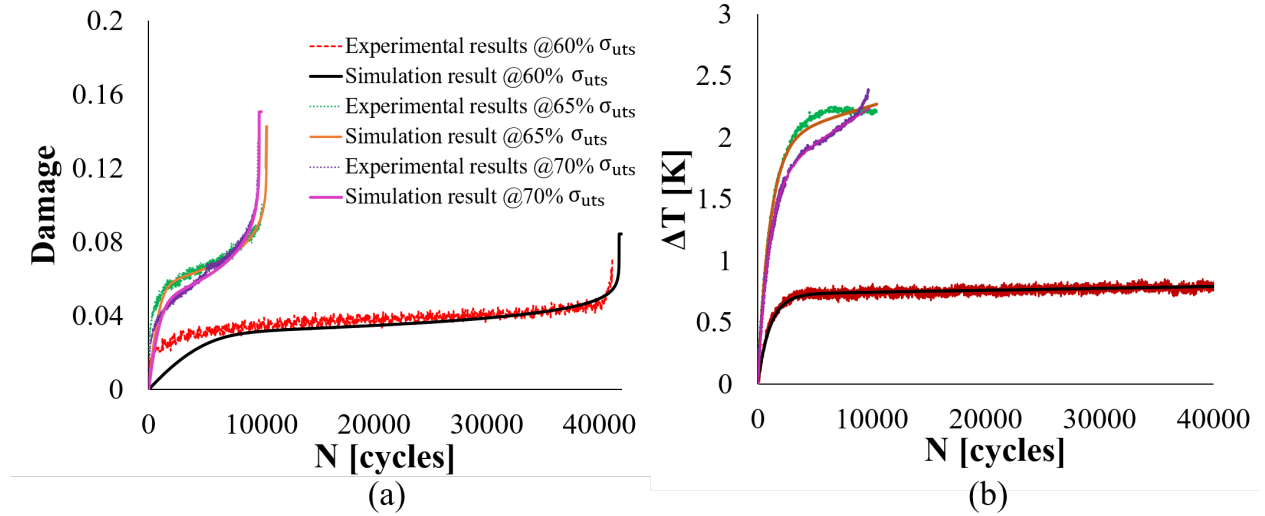


**Figure 6.8:** Cycle-jump algorithm demonstration for a representative Voronoi cell ( $70\% \sigma_{UTS}$ ,  $R = 0.1$ ,  $f = 15$  Hz). **(a)** Applied axial stress  $\sigma_{xx}(N)$ ; uniform cycle-jump intervals are visible during stable Phase-II propagation. **(b)** Axial strain  $\epsilon_{xx}(N)$  accumulating through viscoelastic ratcheting; staircase steps correspond to jump events. **(c)** Composite damage  $D_c(N)$  reproducing Phase-I nucleation, Phase-II plateau, and Phase-III acceleration toward failure. **(d)** Nodal temperature rise  $\Delta T(N)$  reaching  $\approx 1.4$  K at final failure. The cycle-jump solution agrees with the full cycle-by-cycle reference to within 1% while reducing wall-clock time by over two orders of magnitude.

the cell constitutive response through two-step porous-matrix homogenization, reducing the effective matrix properties assigned to each cell. Cell stiffnesses were assembled through Eq. 6.34 to give the coupon-scale modulus trajectory  $E_{xx}(N)/E_{xx}(0)$ .

Figure 6.9 compares predictions to experimental data for all three stress levels (60%, 65%, and  $70\% \sigma_{UTS}$ ). The model reproduces the stress-level-dependent transition from the Phase-II plateau to the Phase-III runaway, including the correct failure-cycle count, across all conditions. The predicted composite damage  $D_c(N)$  tracks the experimental

extensometer trajectories within 5–7% pointwise across the full fatigue life at all three stress levels, and the simultaneous prediction of surface temperature rise  $\Delta T(N)$  (Figure 6.9b) agrees with IRT measurements within experimental scatter. The latter confirms that the frequency-scaled heat-generation law (Eq. 6.32) correctly partitions dissipation between viscoelastic and damage contributions [107, 153]— a nontrivial test, given that the same scalar  $Y_{\text{eq}}$  governs both  $\Delta W_d$  and the damage growth rate.



**Figure 6.9:** Coupon-scale validation under CAF at three stress levels (60%, 65%, 70%  $\sigma_{\text{uts}}$ ;  $R = 0.1$ ;  $f = 15$  Hz). **(a)** Composite damage  $D_c(N)$ : multiscale CDM predictions (solid lines) versus experimentally derived damage trajectories (dotted). The model captures Phase II plateau and Phase III runaway at the correct cycle count without parameter recalibration between stress levels. **(b)** Surface temperature rise  $\Delta T(N)$ : predicted stabilized trajectories (solid) agree with IRT measurements (dotted) within experimental scatter, confirming that the frequency-scaled heat-generation law (Eq. 6.32) correctly partitions viscous and damage dissipation.

### Interrupted staircase fatigue:

Figure 6.10 presents validation against the interrupted staircase fatigue test, in which  $\sigma_{\text{max}}$  is stepped from 30% to 70%  $\sigma_{\text{UTS}}$  in 5% increments of 7,500 cycles each. The accumulated composite damage  $D_c(N)$  (Figure 6.10a) shows quantitative agreement between experiment and model at every step, including the correct burst-damage increments at each step transition — a direct consequence of the exponential Phase-I term  $\Lambda^{\text{eff}} Y_{\text{eq}} e^{-\Delta^{\text{eff}} N}$

re-activating whenever  $Y_{eq}$  jumps at a new load level — and the catastrophic Phase-III run-away during the final 70% block [82]. The surface temperature (Figure 6.10b) reproduces the characteristic sawtooth pattern:  $\Delta T$  rises within each block and resets to near-ambient at each step change. This reset is a direct consequence of the `TIME(1)` variable resetting in the `UMATHT` subroutine at each Abaqus step, which correctly represents the specimen cooling to ambient between loading blocks.

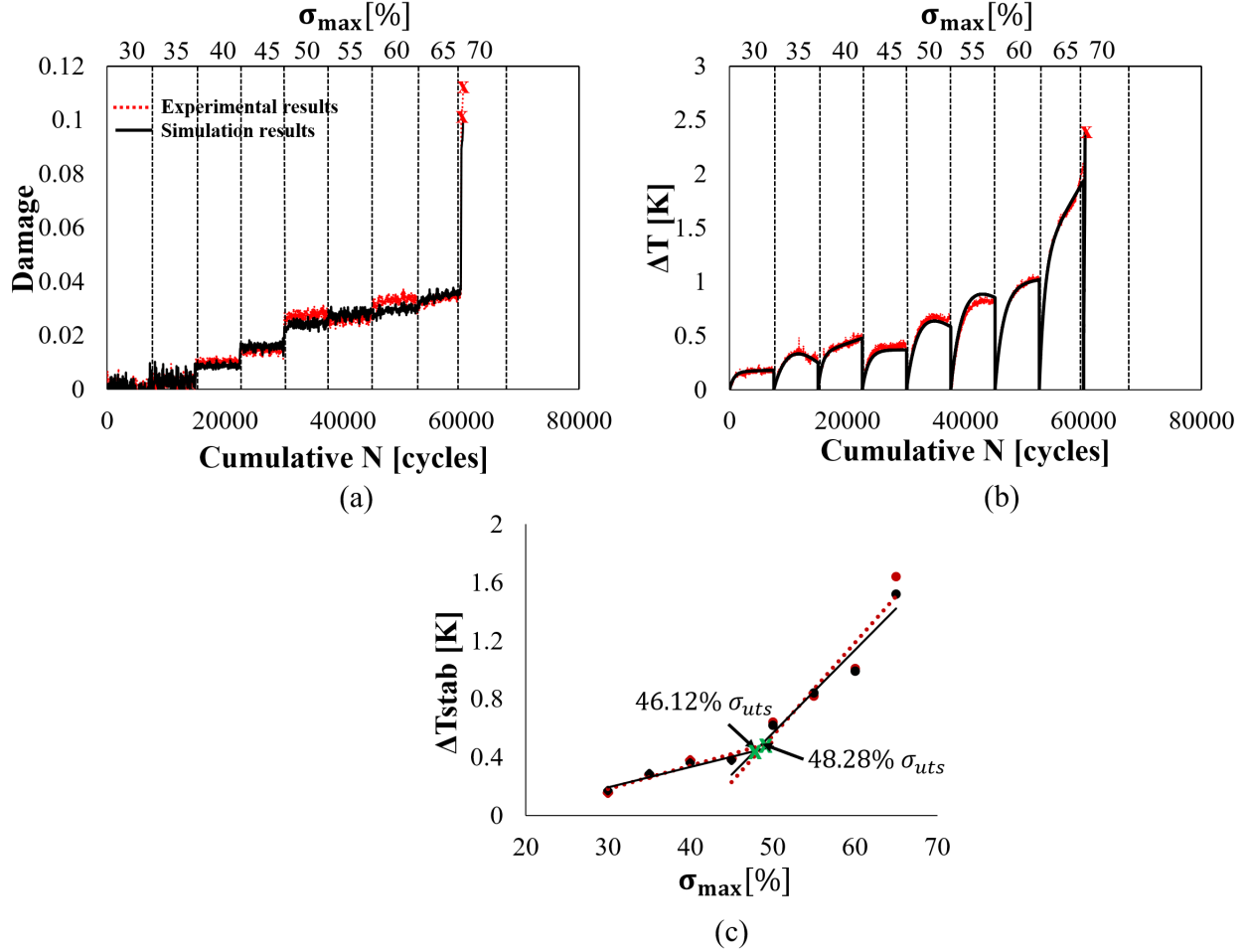
The stabilized block temperature  $\Delta T_{stab}$  versus applied stress fraction (panel c) shows a bilinear trend with an inflection at approximately  $46\% \sigma_{UTS}$ . This inflection marks the stress level at which the equivalent energy release rate first exceeds the endurance threshold  $Y^{th}$ , activating Phase-II damage. It agrees closely with the IRT-derived fatigue limit of approximately  $48\% \sigma_{UTS}$  reported in Chapter 4 [3, 155] — an independent confirmation that the fatigue-limit concept and the CDM activation criterion identify the same physical transition, even though they are derived from different observables (surface temperature slope change vs. thermodynamic threshold crossing).

Taken together, the CAF and interrupted staircase tests validate three distinct aspects of the framework simultaneously: (i) the calibration transfers across stress levels (CAF prediction at three amplitudes with a single parameter set), (ii) the calibration transfers across load-history types (CAF calibration reproduces interrupted staircase without further adjustment), and (iii) the identified fatigue limit matches an independent IRT-derived value from a different experimental protocol. Each of these represents a genuine falsification opportunity that the framework passes.

## 6.5 Conclusions

This chapter developed and validated a multiscale fatigue-limit and life-prediction framework for AM-CM SFTs. The framework couples a full fourth-order Eshelby–Mori–Tanaka homogenization operator, an inverse micromechanical procedure for extracting matrix





**Figure 6.10:** Coupon-scale validation under interrupted staircase fatigue ( $\sigma_{\max}$  from 30% to 70%  $\sigma_{UTS}$  in 5% increments; 7,500 cycles per step;  $R = 0.1$ ,  $f = 15$  Hz). **(a)** Accumulated composite damage  $D_c(N)$ : experimental trajectory (red dotted) and multiscale CDM prediction (black solid) agree at every step, including burst-damage increments at step transitions and the Phase III run-away at the final 70% block. **(b)** Surface temperature rise  $\Delta T(N)$ ; the sawtooth pattern — rising within each block, resetting at each step change — is reproduced by the TIME(1) reset in the UMATHT subroutine. **(c)** Stabilized block temperature  $\Delta T_{\text{stab}}$  vs  $\sigma_{\max} [\% \sigma_{UTS}]$ ; the bilinear inflection at  $\approx 46\text{--}48\% \sigma_{UTS}$  identifies the stress level at which the equivalent driving force  $Y_{\text{eq}}$  first crosses the endurance threshold  $Y^{\text{th}}$ , consistent with the IRT-derived fatigue limit from Chapter 4.

damage from composite modulus measurements, and a sequentially coupled thermomechanical UMAT/UMATHT implementation of an isotropic scalar-damage constitutive law with cycle-jump acceleration. The key contributions are the following.

- i. *Inverse Mori–Tanaka calibration of a scalar matrix damage law:* The full Eshelby–MT operator [131, 138, 139, 156], incorporating the  $\mu$ -CT-measured FLDs and FODs,

was inverted pointwise to recover an RVE-averaged matrix damage evolution  $D_m(N)$  from three composite fatigue tests at 60%, 65%, and 70%  $\sigma_{UTS}$ . The recovered  $D_m(N)$  consistently exceeds the measured  $D_c(N)$  at all cycles and all stress levels, quantifying the fiber-shielding effect [157, 158]: because the fibers carry a disproportionate share of the load and remain elastic, a larger matrix stiffness loss is required to produce a given composite stiffness loss. The extracted  $D_m(N)$  curves serve as the single-parameter-set calibration target for all subsequent CDM fitting.

- ii. *Coupled UMAT/UMATHT with cycle-jump acceleration:* A three-phase matrix CDM law incorporating viscoelasticity [153, 154] and the scalar damage driven by  $Y_{eq}$  was implemented as a sequentially coupled Abaqus subroutine. A cycle-jump algorithm reduced FE wall-clock time by more than two orders of magnitude relative to full cycle-by-cycle integration while maintaining pointwise damage deviations below 1%, making the mesoscale assembly of thousands of Voronoi cells computationally tractable.
- iii. *Microstructure-driven damage divergence:* Under identical loading conditions (70%  $\sigma_{uts}$ ,  $R = 0.1$ ,  $f = 15$  Hz), the cell-level composite damage  $D_c$  at  $N = 10,000$  cycles varied by approximately  $2.5\times$  across three Voronoi cells with distinct fiber volume fractions and packing. The densely packed cell accumulated the most damage because overlapping stress-concentration zones at multiple fiber termini raised  $Y_{eq}$  far above the endurance threshold  $Y^{th}$  earliest and most severely. This finding confirms that local fiber topology governs fatigue damage as directly as the global stress amplitude does, and motivates the microstructure-informed surrogate framework outlined below.
- iv. *Coupon-scale validation without recalibration:* Mesoscale assembly of cell-level predictions reproduced experimentally measured composite damage within 5–7%

and IRT surface temperature within experimental scatter across all three constant-amplitude stress levels and the interrupted staircase fatigue test. The bilinear inflection in the stabilized block temperature curve, identified with the  $Y_{\text{eq}} = Y^{\text{th}}$  crossing at  $\approx 46\% \sigma_{\text{uts}}$ , agrees closely with the independent IRT-derived fatigue limit of  $\approx 48\% \sigma_{\text{uts}}$  from Chapter 4, providing independent confirmation of the physical transition identified by the CDM activation criterion.

### **Future work: machine-learning surrogate:**

While the Mori–Tanaka FE framework achieves the accuracy required for physics-based fatigue prediction, the computational cost of resolving thousands of Voronoi cells over extended-cycle domains remains significant for full-component analysis [150, 152]. Immediate future work will use the datasets generated by these simulations to train a GNN paired with an LSTM surrogate [159]. By representing each Voronoi cell as a fiber-interaction graph and mapping its topology together with the loading quadruplet  $(N, f, R, \sigma_{\text{max}})$  directly to the cycle-dependent stiffness tensor, the surrogate will bypass the nested FE loops and reduce runtime by several orders of magnitude while preserving the underlying damage physics.

## Chapter 7

### Conclusion and Future Work

#### 7.1 Overview

This dissertation develops, experimentally validates, and computationally demonstrates an integrated framework for accelerated fatigue characterization and life prediction of AM-CM 20 wt.% CF-ABS SFTs. This final chapter synthesizes the findings of each chapter, evaluates the framework's limitations, and proposes directions for future research, organized by priority and implementation readiness.

#### 7.2 Summary of Principal Findings

All quantitative claims are directly traceable to experimental data, simulation results, or validated surrogate predictions reported in the corresponding chapter.

- i. The IRT staircase protocol achieved a 96-fold reduction in testing time (5 hours, 3 specimens) relative to conventional S-N testing (>15 days, 18+ specimens), producing HCFS estimates within  $\pm 4\%$  of S-N-derived values for AM-CM SFTs at 15 Hz and  $R = 0.1$ . This result directly closes Gap 1 identified in Chapter 2 and establishes IRT as a validated, resource-efficient alternative to S-N testing for this material class.
- ii. All four IRT thermal indicators ( $\Delta T_{\text{stab}}$ ,  $R_{\theta}$ ,  $R_c$ ,  $S_2$ ) yielded HCFS estimates within a  $\pm 4\%$  band centered at 54%  $\sigma_{\text{uts}}$ .  $\Delta T_{\text{stab}}$  and  $R_c$  exhibited the lowest inter-specimen scatter (coefficients of variation of approximately 1.4% and 6.0%, respectively).

- iii. HCFS increased monotonically from  $52.14 \pm 0.71\% \sigma_{\text{uts}}$  at 5 Hz to  $61.14 \pm 0.85\% \sigma_{\text{uts}}$  at 20 Hz — a 17.3% relative increase driven by frequency-dependent suppression of viscoelastic creep accumulation rather than thermal degradation. Dynamic mechanical analysis confirmed that fatigue surface temperatures (301–303 K) remained well below the ABS glass transition temperature ( $T_g \approx 378$  K), excluding thermal softening as a contributing mechanism. Independent constant-amplitude validation at 60%  $\sigma_{\text{uts}}$  — above the 5 Hz fatigue limit but below the 20 Hz fatigue limit — directly confirmed the IRT-predicted frequency-dependent endurance threshold, addressing Gap 2.
- iv. HCFS decreased monotonically from  $61.14 \pm 0.85\% \sigma_{\text{uts}}$  at  $R = 0.10$  to  $49.42 \pm 0.78\% \sigma_{\text{uts}}$  at  $R = 0.75$  (a 19.2% reduction) and confirming that elevated mean stress, through time-dependent matrix deformation and fiber– matrix debonding, is the dominant driver of fatigue limit reduction in this viscoelastic material.
- v. Fiber orientation produced the widest HCFS range observed in this study: from  $61.95 \pm 0.85\% \sigma_{\text{uts}}$  for 0°-aligned specimens (fiber-dominated axial load transfer) to  $36.18 \pm 0.25\% \sigma_{\text{uts}}$  for 60°-oriented specimens. Off-axis specimens at 45°–90° fell below the HCFS of unreinforced ABS ( $51.85 \pm 0.74\% \sigma_{\text{uts}}$ ), confirming that misaligned fiber ends act as interfacial stress concentrators that actively reduce fatigue resistance relative to the unfilled matrix.
- vi. FFE was frequency-invariant within  $\pm 15\%$  across 5–20 Hz (mean =  $0.0965 \text{ kJ m}^{-3} \text{ K}^{-1}$ , standard deviation = 0.0144), establishing FFE as a rate-independent scalar descriptor of irreversible fatigue damage in AM-CM SFTs and providing a thermodynamic basis for frequency-corrected HCFS estimation — the first such systematic frequency-resolved FFE characterization reported for any SFT system.
- vii. Initial void volume fraction is the single strongest predictor of IRT-derived HCFS across the specimens studied: increasing porosity from 1.41% to 2.86% reduced HCFS by 24.4% (from 63.89% to 48.28%  $\sigma_{\text{uts}}$ ), corresponding to an approximately 11%

reduction in HCFS per unit percentage-point increase in initial void content. This result directly closes Gap 3 and establishes a quantitative process–defect–performance relationship for AM-CM SFTs.

- viii. Multi-stage interrupted  $\mu$ -CT scanning (Before Test  $\rightarrow$  Below Fatigue Limit  $\rightarrow$  Above Fatigue Limit) revealed that void growth below HCFS is spatially diffuse and modest in magnitude (25–65% increase in void fraction), while void growth above HCFS is spatially concentrated at fiber-end neighborhoods and matrix-rich cluster boundaries, with void fraction increasing by 232–370% relative to the pristine state. This dual-zone growth behavior, confirmed for the first time in three dimensions in AM-CM SFTs, reflects the activation of two mechanistically distinct modes of void population growth at the fatigue limit transition.
- ix. Finite element homogenization of Voronoi-discretized  $\mu$ -CT microstructures demonstrated that fiber interaction topology — quantified by local clustering, nearest-neighbor proximity, and orientation distribution within each cell — produces 8–12% cell-to-cell variability in axial stiffness  $E_{33}$  at fixed global volume fraction, a range that mean-field homogenization predicts as identically zero. This result provides the primary mechanistic justification for the topology-preserving surrogate approach.
- x. The GNN–LSTM quasi-static surrogate, trained on 500 Voronoi-cell FE simulations, predicted full nonlinear stress–strain trajectories with  $R^2 = 0.993$  and mean relative error  $<4\%$  across aligned, mixed-orientation, and resin-rich cell topologies, directly addressing Gap 4. The surrogate reproduced topology-driven stiffness variability invisible to conventional scalar-parameterized surrogates.
- xi. Per-cell surrogate inference required less than one second on a single CPU versus several minutes for the equivalent nonlinear FE homogenization on five CPUs — a reduction in computational cost exceeding two orders of magnitude — enabling

coupon-level Voronoi assembly of 500 cells in approximately 60 seconds compared with 25–50 CPU-hours for direct FE simulation.

- xii. The coupled thermomechanical UMAT/UMATHHT subroutine — incorporating a 44-state-variable architecture with viscoelasticity, stiffness degradation model, and a cycle-jump acceleration algorithm — was validated simultaneously against the IRT surface temperature ( $\Delta T_{\text{stab}}$ ) and extensometer stiffness degradation  $E(N)/E_0$  data for AM-CM SFTs. The cycle-jump algorithm achieved a wall-clock time reduction exceeding two orders of magnitude relative to full cycle-by-cycle integration, with a maximum pointwise deviation in  $D(N)$  below 1% across all three fatigue phases.
- xiii. Discrete Voronoi-cell UMAT simulations revealed microstructure-dependent damage evolution: aligned-cluster cells exhibited slower Phase I onset but faster Phase III acceleration than matrix-rich cells under identical far-field loading conditions, driven by fiber-end stress-concentration amplification encoded in the CDM thermodynamic energy release rates  $Y_k$ .

### 7.3 Limitations of the Current Work

Scientific rigor requires that the boundary conditions for the framework’s validated applicability be stated precisely. The following discussion identifies the most consequential limitations, distinguishing those that constrain the current claims from those that simply indicate avenues for further development.

- i. *Monotonically increasing IRT staircase protocol:* The IRT staircase employs monotonically increasing steps in stress amplitude. Damage accumulated in earlier steps may marginally alter the dissipation signature in subsequent steps through a load-sequence effect, introducing a small systematic bias toward higher apparent HCFS values relative to the true constant-amplitude fatigue limit.

- ii. *Single material system:* All experimental data were derived from one fiber-matrix system (20 wt.% carbon fiber in ABS) processed by one manufacturing route (AM-CM). The generalizability of the IRT protocol, the  $\mu$ -CT porosity evolution patterns, the UMAT damage parameters, and the GNN-LSTM surrogate predictions to other SFT systems (short glass fiber/PA66, carbon fiber/PPS, or natural fiber/PLA) or manufacturing routes (conventional injection molding, FDM without compression consolidation) has not been experimentally verified.
- iii. *Uniaxial loading only:* All fatigue characterization employed uniaxial tension-tension loading. Structural components subjected to bending, torsion, or combined multiaxial fatigue may activate damage modes not observed under uniaxial tension (e.g., interlaminar shear delamination, biaxial matrix cracking), and IRT HCFS estimation under multiaxial loading has not been validated for AM-CM SFTs.
- iv. *Ex-situ  $\mu$ -CT porosity evolution tracking:* Multi-stage  $\mu$ -CT scanning was performed during fatigue interruptions with the specimen removed from the test frame. Viscoelastic recovery of the ABS matrix during the off-machine period may partially close microcracks and reduce the apparent void volume fraction, particularly in the Stage II regime. In-situ  $\mu$ -CT with a miniature fatigue loading stage would eliminate this potential relaxation effects.
- v. *Coupon-scale scope:* All experimental validation employs ASTM D638 Type I coupon-scale specimens. The fatigue performance of AM-CM SFT structural components — which may exhibit different through-thickness FOD gradients, stress concentration features (holes, fillets, bolted joints), and residual stress distributions — has not been characterized, and the coupon-to-component scaling of the IRT-derived HCFS remains an open question.
- vi. *Perfect fiber–matrix bonding assumption:* Both the static (Chapter 5) and fatigue (Chapter 6) FE homogenization models assume perfect adhesion at fiber– matrix



interfaces. This assumption is acceptable for pristine specimens below the fatigue limit but becomes increasingly inaccurate above HCFS, where interfacial debonding is the primary damage initiation mechanism. The absence of cohesive zone elements means that the FE-generated surrogate training data underestimates Stage I damage onset rates and may misrepresent the spatial pattern of damage localization.

- vii. *Quasi-static surrogate trained only on monotonic data:* The GNN–LSTM static surrogate (Chapter 5) is trained on monotonic tensile loading trajectories. Extension to cyclic constitutive prediction — including hysteretic energy dissipation loops, mean stress relaxation, and ratcheting behavior — requires retraining on cyclic FE data, which was not generated within the scope of this dissertation.
- viii. *Scalar porosity representation in UMAT:* The UMAT fatigue damage model incorporates porosity via a stage-level, two-step homogenization that updates the effective matrix stiffness at discrete  $\mu$ -CT scan points (BT, BF, AF), but does not resolve the continuous evolution of individual void morphologies within each UMAT increment. The spatial heterogeneity of void growth documented in Chapter 4 is therefore represented only in an averaged sense, potentially missing the localized stress amplification from the most rapidly growing voids that governs the onset of Phase III.

## 7.4 Future Research Directions

The limitations identified in Section 7.3 define a scientifically coherent research agenda that extends naturally from the present framework.

- i. *Cohesive Zone Interface Elements in RUC Models:* The perfect-bonding assumption of Chapters 5 and 6 can be relaxed by introducing bilinear traction-separation cohesive zone elements at fiber-matrix interfaces. Cohesive law parameters (interfacial fracture toughness  $G_{IC}$ ,  $G_{IIC}$ ; peak traction  $\sigma_c$ ,  $\tau_c$ ) can be calibrated from single-fiber push-out or microbond tests on AM-CM SFTs. This extension would enable the RUC FE model

to capture interfacial debonding as an explicit discrete event rather than a smeared CDM variable, producing more physically representative Stage I damage-onset data for the proposed GNN–LSTM fatigue surrogate’s training (Chapter 6) and closing the last principal modeling gap between the current framework and the experimentally observed damage sequence.

- ii. *Multiaxial Fatigue IRT Protocol:* Extension of the IRT methodology to multiaxial fatigue loading — combined tension-torsion, bending, and biaxial in-plane loading — requires a multiaxial thermodynamic indicator framework that decomposes dissipation contributions from each stress component within the complex stress state. The theoretical foundation lies in the multiaxial thermodynamics of irreversible processes (TIP) framework, where the intrinsic dissipation  $d_1$  is a scalar invariant of the full stress tensor rather than of a single uniaxial amplitude. Multiaxial IRT validation would substantially broaden the industrial applicability of the present protocol for components subjected to combined service loads.
- iii. *Probabilistic Fatigue Life Prediction and Structural Reliability:* Once trained on the UMAT-generated cell-level dataset (Chapter 6, proposed future work), a GNN–LSTM fatigue surrogate would offer the computational efficiency needed for Monte Carlo uncertainty quantification (UQ) studies that remain infeasible with the underlying UMAT itself, whose per-cell nonlinear FE solution cost precludes the  $10^4$ – $10^5$  realizations such studies require. A complete probabilistic fatigue life prediction methodology built on this future surrogate would: (i) characterize the statistical distributions of FOD, void volume fraction, void morphology, and fiber length from multi-location  $\mu$ -CT scans across production AM-CM panel; (ii) propagate these microstructural uncertainties through the trained surrogate using Monte Carlo sampling ( $10^4$ – $10^5$  realizations) to generate probability distributions of HCFS and fatigue life  $N_f$ ; and (iii) apply the resulting distributions within a structural reliability framework (FORM

or Monte Carlo) to compute probability of fatigue failure at a specified design life and loading condition. This methodology, once the surrogate is trained and independently validated, would support the development of probabilistic fatigue allowables for AM-CM SFT structural components—a critical enabler for regulatory acceptance in aerospace and automotive certification contexts.

- iv. *Variable-Amplitude and Spectrum Fatigue Extension*: All experimental and computational results in this dissertation employ constant-amplitude fatigue loading. Structural components in service experience variable-amplitude loading spectra — road-load spectra in automotive, gust-load spectra in wind turbines, maneuver spectra in aerospace — that include overloads, underloads, and irregular sequencing, which may accelerate or retard fatigue damage relative to constant-amplitude predictions through load interaction effects. The LSTM architecture proposed for the fatigue surrogate (Chapter 6, not trained within the scope of this dissertation) would be well-suited to this extension in principle, because LSTMs are designed for sequential data processing and can naturally encode load-history dependence: augmenting the input sequence with cycle-by-cycle stress amplitude and ratio variations would require only modification of the LSTM input vector, with no change to the GNN encoder or output architecture. Variable-amplitude IRT testing using standardized load spectra (e.g., FALSTAFF for aerospace, CARLOS for automotive) would provide the experimental dataset needed for the surrogate’s initial training and subsequent validation on variable-amplitude data.

## **7.5 Broader Impact and Industrial Significance**

The contributions of this dissertation are significant not only within the academic community of composite mechanics and materials informatics but also for the industrial stakeholders who develop, qualify, and deploy AM-CM SFT structural components. Three dimensions of industrial impact are identified.

First, the IRT staircase protocol directly addresses the most acute practical bottleneck in AM-CM SFT qualification: the prohibitive time and specimen cost of conventional S-N fatigue characterization for materials still under active process development. By reducing the fatigue qualification timeline from weeks to hours and the specimen count from eighteen to three, the IRT protocol enables AM-CM process optimization cycles that incorporate fatigue performance feedback at every iteration — a capability currently absent and whose absence forces reliance on empirical rules of thumb rather than measured performance data in early-stage structural design.

Second, the computational framework provides the foundation for a new class of material-specific, microstructurally resolved fatigue allowables for AM-CM SFTs. Current airworthiness certification standards (FAA AC 20-107B; EASA CS-23) require building-block testing programs that generate fatigue allowables from statistically significant specimen populations across a matrix of loading conditions — a process requiring years and substantial resources for each new material-process combination. The physics-based multiscale framework of Chapter 6 (Mori–Tanaka homogenization coupled to the UMAT/UMATHHT fatigue damage law), validated against experiments to within 5–7% at the coupon scale, provides a physics-grounded computational alternative that can, in principle, generate statistically representative fatigue allowable distributions from  $\mu$ -CT microstructural inputs and targeted validation tests. Because the mesoscale UMAT assembly remains too computationally expensive for the large Monte Carlo ensembles this application requires, realizing it in practice depends on the proposed GNN–LSTM fatigue surrogate (Chapter 6, future work) being trained and independently validated against the same experimental benchmarks; only then would the combined framework substantially reduce the experimental burden of the building-block process.

Third, the graph-based microstructure representation and the IRT porosity diagnostic have applications extending beyond the specific SFT material class studied here. The GNN architecture for fiber-topology encoding is applicable to any discontinuous-fiber composite

system for which  $\mu$ -CT fiber centerline extraction is feasible — including chopped-tape composites, sheet molding compounds, long-fiber thermoplastics, and FDM-printed short-fiber parts. The  $R_\theta$ -based non-destructive porosity indicator, calibrated here for AM-CM SFTs, provides a methodological template applicable to any IRT-instrumented fatigue test on a polymer-matrix composite in which subcritical porosity is a manufacturing process variable.

## Publications

### Journal Articles

1. **P. Pathak**, V. Kumar, M. M. Khonsari, T. Ricks, S. Srivastava, and S. Gururaja *On Surrogate Modeling of Fatigue Lifetime Prediction Response of AM-CM SFTs Using Graph Neural Networks*, (Under preparation)
2. **P. Pathak**, V. Kumar, T. Ricks, S. Gururaja, and S. Srivastava *On Surrogate Modeling of Static Response of AM Short-Fiber Thermoplastics Using Graph Neural Networks*, Composites Part B: Engineering (Minor revision)
3. **P. Pathak**, V. Kumar, T. Ricks, S. Gururaja, and S. Srivastava *On Surrogate Modeling of Static Response of AM Short-Fiber Thermoplastics Using Graph Neural Networks*, arXiv (2026) <https://doi.org/10.48550/arXiv.2606.28996>
4. **P. Pathak**, K. Bristy, M. M. Khonsari, V. Kumar and S. Gururaja *On the influence of cyclic loading frequency on fatigue limit of short-fiber thermoplastics*, Fatigue and Fracture of Engineering Materials and Structures 45 (2026) 1001–1021. <https://doi.org/10.1111/ffe.70241>
5. J. Rahman, **P. Pathak**, R. Warren, O. Hasan, K.T. Hsiao and S. Gururaja *Effect of Electrically Aligned Carbon Nanofibers Z-threading on the Fatigue Behavior in Unidirectional CFRP Composites via Infrared Thermography*, Composites Part A: Applied Science and Manufacturing 199 (2025) 109193. <https://doi.org/10.1016/j.compositesa.2025.109193>
6. **P. Pathak**, S. Gururaja, *Porosity evolution in additively manufactured compression-molded short-fiber thermoplastics under cyclic loading: Insights from micro-computed*

*tomography and infrared thermography*, Composites Part A: Applied Science and Manufacturing 194 (2025) 108881. <https://doi.org/10.1016/j.compositesa.2025.108881>

7. **P. Pathak**, S. Gururaja, V. Kumar, D. Nuttal, A. Mahmoudi, M. M. Khonsari and U. Vaidya *Examining infrared thermography-based approaches to rapid fatigue characterization of additively manufactured compression molded short fiber thermoplastic composites*, Composite Structures 351 (2025) 118610. <https://doi.org/10.1016/j.compstruct.2024.118610>

### Conference Proceedings

1. **P. Pathak** and S. Gururaja *Fatigue life prediction of additively manufactured compression molded short fiber composites*, American Society for Composites (ASC) 40th Annual Technical Conference, Dayton, OH, October 6-8th, 2025.
2. **P. Pathak**, N. Manoharan, K. Bristy, J. Rahman and S. Gururaja *Accelerated fatigue characterization of advanced composites using infrared thermography*, 24th International Conference on Composite Materials (ICCM24), Baltimore, MD, August 4-8th, 2025.
3. **P. Pathak**, K. Bristy, V. Kumar and S. Gururaja *Effect of Loading Frequency on Fatigue Behavior of Additively Manufactured Short Fiber Thermoplastics via Infrared Thermography*, SEM Annual Conference & Exposition on Experimental and Applied Mechanics, Milwaukee, WI, June 2-5th, 2025.
4. H. Gandhi, **P. Pathak** and S. Gururaja *Effect of Induced Porosity on Fatigue Performance of Additively Manufactured Short-Fiber Thermoplastics Using Infrared Thermography*, SEM Annual Conference & Exposition on Experimental and Applied Mechanics, Milwaukee, WI, June 2-5th, 2025.

5. **P. Pathak** and S. Gururaja *Understanding Fatigue Behavior of Additively Manufactured Compression Molded Short Fiber Reinforced Thermo-plastics with Process Defects*, American Society for Composites (ASC) 39th Annual Technical Conference, San Diego, CA, October 21-24th, 2024 (Presentation alone).
6. **P. Pathak** and S. Gururaja *Effect of process defects on fatigue life of AM-CM composites via infrared thermography*, SEM Annual Conference & Exposition on Experimental and Applied Mechanics, Vancouver, WA, June 3-6th, 2024.
7. **P. Pathak** and S. Gururaja *Rapid fatigue characterization of additively manufactured polymer composites using infrared thermograph*, 15th International Conference of Fracture (ICF15), Atlanta, GA, June 11-16th, 2023 (Poster Presentation).
8. N. Manoharan, **P. Pathak**, S. Gururaja, V. Kumar and U. Vaidya *Rapid fatigue characterization via infrared thermography of am-cm composites*, SEM Annual Conference & Exposition on Experimental and Applied Mechanics, Orlando, FL, June 5-8th, 2023.



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## Appendix A

### Viscoelastic characterization

This appendix presents the two independent material characterization measurements: the glass transition temperature of the CF-ABS composite using differential scanning calorimetry (DSC), and the three-term Prony series calibration of the neat ABS matrix using DMA.

#### A.1 Test Conditions

Table A.1 reports the DMA test conditions, and Table A.2 the DSC test conditions, as recorded by the instrument software (TA Instruments Trios) at the time of testing.

**Table A.1:** DMA test conditions for the ABS matrix (Instrument type: Discovery HR20, Auburn University).

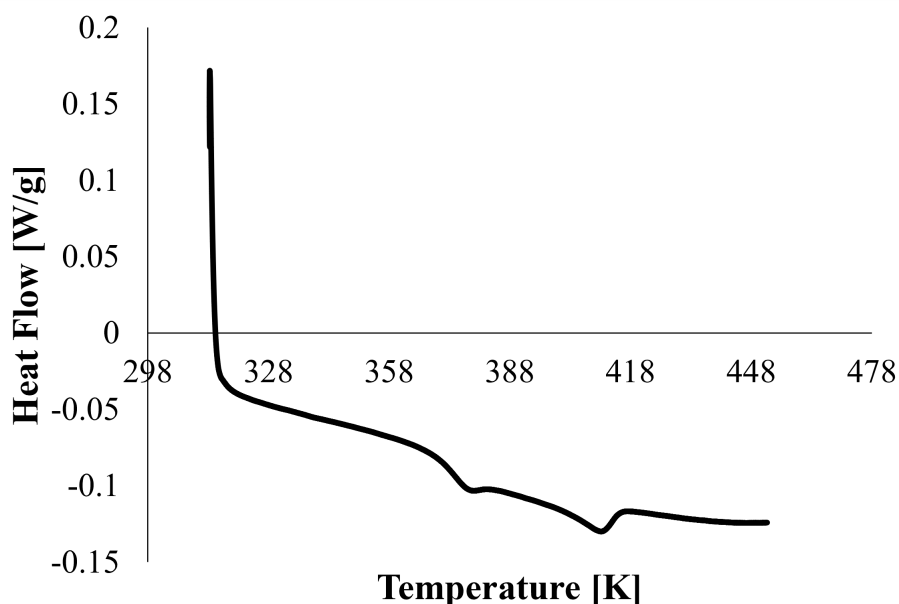
| Parameter                                                      | Value                                |
|----------------------------------------------------------------|--------------------------------------|
| Geometry                                                       | Rectangular solid sample             |
| Specimen length                                                | 5.078 mm                             |
| Clamp face                                                     | 4.5 mm                               |
| <i>Master curve construction (isothermal frequency sweeps)</i> |                                      |
| Temperature range                                              | 298–493K, 5K increments              |
| Frequency range per isotherm                                   | $\approx 0.89$ –94 Hz                |
| Reference temperature                                          | $T_{\text{ref}} = 298$ K             |
| <i>Glass transition (temperature ramp)</i>                     |                                      |
| Oscillation frequency                                          | 10 rad/s ( $\approx 1.59$ Hz, fixed) |
| Temperature range                                              | 308.2–423.2C                         |
| Ramp rate                                                      | 3.0C/min                             |
| Oscillation displacement                                       | 0.00243–0.00261 rad                  |
| Oscillation torque                                             | 11.5–8392 $\mu\text{N}\cdot\text{m}$ |

**Table A.2:** DSC test conditions (Instrument type: DSC25, Auburn University).

| Parameter             | Value                                             |
|-----------------------|---------------------------------------------------|
| Sample mass           | 6.92 mg                                           |
| Pan type              | Tzero aluminum, hermetic                          |
| Purge gas             | Nitrogen, 50 mL/min                               |
| Procedure             | Heat–Cool–Heat                                    |
| Segment 1             | Ramp 278.00K/min to 453K                          |
| Segment 2             | Ramp 278.00K/min to 453K                          |
| Segment 3             | Ramp 278.00K/min to 453K                          |
| Sampling interval     | 0.1 s/pt                                          |
| $T_g$ determined from | Segment 3 (second heat), removing thermal history |

## A.2 Glass Transition Temperature

The glass transition temperature reported in Section 6.3.3 ( $T_g \approx 374$  K) is determined from DSC, using the inflection point (point of maximum heat-flow slope) of the second-heat curve (Figure A.1), consistent with the small endothermic enthalpy-relaxation overshoot visible immediately above the transition. This value is used as the reference  $T_g$  throughout this dissertation.



**Figure A.1:** DSC glass transition determination for CF-ABS. Normalized heat flow versus temperature.

### A.3 Master Curve Reference Temperature and Time–Temperature Superposition (TTS) Shifting

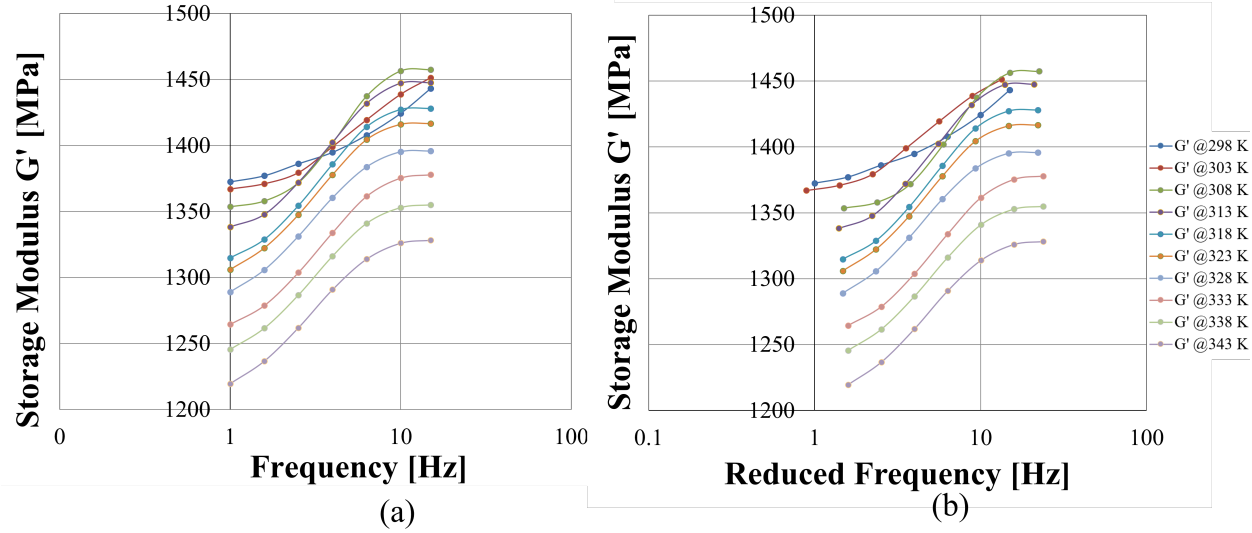
The master curve reference temperature is  $T_{\text{ref}} = 298$  K, chosen to represent the actual operating condition of the fatigue tests in this dissertation, which were conducted in the 298–310K range, rather than the material's  $T_g$ . This places the master curve within the same glassy-state regime as the fatigue tests it is used to model, approximately 60–75 K below  $T_g$ .

The master curve is constructed by superposing isothermal frequency sweeps at ten temperatures spanning this range and beyond (298–343K) onto the 298 K reference isotherm using horizontal time–temperature shift factors  $a_T$ , listed in Table A.3. Figure A.2 shows this shifting explicitly: panel (a) plots the raw, unshifted isotherms, each occupying a distinct frequency window; panel (b) shows the same data after multiplying each isotherm's frequency axis by its  $a_T$ , collapsing the individual isotherms onto a single continuous master curve at  $T_{\text{ref}}$ .

**Table A.3:** Horizontal shift factors  $a_T$  used to construct the ABS matrix master curve at  $T_{\text{ref}} = 298$  K.

| Temperature (K) | $a_T$ |
|-----------------|-------|
| 298             | 1.000 |
| 303             | 0.891 |
| 308             | 1.502 |
| 313             | 1.399 |
| 318             | 1.477 |
| 323             | 1.477 |
| 328             | 1.477 |
| 333             | 1.592 |
| 338             | 1.592 |
| 343             | 1.592 |

A small crossover appears among the 298–308K isotherms at the highest frequencies (10–15 Hz), well under 1% of the modulus range; the expected ordering holds cleanly elsewhere, and this does not affect the Prony calibration (Section A.4), which is fit to binned averages across the full dataset rather than any single isotherm.



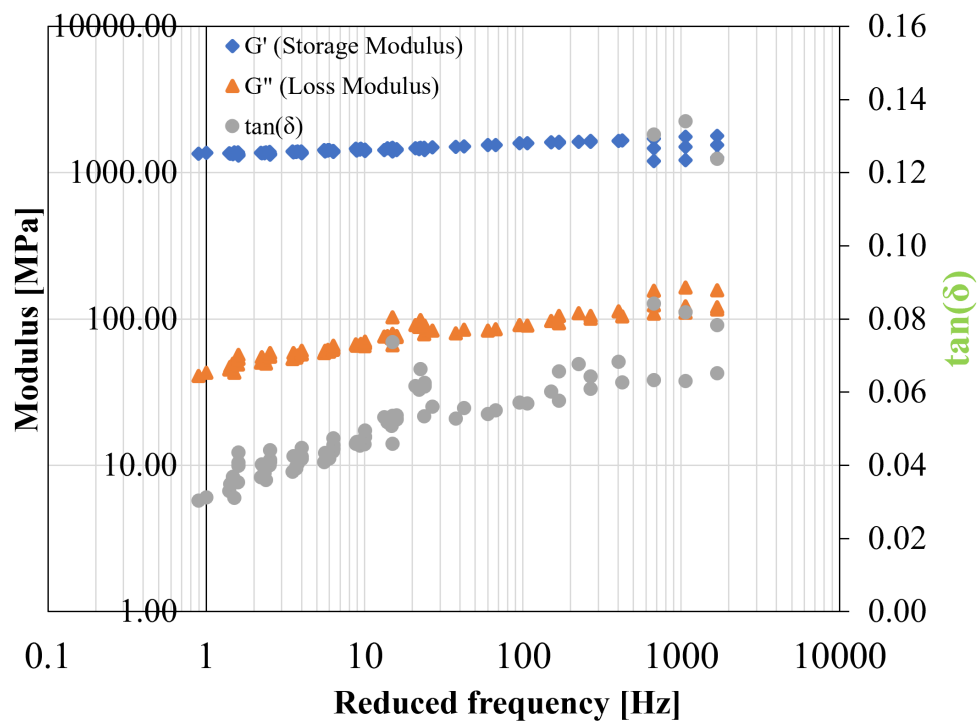
**Figure A.2:** Time–temperature superposition of the ABS matrix DMA data. **(a)** Raw isothermal frequency sweeps, 298–343K, each occupying a distinct frequency window. **(b)** The same isotherms after applying the shift factors of Table A.3, collapsing onto a single master curve at  $T_{\text{ref}} = 298$  K.

#### A.4 Prony Series Calibration of the ABS Matrix

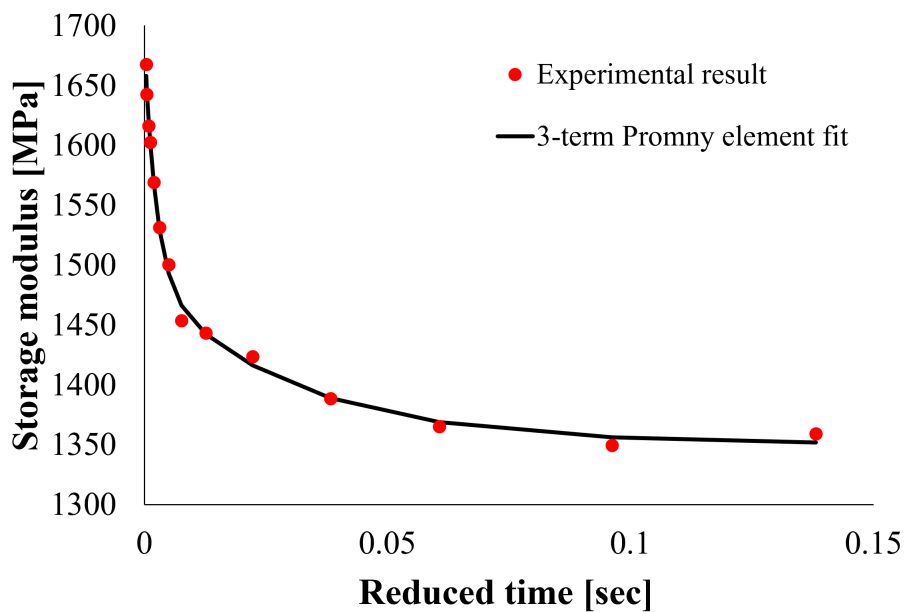
Figure A.3 presents the full master curve in the standard log–log TTS format: storage modulus  $G'$ , loss modulus  $G''$ , and  $\tan(\delta)$ , all versus reduced frequency at  $T_{\text{ref}} = 298$  K. As expected for a glassy polymer well below  $T_g$ ,  $\tan(\delta)$  increases with frequency across the measured range ( $\approx 0.03$  to  $\approx 0.09$ ), indicating increasing viscous dissipation at higher loading rates consistent with the frequency-dependent fatigue behavior discussed in Chapter 3 (Section 2.4.2).

The Prony series itself is calibrated in the time domain, on the same master curve, because the Chapter 6 UMAT implements the viscoelastic branches as a time-domain recursive update (Eq. 6.15) integrated directly over time, with the reduced-time axis obtained from the standard interconversion of the frequency-domain data above.

Table A.4 reports the calibrated coefficients.



**Figure A.3:** ABS matrix DMA master curve in standard log–log format: storage modulus  $G'$ , loss modulus  $G''$ , and  $\tan(\delta)$  versus reduced frequency at  $T_{\text{ref}} = 298\text{K}$ .



**Figure A.4:** DMA storage modulus master curve for the neat ABS matrix ( $T_{\text{ref}} = 298\text{K}$ ) with the calibrated three-term Prony series fit (Table A.4).



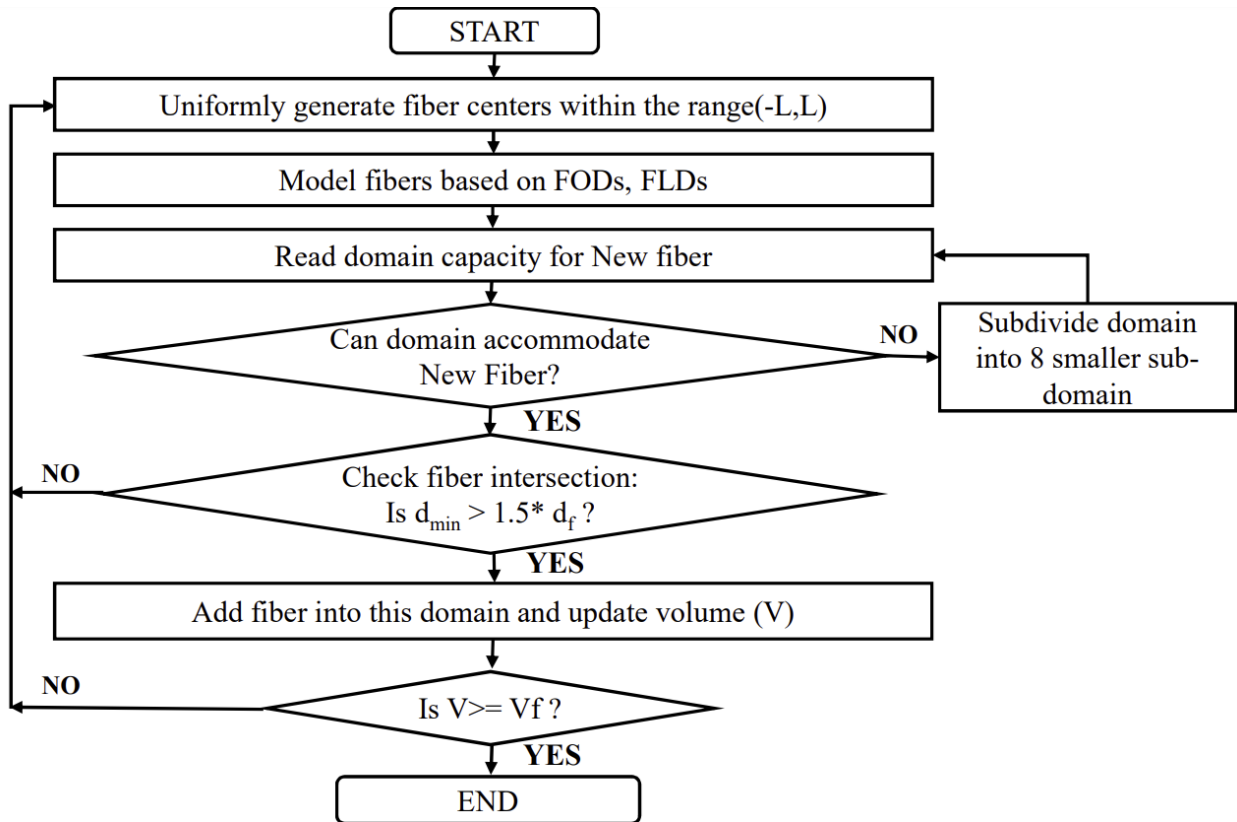
**Table A.4:** Three-term Prony series coefficients calibrated to the ABS matrix DMA master curve ( $T_{\text{ref}} = 298\text{K}$ ,  $R^2 = 0.996$ ).

| Term                | Modulus (MPa) | Relaxation time $\tau_i$ (s) |
|---------------------|---------------|------------------------------|
| $G_e$ (equilibrium) | 1350.6        | —                            |
| $G_1$ (branch 1)    | 199.1         | 0.00242                      |
| $G_2$ (branch 2)    | 44.4          | 0.0298                       |
| $G_3$ (branch 3)    | 94.1          | 0.0298                       |

## Appendix B

### Octree algorithm

As the domain reaches its  $n$ -fiber capacity, it is subdivided into eight smaller subdomains. The placement of the  $(n + 1)^{th}$  fiber is validated for intersections within its assigned subdomain. This recursive subdivision continues until the desired fiber volume fraction is achieved. The same approach is applied to model porosity. This method achieves the target packing density for fibers and pores, resulting in a 3D-RUC model.

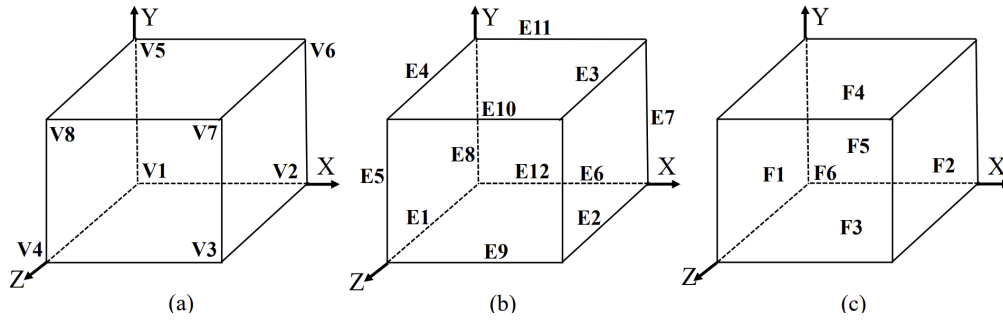


**Figure B.1:** Octree algorithm for constituent packing.

## Appendix C

### Periodic Boundary Conditions

Periodic Boundary Conditions (PBCs) are essential for finite element analysis (FEA)-based numerical homogenization using 3D-Repeated Unit Cells (RUCs). In ABAQUS/CAE, PBCs are implemented using multi-point constraint equations. They ensure the spatially repeating nature of the unit cell by relating the relative displacements between corresponding points on opposite faces of a cuboidal unit cell to the macroscopic strains.



**Figure C.1:** Vertex, edge, and face numbering convention for periodic boundary condition application. (a) Faces (b) Edges (c) Vertices.

For a cuboidal RUC with dimensions  $L \times B \times D$ , the relative displacements between a point  $P(x, y, z)$  on the boundary and its translated image  $P'(x', y', z')$  are given by the following relations:

$$u' - u = (x' - x)\epsilon_{xx}^o + (y' - y)\gamma_{xy}^o + (z' - z)\gamma_{xz}^o$$

$$v' - v = (y' - y)\epsilon_{yy}^o + (z' - z)\gamma_{yz}^o$$

$$w' - w = (z' - z)\epsilon_{zz}^o$$

Here,  $u, v, w$  are the displacements in the  $x, y, z$  directions, respectively, and  $\epsilon_{xx}^o, \epsilon_{yy}^o, \epsilon_{zz}^o, \gamma_{xy}^o, \gamma_{yz}^o, \gamma_{xz}^o$  are the macroscopic strain components. Quantities with a prime (') refer to the corresponding points in the adjacent unit cell.

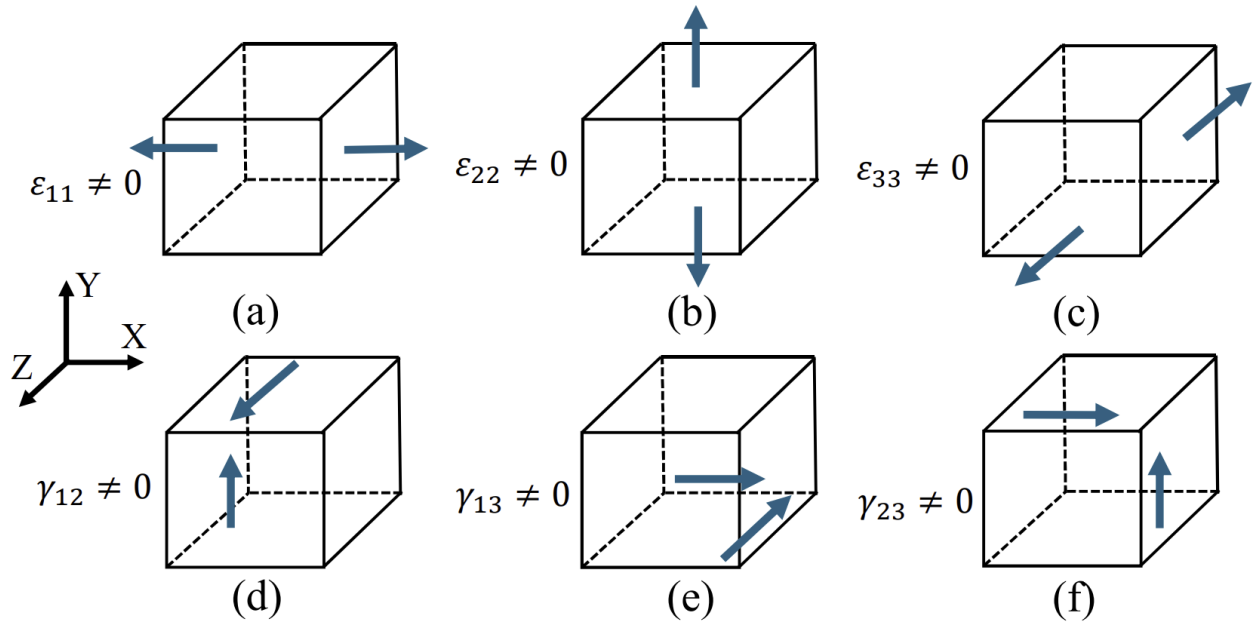
To enforce PBCs, the relative displacements between points on opposing faces are expressed as:

$$\begin{aligned}
\left( v|_{x=-\frac{L}{2}} - v|_{x=\frac{L}{2}} \right) &= 0 \\
\left( w|_{x=-\frac{L}{2}} - w|_{x=\frac{L}{2}} \right) &= 0 \\
\left( u|_{y=-\frac{B}{2}} - u|_{y=\frac{B}{2}} \right) &= B\epsilon_{xy}^o \\
\left( u|_{x=-\frac{L}{2}} - u|_{x=\frac{L}{2}} \right) &= L\epsilon_{xx}^o \\
\left( v|_{y=-\frac{B}{2}} - v|_{y=\frac{B}{2}} \right) &= B\epsilon_{yy}^o \\
\left( w|_{z=H} - w|_{z=0} \right) &= H\epsilon_{zz}^o \\
\left( w|_{z=-\frac{B}{2}} - w|_{z=\frac{B}{2}} \right) &= 0 \\
\left( u|_{z=H} - u|_{z=0} \right) &= H\epsilon_{xz}^o \\
\left( v|_{z=H} - v|_{z=0} \right) &= H\epsilon_{yz}^o
\end{aligned}$$

The faces of the RUC are further subdivided into vertex nodes, edge nodes, and internal face nodes (excluding vertices and edges). Three edges share each vertex, and two faces share each edge. Therefore, the constraint equations for edges and vertices are defined as follows:

| Face equations                                                                         | Edge equations                                                                                                                                                                                                                                                                                           | Vertex equations                                                                                                                                                                                                                                            |
|----------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| $U_{F2} - U_{F1} = U_{12}$<br>$U_{F4} - U_{F3} = U_{34}$<br>$U_{F6} - U_{F5} = U_{56}$ | $U_{E2} - U_{E1} = U_{12}$<br>$U_{E3} - U_{E1} = U_{12} + U_{34}$<br>$U_{E4} - U_{E1} = U_{34}$<br>$U_{E6} - U_{E5} = U_{12}$<br>$U_{E7} - U_{E5} = U_{12} + U_{56}$<br>$U_{E8} - U_{E5} = U_{56}$<br>$U_{E10} - U_{E9} = U_{34}$<br>$U_{E11} - U_{E9} = U_{34} + U_{56}$<br>$U_{E12} - U_{E9} = U_{56}$ | $U_{V2} - U_{V1} = U_{12}$<br>$U_{V3} - U_{V1} = U_{12} + U_{34}$<br>$U_{V4} - U_{V1} = U_{34}$<br>$U_{V5} - U_{V1} = U_{56}$<br>$U_{V6} - U_{V1} = U_{12} + U_{56}$<br>$U_{V7} - U_{V1} = U_{56} + U_{12} + U_{34}$<br>$U_{V8} - U_{V1} = U_{34} + U_{56}$ |

**Table C.1:** Equations for Faces, Edges, and Vertices



**Figure C.2:** All six load cases: three normal loads and three shear loads. (a) Along the x-axis, (b) Along the y-axis, (c) Along the z-axis, (d) Along yz plane, (e) Along zx plane, and (f) Along xy plane

### Effective property estimation

The stress and strain fields in the RUC are obtained via finite element analysis (FEA) for each load case, with volume-averaged stresses and strains calculated during post-processing using the following relations:

$$\bar{\sigma}_{ij} = \frac{1}{V} \sum_{e=1}^{N_e} \sum_{k=1}^{N_{int}} \sigma_{ij}^{k,e} V^{k,e} \quad (C.1)$$

$$\bar{\epsilon}_{ij} = \frac{1}{V} \sum_{e=1}^{N_e} \sum_{k=1}^{N_{\text{int}}} \epsilon_{ij}^{k,e} V^{k,e} \quad (\text{C.2})$$

where:

- $\bar{\epsilon}_{ij}$  is the volume-averaged strain tensor,
- $\bar{\sigma}_{ij}$  is the volume-averaged stress tensor,
- $N_e$  is the total number of elements,
- $N_{\text{int}}$  is the number of integration points per element,
- $\epsilon_{ij}^{k,e}$  is the strain tensor at the  $k$ -th integration point in the  $e$ -th element,
- $\sigma_{ij}^{k,e}$  is the stress tensor at the  $k$ -th integration point in the  $e$ -th element,
- $V^{k,e}$  is the volume or weight of the  $k$ -th integration point in the  $e$ -th element,
- $V = \sum_{e=1}^{N_e} \sum_{k=1}^{N_{\text{int}}} V^{k,e}$  is the total volume of the RUC.

The stiffness matrix  $C_{ijkl}$  is derived from the volume-averaged stresses and strains obtained for six load cases. The compliance matrix  $S_{ijkl}$  is obtained by inverting the stiffness matrix. The effective elastic properties of the unit cell are then expressed as follows:

$$E_1 = \frac{1}{S_{11}}, \quad E_2 = \frac{1}{S_{22}}, \quad E_3 = \frac{1}{S_{33}} \quad (\text{C.3})$$

$$\nu_{12} = -\frac{S_{12}}{S_{11}}, \quad \nu_{23} = -\frac{S_{23}}{S_{22}}, \quad \nu_{13} = -\frac{S_{13}}{S_{33}} \quad (\text{C.4})$$

$$G_{23} = \frac{1}{S_{44}}, \quad G_{13} = \frac{1}{S_{55}}, \quad G_{12} = \frac{1}{S_{66}} \quad (\text{C.5})$$

## Appendix D

### Parametric Finite-Element Validation of the Edge Weight Function

#### Parametric Finite-Element Validation of the Edge Weight Function

The edge weight function (Equation 2.8) embedded two physically motivated assumptions regarding pairwise fiber–fiber load transfer: (i) that matrix-mediated stress transfer between proximal fiber ends decayed with increasing fiber–fiber separation, and (ii) that load-transfer efficiency depended on relative fiber orientation through two distinct mechanisms — a dominant cosine-dependent axial shear-lag coupling and a residual orientation-independent transverse stress concentration. To confirm the physical basis of both terms in the CF–ABS material system at geometries consistent with  $\mu$ -CT observations, a systematic parametric finite-element study was conducted using a two-fiber RUC model.

The two-fiber configuration was chosen deliberately to isolate the pairwise interaction mechanism underlying the edge weight construction. As discussed in Section 5.2.3, Equation 5.9 governed physics at the level of individual fiber pairs; multi-fiber effects were handled through GNN message-passing aggregation. The two-fiber RUC therefore represented the minimal and most direct unit for validating the functional form of Equation 2.8 against observable pairwise stress transfer behavior in CF–ABS.

#### Two-fiber RUC model geometry

The model consisted of two cylindrical carbon fibers of equal length  $L_{f1} = L_{f2} = 50 \mu\text{m}$  and radius  $r_f = 4 \mu\text{m}$  embedded within an ABS matrix cuboid (Figure A2). The position and orientation of the first fiber were fixed in all analyses. The second fiber was varied such that the end-to-end separation  $L_{\text{gap}}$  ranged from 20 to 70  $\mu\text{m}$  in six increments, and the

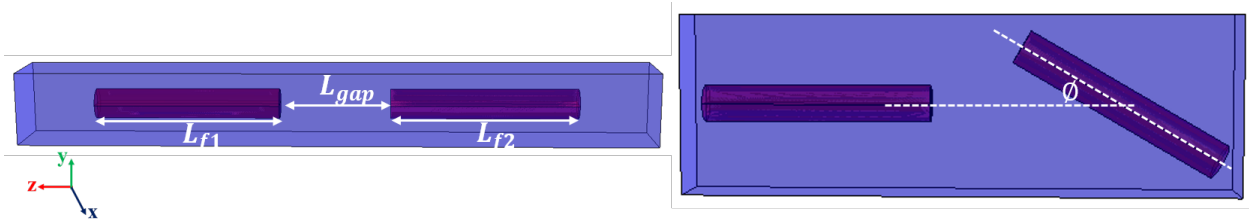
relative orientation angle  $\phi$  took values of  $0^\circ$ ,  $30^\circ$ ,  $60^\circ$ , and  $90^\circ$ , yielding 24 parametric cases. All cases were analyzed under uniaxial tensile strain  $\varepsilon_0 = 4\%$  applied along the primary fiber longitudinal direction, consistent with the homogenization protocol of Section 2.3.3. For angled configurations, the RUC dimensions were adjusted to accommodate the tilted fiber geometry while keeping fiber dimensions fixed ( $L_f = 50 \mu\text{m}$ ,  $r_f = 4 \mu\text{m}$ ), resulting in orientation-dependent fiber volume fractions:  $V_f = 7.86\%$  at  $0^\circ$ ,  $6.60\%$  at  $30^\circ$ ,  $5.60\%$  at  $60^\circ$ , and  $4.83\%$  at  $90^\circ$ .

### Interfacial shear stress extraction

For each parametric case, the interfacial shear stress resultant:

$$\tau = \sqrt{\tau_{12}^2 + \tau_{13}^2 + \tau_{23}^2} \quad (\text{D.1})$$

was extracted at the first matrix integration point immediately adjacent to the fiber–matrix interface along the full fiber axis from  $z = 0$  to  $z = L_f$ . The peak interfacial shear stress  $\tau_{\text{peak}}$  was identified for each case and, to enable consistent comparison across orientations with differing fiber volume fractions, normalized by the local  $V_f$  in Figure D.2 (b).



**Figure D.1:** Two-fiber RUC model of CF–ABS used for parametric shear-lag studies. **Left:**  $\phi = 0^\circ$  with fiber lengths  $L_{f1}$ ,  $L_{f2}$  and end-to-end separation  $L_{\text{gap}}$  labeled. **Right:**  $\phi = 30^\circ$  case.

### Validation of the distance-decay term.

Figure D.2 (a) presented the  $\tau(z)$  profiles for all 24 parametric cases. Across all four fiber orientations, interfacial shear stress concentrated at both fiber termini, confirming that end-to-end proximity governed pairwise load transfer regardless of orientation. Within each orientation group,  $\tau_{\text{peak}}$  decreased monotonically with increasing  $L_{\text{gap}}$ : at  $0^\circ$ ,  $\tau_{\text{peak}}$  decreased



by 15–22% as  $L_{gap}$  increased from 20 to 70  $\mu\text{m}$ ; a consistent monotonic trend was observed at 30°. This monotonic distance-dependent attenuation of pairwise stress transfer directly confirmed the physical basis of the exponential decay term  $\exp(-d_{pq}/L_c)$  in Equation 2.8. At 60° and 90°, the gap effect was negligible (less than 8%), confirming that the distance-decay mechanism was physically operative only when fibers were participating in axial shear-lag-governed load transfer — precisely the condition captured by the orientation-dependent component.

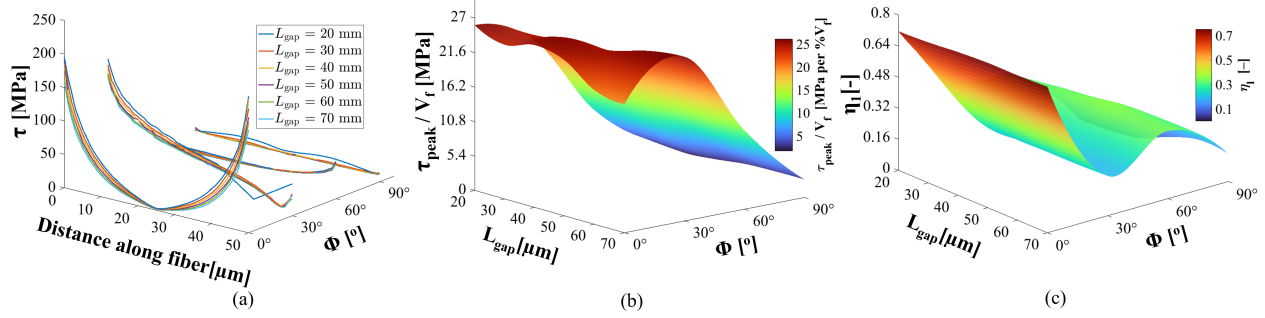
Validation of the two-component orientation factor.

Figure D.2 (b) revealed two physically distinct orientation regimes motivating the structure of  $(0.9|\mathbf{t}_p \cdot \mathbf{t}_q| + 0.10)$  in Equation 2.8. The  $V_f$ -normalized peak stress decreased systematically with misalignment — from 25–32 MPa per % $V_f$ , at 0° to 2–7 MPa per % $V_f$ , at 90° — an 8–10-fold reduction that validated the dominant cosine-dependent axial shear-lag term. Critically, even at 90° a non-negligible residual of 2–7 MPa per % $V_f$  persisted, arising from transverse stress concentration due to fiber–matrix stiffness mismatch rather than axial shear-lag. This residual was gap-insensitive (less than 8% variation across the full  $L_{gap}$  range), confirming its orientation-independent character. The observed residual fraction of 0.08–0.22 relative to the 0° maximum directly yielded the constant weight of 0.10 in Equation 2.8, with the complementary 0.9 assigned to the cosine-dependent term.

Fiber length efficiency

The fiber length efficiency  $\eta_l$ , presented as a three-dimensional surface in Figure D.2 (c), quantified the fraction of theoretical fiber stiffness contribution activated over the actual fiber length as directly observed from the two-fiber FEA results. Values of  $\eta_l = 0.72$ –0.75 for 0° fiber pairs confirmed that at the fiber lengths and separation distances present in the  $\mu$ -CT microstructure, pairwise fiber–fiber interaction was strongly active and a large fraction of available reinforcement efficiency was realized through end-to-end load transfer. For 30° fibers,  $\eta_l = 0.20$ –0.38, indicating partial activation consistent with the intermediate

orientation behavior described above. These values were reported directly as observable two-fiber FEA results characterizing pairwise interaction efficiency, without reference to single-fiber analytical models.



**Figure D.2:** Shear-lag response of two-fiber CF–ABS RVEs across all 24 parametric cases (four orientations  $\times$  six gap distances). (a) Absolute interfacial shear stress  $\tau(z)$  profiles extracted along the matrix–fiber interface path. Each set of curves corresponds to one fiber orientation ( $\phi = 0^\circ, 30^\circ, 60^\circ, 90^\circ$ ), with individual curves representing gap distances  $L_{\text{gap}} = 20\text{--}70$  mm. (b)  $V_f$ -normalised peak interfacial shear stress  $\tau_{\text{peak}}/V_f$  [MPa per % $V_f$ ] as a three-dimensional surface over the  $L_{\text{gap}}\text{--}\phi$  parameter space. Normalisation by local fiber volume fraction removes the geometric  $V_f$  variation introduced by the tilted-fiber box geometry. (c) Fiber length efficiency  $\eta_l$  estimated from the data-driven exponential decay of the normalised  $\tau$  profile, shown as a three-dimensional surface over the  $L_{\text{gap}}\text{--}\phi$  parameter space.

## Appendix E

### GNN Architecture Details and Training Procedure

#### GNN Architecture Details and Training Procedure

Figure E.1 provides a detailed schematic of the GNN architecture used for region-level microstructural embedding. The five major components were as follows.

##### GNN encoder

Fiber node features were 8-dimensional: fiber length, per-fiber volume fraction ( $V_{f,n}$ ), and three-dimensional start and end coordinates ( $\mathbf{x}_n^{(s)}, \mathbf{x}_n^{(e)}$ ). These features were projected from 8 to 64 dimensions via a linear layer with GELU activation. Two stacked graph convolutional layers (hidden dimension 64) with residual connections, layer normalization, and dropout (rate 0.2) performed degree-normalized weighted message passing (Eq. 5.9). Masked global mean pooling aggregated active node embeddings into a 64-dimensional graph-level representation, which was projected to a 16-dimensional cell embedding  $z_{\Omega_c} \in \mathbb{R}^{16}$  via a linear layer. An auxiliary head (Linear(16,32), ReLU, Dropout(0.1), Linear(32,4)) predicted the four normalized physics supervision targets: initial modulus, peak stress, peak strain, and post-peak softening rate.

##### LSTM

Input dimension was 21: four strain features ( $\varepsilon_t/\varepsilon_{pk}, (\varepsilon_t/\varepsilon_{pk})^2, (\varepsilon_t/\varepsilon_{pk})^3, \ln(1+\varepsilon_t/\varepsilon_{pk})$ ), plus  $V_{f,\Omega_c}$ , and the 16-dimensional  $z_{\Omega_c}$ . Two stacked LSTM layers with hidden dimension 128 and inter-layer dropout 0.25 processed the strain sequence.

Output network.

The LSTM hidden state ( $\mathbb{R}^{128}$ ) was concatenated with  $z_{\Omega_c}$  ( $\mathbb{R}^{16}$ ) via a skip connection at every time step, producing a 144-dimensional input to a three-layer residual MLP ( $144 \rightarrow 64 \rightarrow 32 \rightarrow 1$ , GELU activations), followed by Softplus to enforce non-negative stress predictions.

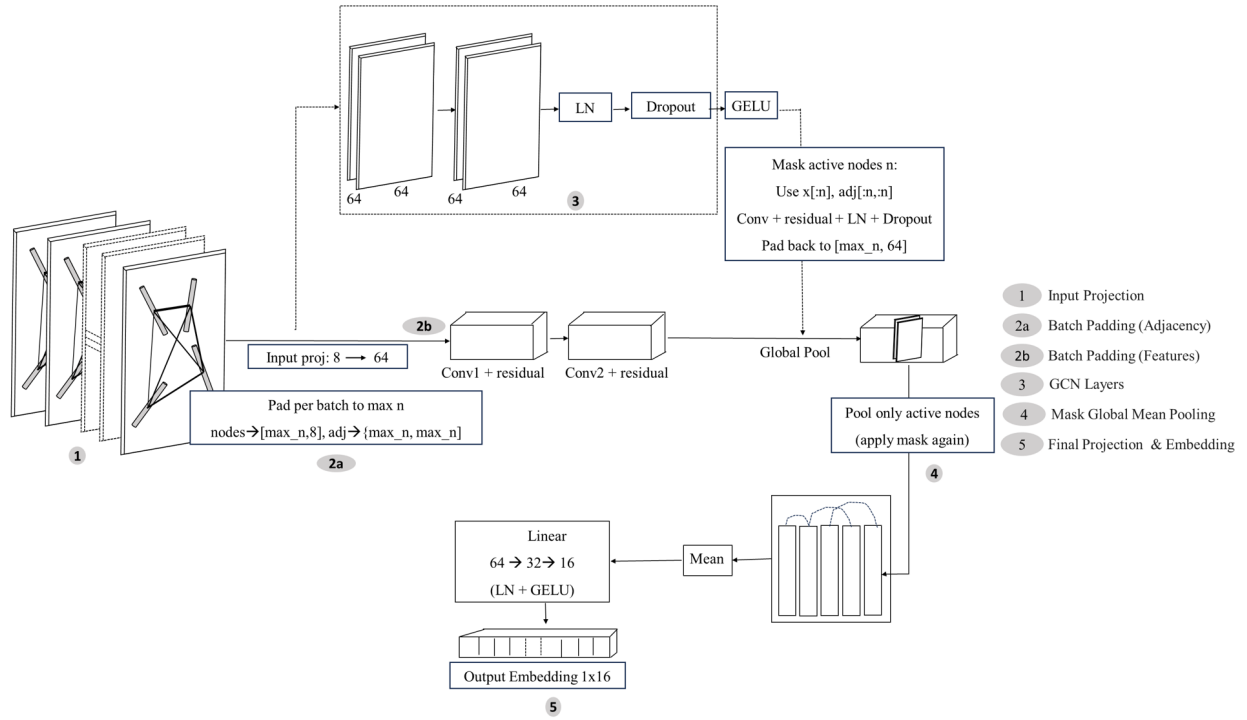
Random Forest physics regressor.

After GNN–LSTM convergence, a Random Forest regressor (300 trees, MultiOutputRegressor) was trained on the concatenation of  $V_{f,\Omega_c}$  and the frozen GNN embedding  $z_{\Omega_c}$  to predict the physical amplitude targets  $[\hat{E}, \hat{\sigma}_{pk}, \hat{\epsilon}_{pk}]$  for inference on unseen microstructures. The Random Forest was trained post-hoc using frozen embeddings because jointly trained auxiliary heads risk distribution shift on unseen cells; a non-parametric regressor applied to frozen embeddings provided more robust generalization without additional FE simulations.

Table A1 summarizes the complete training hyperparameters used for GNN–LSTM optimization.

*Batch size note:* A batch size of 1 was used because Voronoi cells contained variable numbers of fibers, making batched graph processing require variable-size node-feature padding of variable complexity. Processing cells sequentially avoided padding overhead while maintaining training stability through gradient norm clipping.

The 500-cell dataset was partitioned using stratified random shuffling (seed 42) rather than a sequential or sorted split, to ensure that training, validation, and testing subsets each contained representative distributions of fiber count, local volume fraction, and orientation. A sorted split would risk placing all low-fiber-count or high- $V_f$  cells within a single subset, producing an out-of-distribution validation set that yielded overoptimistic generalization estimates.



**Figure E.1:** Detailed schematic of the GNN encoder for cell-level microstructural embedding. Five processing stages are shown: (1) *Input Projection* — 8-dimensional node features projected to 64 dimensions via a linear layer with GELU activation; (2a–2b) *Batch Padding* — adjacency matrices and node feature tensors padded to  $[\max_n, \max_n]$  and  $[\max_n, 64]$  respectively, with padding masks identifying active nodes; (3) *GCN Layers* — two stacked graph convolutional layers with residual connections, layer normalization, and dropout (rate 0.2), operating on active nodes only (Equation 5.9); (4) *Masked Global Mean Pooling* — active node embeddings aggregated to a 64-dimensional graph-level representation; (5) *Final Projection and Embedding* — linear network ( $64 \rightarrow 32 \rightarrow 16$ , LN + GELU) producing the cell embedding  $z_{\Omega_c} \in \mathbb{R}^{16}$ .

**Table E.1:** Training hyperparameters used for GNN–LSTM model optimization.

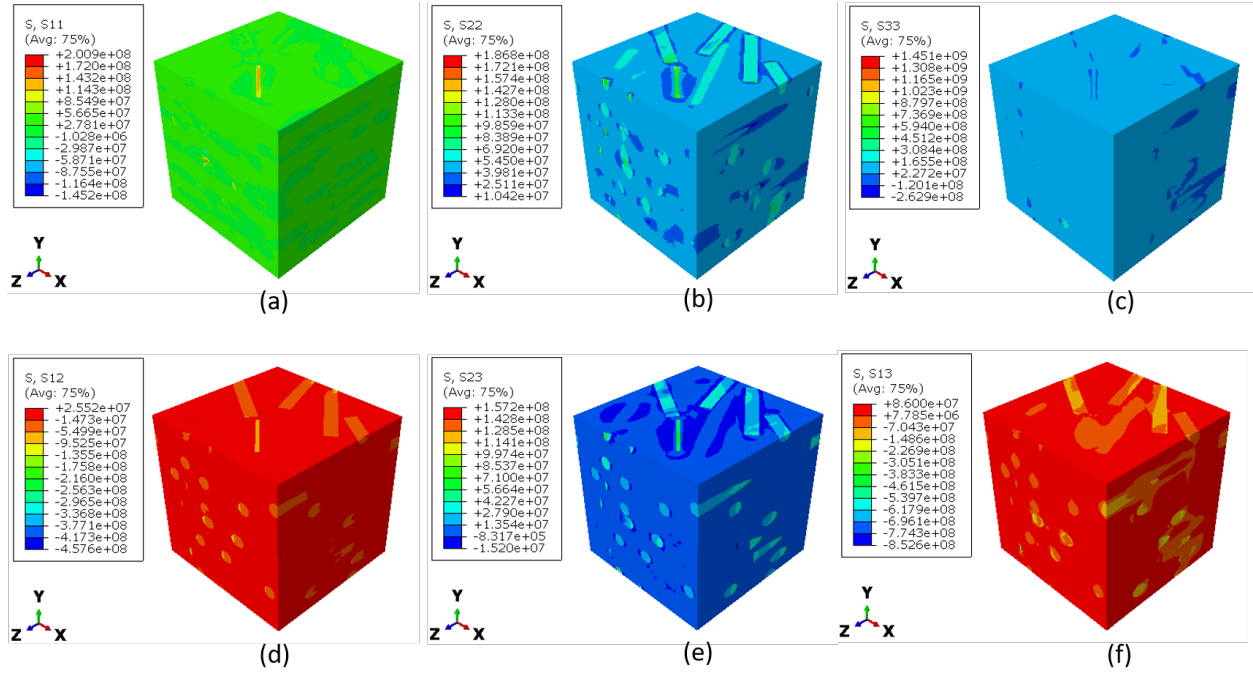
| Parameter                 | Value                                                |
|---------------------------|------------------------------------------------------|
| Optimizer                 | AdamW                                                |
| Initial learning rate     | $5 \times 10^{-4}$                                   |
| Weight decay              | $2 \times 10^{-4}$                                   |
| LR scheduler              | ReduceLROnPlateau (factor 0.5, patience 15 epochs)   |
| Minimum learning rate     | $10^{-6}$                                            |
| Gradient clip norm        | 1.0                                                  |
| Batch size                | 1                                                    |
| Maximum epochs            | 800                                                  |
| Early stopping patience   | 80 epochs (validation loss)                          |
| Primary loss              | Strain-weighted Huber ( $\delta = 0.1$ )             |
| $\lambda_{\text{mono}}$   | 0.05                                                 |
| $\lambda_{\text{smooth}}$ | 0.001                                                |
| $\lambda_{\text{zero}}$   | 0.02                                                 |
| $\lambda_{\text{aux}}$    | 0.3                                                  |
| $\lambda_{\text{peak}}$   | 0.5                                                  |
| Train / Val / Test split  | 70% / 15% / 15% (stratified random shuffle, seed 42) |
| GNN hidden dimension      | 64                                                   |
| GNN embedding dimension   | 16                                                   |
| GNN layers                | 2 (GCNConv + residual + LN + Dropout 0.2)            |
| LSTM hidden dimension     | 128                                                  |
| LSTM layers               | 2 (inter-layer Dropout 0.25)                         |
| RF estimators             | 300 (MultiOutputRegressor)                           |

## **Appendix F**

### **Full Six-Mode Constitutive Response of the Discrete Cell**

#### **Full Six-Mode Constitutive Response of the Discrete Cell**

To verify that the discrete-cell FE homogenization produces physically consistent constitutive responses under all six independent loading modes, Figure F.1 presents the full von Mises stress fields for a representative Voronoi cell subjected to three normal and three in-plane shear loading cases. Under normal loading in the x- and y-directions (Figure F.1a–b), stress is distributed relatively uniformly through the matrix, consistent with matrix-dominated transverse response and the comparatively small contribution of off-axis fibers to transverse stiffness. Under normal loading in the z-direction (fiber-aligned, Figure F.1c), pronounced stress localization occurs along fiber axes, confirming efficient axial load transfer. Under in-plane shear loading (Figure F.1d–f), stress concentrations develop in matrix ligaments between adjacent fibers, consistent with shear-lag-governed inter-fiber coupling. These results confirm that the discrete-cell FE implementation correctly captures the anisotropic, topology-sensitive constitutive behavior that the GNN–LSTM surrogate is trained to reproduce.



**Figure F.1:** Full six-mode constitutive response of a representative discrete Voronoi cell from finite-element homogenization. Von Mises stress fields are shown under: (a) normal loading in the x-direction ( $\sigma_{11}$ ); (b) normal loading in the y-direction ( $\sigma_{22}$ ); (c) normal loading in the fiber-aligned z-direction ( $\sigma_{33}$ ); (d) in-plane shear in the x-y plane ( $\sigma_{12}$ ); (e) out-of-plane shear in the y-z plane ( $\sigma_{23}$ ); (f) out-of-plane shear in the x-z plane ( $\sigma_{13}$ ). The contrasting stress patterns under normal versus shear loading confirm that the cell's constitutive response is strongly anisotropic and topology-sensitive.