An Empirically Validated Multiscale Continuum Damage Model for Thermoplastic Polymers Subjected to Variable Strain Rates

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An empirically validated multiscale continuum damage model for thermoplastic polymers subjected to variable strain rates

By
David K. Francis

A Dissertation
Submitted to the Faculty of Mississippi State University
in Partial Fulfillment of the Requirements
for the Degree of Doctorate of Philosophy
in Mechanical Engineering
in the Department of Mechanical Engineering

Mississippi State, Mississippi
May 2013
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David K. Francis

2013
An empirically validated multiscale continuum damage model for thermoplastic polymers subjected to variable strain rates

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Approved:

<table>
<thead>
<tr>
<th>Mark F. Horstemeyer</th>
<th>Jean-Luc Bouvard</th>
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<tr>
<td>Professor</td>
<td>Assistant Professor</td>
</tr>
<tr>
<td>Mechanical Engineering</td>
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<tr>
<td>(Major Professor)</td>
<td>(Committee Member)</td>
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<tr>
<th>Thomas E. Lacy Jr.</th>
<th>Hongjoo Rhee</th>
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<tr>
<td>Professor</td>
<td>Assistant Research Professor</td>
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<td>Aerospace Engineering</td>
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<tr>
<td>(Committee Member)</td>
<td>(Committee Member)</td>
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<tr>
<th>Kalyan K. Srinivasan</th>
<th>Sarah A. Rajala</th>
</tr>
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<tr>
<td>Associate Professor</td>
<td>Dean of the James Worth</td>
</tr>
<tr>
<td>Mechanical Engineering</td>
<td>Bagley College of Engineering</td>
</tr>
<tr>
<td>(Graduate Coordinator)</td>
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</table>
Name: David K. Francis

Date of Degree: May 10, 2013

Institution: Mississippi State University

Major Field: Mechanical Engineering

Major Professor: Dr. Mark F. Horstemeyer

Title of Study: An empirically validated multiscale continuum damage model for thermoplastic polymers subjected to variable strain rates

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Candidate for Degree of Doctorate of Philosophy

This dissertation proposes a modified internal state variable (ISV) inelastic damage model that was motivated by experimental structure–property relations of thermoplastics. In particular, a new damage model was developed for glassy, amorphous thermoplastics. ISV evolution equations are defined through thermodynamics, kinematics, and kinetics for isotropic damage arising from two different inclusion types: pores and particles. The damage arising from the particles and crazes is accounted for by three processes: damage nucleation, growth, and coalescence. Damage nucleation is defined as the number density of voids/crazes. The associated ISV rate equation is a function of stress state, molecular weight, fracture toughness, particle size, particle volume fraction, temperature, and strain rate. The damage growth is based upon a single void growing and its growth is defined by an ISV rate equation that is a function of stress state, strain rate sensitivity, and strain rate. The coalescence ISV equation enables interaction between voids and crazes and is a function of the nearest
neighbor distance between voids/crazes, size of voids/crazes, temperature, and strain rate. The damage arising from pre-existing voids employs the Cocks–Ashby void growth rule. The total void volume fraction is a summation of the damage arising from particles, pores, and crazes. Micromechanical modeling results for a single void compare well to experimental findings garnered from the literature. This formulation is then implemented into a finite element analysis. For damage evolution, comparisons are made between a one-dimensional material point simulator and a three-dimensional finite element (FE) simulation. Finally, good agreement is found between impact experiments and FE impact simulations using the implemented model.

Key words: Damage modeling, Thermoplastics, Internal State Variable, Constitutive Behavior, Viscoplastic Material
DEDICATION

I dedicate this work contained within these pages to the Triune God: the Father, Son, and Holy Spirit; for in Him, all things hold together—including polymers. The efforts of the past few years have been out of both obedience and joy. Obedience in that God told the first human to “subdue the earth” and all scientific and engineering efforts since then are simply an attempt to follow that command by working with what he has given us. Joy in that God has gifted his children to do that task. Any good or scientific progress contained in these pages can only be attributed to his goodness in gifting me and the community around me. And any unhelpful or incorrect ideas can be attributed to the fact that this creation, including the human mind, is fallen and corrupt: “for now we see in a mirror dimly.” Toti Deo Gloria!
ACKNOWLEDGEMENTS

If it takes a village to raise a child, as they say, what kind of community does it take to raise a graduate student? I’m not sure I have the complete answer, but I’d like to take the following paragraphs to express my thankfulness towards that diverse community that has molded me as a scientist, engineer, experimentalist, theorist, coder, writer, leader, student, etc.

First and foremost, I would like to thank and acknowledge my major adviser Mark Horstemeyer. Truly there are few parts of my life where his influence cannot be seen. He is devoted in creating the complete and well-rounded engineer. His vision for what a PhD degree represents is what initially drew me in and I am thankful for the journey I’ve traveled under his leadership.

My thanks go to others on my committee: To Jean-Luc Bouvard for his patience, teaching, and leadership as the lead of my funded research, and to Thomas Lacy Jr. for introducing me to continuum mechanics, for his vision in analyzing engineering issues from multiple angles, and for teaching me how to be a more effective technical communicator.

There are many others at CAVS who have been helpful and supportive: Doug Bammann with his insatiable appetite for inelasticity, Youssef Hammi the go-to researcher for all material modeling coding issues, Mark Tschopp for instilling a drive
for excellence in all aspects of research, Stephen Horstemeyer for his laboratory aid, and Andy Oppedal for sharing in the joy of typography. The teeming hordes of CAVS grad students have also made this experience much fun. I’ll simply list some of them in the order I remember meeting them because there are too many stories to tell in this short section: Raj Prabu, Neil Williams, Jason Simmons, Jason Fountain, Jairus Bernard, Wilburn Whittington, Crawford Baird, Radu Florea, Yustianto Tjiptowidjojo, Brian Denton, Denver Seely, William Lawrimore, NaYeon Lee, Kyle Johnson, and Jeremiah Deang.

Finally, I must thank and praise my wonderful wife Emily. She has been a constant source of encouragement and help in the ups and downs. She’s taken on many roles during my schooling. For the first few years she had a full-time job, but now she has the bigger responsibility of raising our one-year-old, Lucy. As Paul wrote “I thank my God every time I remember you.” Looking back down this five year path we’ve traveled together makes me want to pick up the pace to see what around the next bend . . . and we will.

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The opinions of the authors expressed herein do not necessarily state or reflect those of the United States Government or the DoA and shall not be used for advertising or product endorsement purposes. The authors would also like to thank the Center for Advanced Vehicular Systems (CAVS) at Mississippi State University for their support. This work was performed at the Center for Advanced Vehicular Systems (CAVS) at Mississippi State University. CAVS acknowledges the collaboration provided through the SIMULIA Research & Development program under which licenses of Abaqus were provided.
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LIST OF SYMBOLS, ABBREVIATIONS, AND NOMENCLATURE

ABS  Acrylonitrile butadiene styrene

FE  Finite element

GTN  Gurson–Tvergaard–Needleman model

ILD  Intervoid ligament distance

ISV  Internal state variable

PC  Polycarbonate

PP  Polypropylene

SEM  Scanning electron microscope

\( a_\eta \)  Stress state parameter for particle–void nucleation

\( b_\eta \)  Stress state parameter for particle–void nucleation

\( \bar{b} \)  Stress resulting from the tensorial strain-like ISV for large strain hardening at the intermediate configuration \( \vec{B} \), second rank tensor

\( b' \)  Deviatoric part of \( b \) at the intermediate configuration \( \vec{B} \), second rank tensor

\( \mathcal{B} \)  Current configuration

\( \mathcal{B}_0 \)  Reference configuration

\( \vec{B} \)  First intermediate configuration

\( \vec{\mathcal{B}} \)  Second intermediate configuration
\( \bar{B} \) Third intermediate configuration

\( B_p \) Left Cauchy–Green plastic deformation second rank tensor

\( c \) Coalescence

\( \dot{c} \) Coalescence rate

\( c_\eta \) Stress state parameter for particle–void nucleation

\( C_i \) Material parameters \((i = 1, 2, \ldots, 18)\)

\( C_V \) Heat capacity per unit volume

\( C_{\alpha_1} \) Material parameter for \( \bar{\alpha} \)

\( C_{\alpha_2} \) Material parameter for \( \bar{\alpha} \)

\( C_b \) Stress state parameter for \( \bar{b} \)

\( C_{\text{BUD}} \) Coefficient for Budiansky void growth model

\( C_{\text{coal}_1} \) Coalescence parameter due to crazing from particles

\( C_{\text{coal}_2} \) Coalescence parameter due to general matrix crazing

\( C_{\text{coal}_3} \) Impingement coalescence parameter

\( C_{c\theta} \) Temperature material parameter for void impingement

\( C_{\bar{\kappa}_1} \) Stress state parameter for \( \bar{\kappa}_1 \)

\( C_{\bar{\kappa}_2} \) Stress state parameter for \( \bar{\kappa}_2 \)

\( C_{\eta_c\theta} \) Temperature material parameter for craze nucleation

\( C_{\eta_p\theta} \) Temperature material parameter for particle nucleation

\( C \) Total Cauchy-Green deformation tensor at the reference configuration, second rank tensor
\(C_p\) Plastic Cauchy-Green deformation tensor at the reference configuration, second rank tensor

\(\bar{C}_d\) Damage Cauchy-Green deformation tensor at the intermediate configuration \(\bar{B}\), second rank tensor

\(\bar{C}_t\) Thermal Cauchy-Green deformation tensor at the intermediate configuration \(\bar{B}\), second rank tensor

\(\bar{C}_e\) Elastic Cauchy-Green deformation tensor at the intermediate configuration \(\bar{B}\), second rank tensor

\(d\) Average particle diameter for particle nucleation

\(d_0\) Average particle diameter

\(d_\eta\) Stress state parameter for craze nucleation

\(d_{\text{NN}}\) Nearest neighbor distance

\(\bar{D}\) Total rate of deformation tensor at intermediate configuration, second rank tensor

\(\bar{D}_d\) Damage rate of deformation tensor at the intermediate configuration \(\bar{B}\), second rank tensor

\(\bar{D}_p\) Plastic rate of deformation tensor at the intermediate configuration \(\bar{B}\), second rank tensor

\(\bar{D}_t\) Thermal rate of deformation tensor at the intermediate configuration \(\bar{B}\), second rank tensor

\(\bar{D}_r\) Combined elastic, plastic, and thermal rate of deformation tensor at the intermediate configuration \(\bar{B}\), second rank tensor
\( e_\eta \) Stress state parameter for craze nucleation

\( \bar{e}_V \) Specific energy per unit volume

\( \dot{e}_V \) Time rate of change of the specific energy per unit volume

\( E \) Young’s modulus

\( E_1 \) Material parameter for Young’s modulus

\( E_{\text{ref}} \) Reference material parameter for Young’s modulus

\( E_V \) Volumetric strain

\( E \) Total Green-Lagrangian strain tensor at the reference configuration, second rank tensor

\( E_p \) Plastic Green-Lagrangian strain tensor at the reference configuration, second rank tensor

\( \tilde{E}_d \) Damage Green-Lagrangian strain tensor at the intermediate configuration

\( \tilde{B} \), second rank tensor

\( \tilde{E}_t \) Thermal Green-Lagrangian strain tensor at the intermediate configuration

\( \tilde{B} \), second rank tensor

\( \tilde{E}_e \) Elastic Green-Lagrangian strain tensor at the intermediate configuration

\( \tilde{B} \), second rank tensor

\( \dot{\tilde{E}}_e \) Elastic Green-Lagrangian strain rate tensor at the intermediate configuration

\( \tilde{B} \), second rank tensor

\( f \) Initial volume fraction of particles

\( f_\eta \) Stress state parameter for craze nucleation

\( f_\theta \) Temperature dependent variable for thermal expansion

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\( F_t \)  Singular value found in isotropic diagonal tensor \( F_t \)

\( F \)  Total deformation gradient tensor

\( F_e \)  Elastic deformation gradient tensor

\( F_d \)  Volumetric plastic (damage) deformation gradient tensor

\( F_p \)  Deviatoric plastic deformation gradient tensor

\( F_t \)  Thermal deformation gradient tensor

\( F_c \)  Combined elastic, plastic, and thermal deformation gradient tensor

\( g \)  Generalized length scale parameter for craze nucleation

\( g_0 \)  Temperature dependent function for \( \xi_1 \)

\( h \)  Strain rate function for craze nucleation

\( H_1 \)  Hardening modulus for \( \xi_1 \)

\( H_2 \)  Hardening modulus for \( \xi_2 \)

\( I_1 \)  First invariant of stress

\( I_2 \)  Second invariant of stress

\( I_3 \)  Third invariant of stress

\( J \)  Total Jacobian

\( J_d \)  Volumetric plastic (damage) Jacobian

\( J_e \)  Elastic Jacobian

\( J_p \)  Deviatoric plastic Jacobian

\( J_t \)  Thermal Jacobian

\( J_1 \)  First invariant of the deviatoric stress

\( J_2 \)  Second invariant of the deviatoric stress
\( J_3 \)  
Third invariant of the deviatoric stress

\( k \)  
Scalar thermal conductivity

\( k_B \)  
Boltzmann’s constant

\( K \)  
Bulk modulus

\( K_{lc} \)  
Critical fracture toughness

\( l \)  
Velocity gradient in the current configuration

\( l_e \)  
Elastic velocity gradient at the current configuration, second rank tensor

\( l_d \)  
Damage velocity gradient at the current configuration, second rank tensor

\( l_p \)  
Plastic velocity gradient at the current configuration, second rank tensor

\( l_t \)  
Thermal velocity gradient at the current configuration, second rank tensor

\( l_* \)  
Combined elastic, plastic, and thermal velocity gradient at the current configuration, second rank tensor

\( \bar{L} \)  
Velocity gradient at the intermediate configuration \( \bar{B} \), second rank tensor

\( \bar{L}_e \)  
Elastic velocity gradient at the intermediate configuration \( \bar{B} \), second rank tensor

\( \bar{L}_d \)  
Damage velocity gradient at the intermediate configuration \( \bar{B} \), second rank tensor

\( \hat{L}_d \)  
Damage velocity gradient at the intermediate configuration \( \bar{B} \), second rank tensor

\( L_p \)  
Plastic velocity gradient at the intermediate configuration \( B \), second rank tensor
\( \mathbf{L}_t \)  Thermal velocity gradient at the intermediate configuration \( \mathbf{B} \), second rank tensor

\( \mathbf{L}_s \)  Combined elastic, plastic, and thermal velocity gradient at the intermediate configuration \( \mathbf{B} \), second rank tensor

\( m \)  Strain rate sensitivity parameter

\( M_w \)  Molecular weight

\( \mathbf{M} \)  Mandel stress, second rank tensor

\( \mathbf{M}' \)  Deviatoric part of the Mandel stress, second rank tensor

\( n \)  Parameter for molecular chain segment cooperative behavior

\( n_{\text{ed}} \)  Entanglement density

\( \mathbf{n}_i \)  Principal directions of the right stretch tensor

\( \mathbf{N}_p \)  Direction of plastic flow at the intermediate configuration \( \mathbf{B} \), second rank tensor

\( p \)  Hydrostatic pressure

\( \mathbf{Q} \)  Heat flux per area, second rank tensor

\( r_p \)  Plastic zone size

\( r_s \)  Static recovery

\( R \)  universal gas constant

\( R_s \)  Static recovery

\( \mathbf{R}_V \)  Heat source per unit volume

\( \mathbf{R} \)  Rotation second rank tensor

\( \dot{s}_V \)  Specific entropy per unit volume
\( \dot{s}_V \) Time rate of change of the specific entropy per unit volume

\( \bar{S} \) Second Piola–Kirchhoff stress at the intermediate configuration \( \bar{B} \), second rank tensor

\( \tilde{S}' \) Deviatoric part of the Second Piola–Kirchhoff stress at the intermediate configuration \( \bar{B} \), second rank tensor

\( \tilde{t}_d \) Value for each diagonal of the isotropic tensor \( \bar{U}_d \)

\( T_g \) Glass transition temperature

\( U \) Right stretch second rank tensor

\( \bar{U}_d \) Damage right stretch tensor at the intermediate configuration \( \bar{B} \), second rank tensor

\( \tilde{U}_d \) Damage right stretch tensor at the intermediate configuration \( \bar{B} \), second rank tensor

\( V \) Activation volume

\( V_V \) Void volume

\( \dot{V} \) Volume at the intermediate configuration \( \bar{B} \)

\( \bar{V} \) Volume at the intermediate configuration \( \bar{B} \)

\( \bar{W} \) Total spin tensor

\( \bar{W}_d \) Damage spin second rank tensor at the intermediate configuration \( \bar{B} \)

\( \bar{W}_e \) Elastic spin second rank tensor at the intermediate configuration \( \bar{B} \)

\( \bar{W}_p \) Plastic spin second rank tensor at the intermediate configuration \( \bar{B} \)

\( \bar{W}_t \) Thermal spin second rank tensor at the intermediate configuration \( \bar{B} \)
\( \bar{W} \) Combined elastic, plastic, and thermal spin second rank tensor at the intermediate configuration \( \bar{B} \)

\( Y \) Yield surface

\( z \) Material constant for impingement

\( \bar{\alpha} \) Strain-like ISV for large strain hardening at the intermediate configuration \( \bar{B} \), second rank tensor

\( \alpha_p \) Pressure sensitivity parameter

\( \alpha_{th} \) Coefficient of thermal expansion

\( \gamma \) Shear strain

\( \dot{\gamma}_p \) Scalar plastic shear strain rate

\( \dot{\gamma}_{0p} \) Scalar reference plastic shear strain rate

\( \Delta H_\beta \) Activation energy

\( \Delta \theta \) Change in temperature

\( \varepsilon \) Scalar strain

\( \dot{\varepsilon} \) Scalar strain rate

\( \zeta \) Arrhenius temperature dependence for craze nucleation

\( \eta_{\text{craze}} \) Number of craze nucleation sites per volume

\( \dot{\eta}_{\text{craze}} \) Time rate of change of \( \eta_{\text{craze}} \)

\( \eta_{\text{particles}} \) Number of void nucleation site from particles

\( \dot{\eta}_{\text{craze}} \) Time rate of change of \( \eta_{\text{particles}} \)

\( \theta \) Temperature

\( \theta_{\text{ref}} \) Reference temperature
$\kappa_1$ Stress-like quantity related to $\xi_1$, scalar

$\kappa_2$ Stress-like quantity related to $\xi_2$, scalar

$\lambda$ Lamé’s first parameter

$\lambda_i$ Principal values of the right stretch tensor ($i = 1, 2, 3$)

$\lambda_i^\alpha$ Principal values of $\bar{\alpha}$ ($i = 1, 2, 3$)

$\lambda_L$ Network locking stretch

$\lambda_p$ Effective plastic stretch

$\mu$ Shear modulus

$\mu_B$ Rubbery modulus incorporating the backstress

$\mu_R$ Rubbery modulus

$\nu$ Single void growth

$\dot{\nu}$ Single void growth rate

$\nu_p$ Poisson’s Ratio

$\bar{\xi}_1$ Internal strain induced by entanglement points at the intermediate configuration $\bar{B}$, scalar

$\dot{\bar{\xi}}_1$ Internal strain rate induced by entanglement points at the intermediate configuration $\bar{B}$, scalar

$\bar{\xi}^*$ Internal strain-like qualities for chain slip at the intermediate configuration $\bar{B}$, scalar

$\dot{\bar{\xi}}^*$ Internal strain rate-like qualities for chain slip at the intermediate configuration $\bar{B}$, scalar

$\bar{\xi}_{sat}$ Saturation value for $\bar{\xi}^*$ at the intermediate configuration $\bar{B}$, scalar
**\(\xi_0^*\)** Beginning value for \(\xi^*\) at the intermediate configuration \(\bar{\mathcal{B}}\), scalar

**\(\xi_2\)** Internal strain induced by large strain chain alignment/coiling at the intermediate configuration \(\bar{\mathcal{B}}\), scalar

**\(\dot{\xi}_2\)** Internal strain rate induced by large strain chain alignment/coiling at the intermediate configuration \(\bar{\mathcal{B}}\), scalar

**\(\bar{\xi}_2^{\text{sat}}\)** Saturation value for \(\bar{\xi}_2\) at the intermediate configuration \(\bar{\mathcal{B}}\), scalar

**\(\bar{\pi}\)** Effective pressure at the intermediate configuration \(\bar{\mathcal{B}}\), scalar

**\(\bar{\Pi}\)** A set of kinematic-like ISVs, no rank

**\(\rho\)** Density

**\(\sigma_e\)** von Mises equivalent stress

**\(\sigma_y\)** Yield stress

**\(\sigma\)** Cauchy stress at the current configuration \(\mathcal{B}\), second rank tensor

**\(\dot{\sigma}\)** Cauchy stress rate at the current configuration \(\mathcal{B}\), second rank tensor

**\(\ddot{\sigma}\)** Co-rotational Jaumann rate of the Cauchy stress at the current configuration \(\mathcal{B}\), second rank tensor

**\(\sigma'\)** Deviatoric part of the Cauchy stress

**\(\tau\)** First Piola–Kirchhoff stress at the reference configuration \(\mathcal{B}_0\), second rank tensor

**\(\bar{\tau}\)** Equivalent shear stress at the intermediate configuration \(\bar{\mathcal{B}}\), scalar

**\(\bar{\tau}_{\text{eq}}\)** Modified equivalent shear stress at the intermediate configuration \(\bar{\mathcal{B}}\), scalar

**\(\phi\)** Total void volume fraction (damage)

**\(\dot{\phi}\)** Time rate of change for the total void volume fraction
\( \dot{\phi}_{\text{total}} \) Time rate of change for the total void volume fraction

\( \dot{\phi}_{\text{crazing}} \) Void volume fraction from crazing

\( \dot{\phi}_{\text{crazing}} \) Time rate of change of the void volume fraction from crazing

\( \dot{\phi}_{\text{particles}} \) Void volume fraction from particle damage

\( \dot{\phi}_{\text{particles}} \) Time rate of change of the void volume fraction from particle damage

\( \dot{\phi}_{\text{pores}} \) Void volume fraction from pre-existing pores

\( \dot{\phi}_{\text{pores}} \) Time rate of change of the void volume fraction from pre-existing pore growth

\( \chi \) Triaxiality function for Cocks–Ashby function

\( \bar{\psi}_V \) Helmholtz free energy per unit volume

\( \dot{\bar{\psi}}_V \) Time rate of change of the Helmholtz free energy per unit volume

\( \omega \) Ratio of plastic work transferred to temperature change

Mathematical Symbols

\( \otimes \) Tensor direct product symbol

\( : \) Scalar product of two tensors symbol

\( \cdot \) Inner product symbol

\( \exp() \) Exponential function

\( \text{tr}() \) Trace of a tensor

\( \sinh() \) Hyperbolic sine function
CHAPTER 1

INTRODUCTION

1.1 Summary

The goal of this dissertation is to develop a macroscale damage continuum model coupled to an inelastic thermoplastic model. The research objectives of this dissertation are to expand the experimental database and improve computational resources for thermoplastics by (i) creating a thermoplastic material database with mechanical behavior and fracture surface morphology for three materials—acrylonitrile butadiene styrene (ABS), polycarbonate (PC), and polypropylene (PP), (ii) developing an inelastic macroscale material model to capture viscoelastic, plastic, thermal, and damage dissipative behavior, and (iii) implementing the model into a finite element (FE) code that is validated by experimental impact testing data. The experimental database contains various dependencies’ (e.g., temperature, stress state, strain rate) effect on three thermoplastics under mechanical loads. From mechanical testing, material properties will be derived and correlated to the structure observed from tensile fracture surfaces. Beginning with the work from Bouvard et al. [2013], isotropic damage will be included in the kinematics and thermodynamics formulation in such a way to naturally degrade the elastic modulus, in a manner similar to Bammann and Solanki [2010] where each internal state variable (ISV) is multiplied by a damage
deformation entity. Finally, the model will be implemented into a FE code. The model will be calibrated with a material point simulator and validated with impact experiments for PC.

1.2 Intellectual Merit

This project will be the first to develop an inelastic damage macroscale model that employs microstructural data to predict fracture and failure for a thermoplastic. Failure criteria exist for other thermoplastic continuum models in the literature, but none robust enough to take into account initial void fraction, number of voids nucleated due to particles, nucleation density of crazes, void growth due to particles, volume fraction of crazes, nearest neighbor distances between voids, and the interaction effects between each void producing mechanism. The damage model is then be implemented into a user subroutine for a FE analysis.

1.3 Broader Impacts

The inclusion of a physically based ISV inelastic–damage model for thermoplastics will be the first into the polymer community. Horstemeyer and Wang [2003] demonstrated how robust modeling can predict failure and lead to optimization for metals components. In the same spirit, accurate modeling is needed for thermoplastics for both failure prediction and component optimization as they are being used more widely in structural and vehicular designs. While thermoplastic modeling is continually improving in predicting mechanical behavior, damage modeling for thermoplastics has remained mainly basic and phenomenological. Once thermoplastic
fracture is characterized, models can then incorporate fracture data so that designs using thermoplastics can then be optimized, thus leading to both lighter weight and safer vehicles and structures.

1.4 Background

Damage modeling in polymers is becoming much more common in the literature over the past few decades. For thermoplastics, the bulk of modeling damage in polymers employs the classic work by Gurson [1977], which uses a yield condition that is a function of the void volume fraction. Lazzeri and Bucknall [1993, 1995] proposed and applied a modified Gurson model to rubber-toughened polymers to account for dilatational yielding. Jeong and Pan [1995] generalized Gurson’s yield criterion to take into account pressure sensitivity, which reduced to Coulomb’s yield criterion when the void volume fraction was zero. Later, Jeong [2002] implemented the same model into an FE code and also added tensile hydrostatic pressure effects. To account for rupture due to vapor pressure in polymer electronic packaging components, Guo and Cheng [2002] implemented the modified Gurson–Tvergaard model [Tvergaard, 1989], which employs a microscopic stress tensor and the void volume fraction as ISVs, within an FE code. Damage in rubber-modified epoxies was modeled by both Kody and Lesser [1999] and Imanaka et al. [2003] with Gurson-type constitutive equations. Because the Gurson formulation was originally applied to metals, which fracture at small strains compared to ductile polymers, using this formulation overestimates the yield stress in polymers. Therefore, Pijnenburg and der Giessen [2001] modified the model to account
elasticity effects and shear banding. The same issue of polymer fracture at large strains is also dealt with in Steenbrink et al. [1997] and Steenbrink and van der Giessen [1997]. Recently, Zaïri et al. [2008] extended the Bodner–Partom model [Bodner and Partom, 1975] with a modified Gurson model [Tvergaard, 1981] in a thorough experimental/computational approach to accurately predict the inelastic mechanical behavior including damage. Challier et al. [2006] studied polyvinylidene fluoride (PVDF) fracture mechanisms and then used mechanical testing and microscopic observations to fit the Gurson–Tvergaard–Needleman (GTN) model (Tvergaard [1982]; Tvergaard and Needleman [1984]) in an FE analysis. Laiarinandrasana et al. [2009] studied mechanical behavior of PVDF at lower temperatures, which altered the mechanical response by increasing the yield stress and decreasing elongation to failure. They fit the GTN model to correspond to the material properties’ temperature dependence following Khan et al. [2006]. The GTN model was also compared to Bridgman tests to capture triaxiality effects in a polyamide by Boisot et al. [2011].

Other failure criteria, apart from Gurson, have been developed as well for polymers. Gearing and Anand [2004a] employed two parameters into an FE analysis to distinguish between brittle and ductile failure. In their model, if a local elastic volumetric strain threshold was passed, brittle fracture ensued, but if an effective plastic stretch threshold was passed, ductile fracture ensued. In the FE analysis, once a critical strain was reached in an element, the element was removed. To model crazing and molecular chain-scission related failure, a similar failure criterion was developed by Gearing and Anand [2004b] where craze breakdown or molecular chain-scission occurred when a
critical strain value was reached. Benzerga et al. [2009] used the critical craze stress approach from Gearing and Anand [2004b] to simulate crack growth between fibers and voids in fiber-reinforced thermosetting and thermoplastic polymer composites.

When developing an ISV formulation for damage progression in polymers, a metal plasticity and damage paradigm may be used to establish an initial framework. In particular, void nucleation, void growth, and void coalescence (void impingement and shear banding from the void sheet mechanism) have been observed. For example, Fond and Schirrer [1996] studied the void nucleation mechanisms analytically on rubber toughened polymers. Later, Fond [2001] presented a thorough review on void growth models for rubbers, which all started from the basis of continuum damage mechanics in metals. While making a distinction between void growth in rubbers compared to metals, Fond [2001] pointed to void instability in rubber due to coalescence effects. G’Sell et al. [2002] showed experimentally that for glassy thermoplastic and reinforced-blends experience damage progression via crazing and void nucleation, growth, and coalescence. G’Sell et al. [2002] showed clearly that damage progression caused the onset of localization and necking similar to metals (cf., Horstemeyer [2000]; Horstemeyer and Ramaswamy [2000]). The failure analysis by Francis et al. [2012] on a PP component showed pre-existing voids exacerbated failure. After studying spherulite sizes in PP, Way et al. [1974] concluded that spherulite size in semi-crystalline polymers is analogous to the grain size in metals. Hagerman [1973] studied the crazing rates in an ABS material.
1.5 Dissertation Structure

The following dissertation is divided into five chapters. Chapter 2 begins with an experiential study of three thermoplastics in which the strain rate dependence, temperature dependence, and stress state dependence on the mechanical behavior are investigated. Quasi-static and high strain rate compression behavior is studied first and then quasi-static tension and torsion analyses follow. Chapter 2 ends with a section regarding fracture morphology of tensile tests. The experimental study lays the foundation for the theory developed later. In Chapter 3, a thermomechanical inelastic ISV model that incorporates damage for glassy, amorphous thermoplastics is proposed. The development of the model is broken down into kinematic, thermodynamic, and kinetic parts. Chapter 4 documents the implementation, calibration, and validation of the model. Finally, in Chapter 5, a summary is given and a future work section highlights four distinct areas to explore. Two appendices are given to supplement the work. The first appendix discusses the improper usage of stress invariants commonly used in solid mechanics. The second appendix documents the inelastic model used in Chapter 5.
CHAPTER 2

EXPERIMENTAL RESULTS FROM QUASI-STATIC AND HIGH STRAIN RATE MECHANICAL TESTING OF POLYCARBONATE, ACRYLONITRILE BUTADIENE STYRENE, AND POLYPROPYLENE

2.1 Material

A combination of variable strain rate compression, tensile, and torsion tests were performed on three thermoplastics: PC, ABS, and isotactic PP. The three thermoplastics in this study have fundamentally different microstructures but are all commonly used in engineering design. Table 2.1 lists the supplier and material information pertinent for each thermoplastic. PCs are amorphous clear thermoplastics that exhibit good dimensional stability, electrical properties, thermal stability, and impact strengths. They are used in many applications, such as canopies for supersonic aircraft, bubble helmets for astronauts, break-resistant windows, and bullet-resistant laminates for armored vehicles. ABSs are common thermoplastics used to make lightweight, rigid, molded products such as piping, musical instruments, toys, golf club head inserts, automotive body parts, wheel covers, and protective head gear. ABSs are copolymers consisting of an amorphous styrene-acrylonitrile (SAN) thermoplastic copolymer with a grafted rubbery phase. SAN is a simple random copolymer composed of styrene and acrylonitrile. PPs are semi-crystalline thermoplastics used
for automotive, household, and construction industry applications. The chemical structures of ABS, PC, and PP are illustrated in Figure 2.1.

2.2 Compression Testing
2.2.1 Experimental Procedures
2.2.1.1 Quasi-Static Strain Rate Testing

Cylindrical compression specimens were machined from 25.4 mm thick sheet material of PC, ABS, and PP. The specimens had a diameter of 12.7 mm and a height of 6.35 mm. The axis of each specimen was parallel to the thickness direction (see Figure 2.2 for a schematic of specimen orientation). These specimens were used in both quasi-static and high strain rate compression testing. Quasi-static strain rate testing was conducted on an Instron 5882 load frame. For each test, specimens were compressed along the specimen’s axis between two platens up to 100% true strain and then unloaded completely. For each strain rate and temperature, three repeat tests were performed. To investigate the quasi-static strain rate sensitivity of each thermoplastic, three engineering strain rates were used: 0.1/s, 0.01/s, and 0.001/s. To explore the environmental temperature sensitivity of each thermoplastic, four different temperatures were used: a sub-zero Celcius temperature, ambient tempera-

Table 2.1 Thermoplastic material suppliers, manufacturers, and grade name details.

<table>
<thead>
<tr>
<th>Material</th>
<th>Supplier</th>
<th>Manufacturer</th>
<th>Grade Name</th>
</tr>
</thead>
<tbody>
<tr>
<td>PC</td>
<td>McMaster</td>
<td>Sheffield Plastics</td>
<td>HYZOD®</td>
</tr>
<tr>
<td>ABS</td>
<td>McMaster</td>
<td>King Plastic Corp.</td>
<td>ABS copolymer</td>
</tr>
<tr>
<td>PP</td>
<td>McMaster</td>
<td>Poly-Hi Solidur Inc.</td>
<td>White polypropylene</td>
</tr>
</tbody>
</table>
Figure 2.1 Chemical structures of three thermoplastics.

The chemical structure of (a) polycarbonate, (b) acrylonitrile butadiene styrene, and (c) polypropylene.
ture, and two temperatures above room temperature. For PC and ABS, for the two temperatures above room temperature, one was below $T_g$ and one was above $T_g$. Each material’s $T_g$ was determined from dynamic mechanical analysis testing. The testing temperatures and $T_g$ are listed in Table 2.2.

To minimize barreling and minimize friction, molybdenum disulfide lubricant was spread on the contact points between the platens and specimen. For tests performed at temperatures other than room temperature, an environmental chamber was placed around the platens and specimen. The temperature was held at the desired temperature for one hour before loading to guarantee thermal equilibrium in the specimen.

Table 2.2 Test matrix for temperature dependent uni-axial compression tests. All temperatures in degrees Celsius.

<table>
<thead>
<tr>
<th>Material</th>
<th>$T_g$</th>
<th>Cold</th>
<th>Ambient</th>
<th>$T &gt;$ Ambient</th>
<th>$T \gg$ Ambient</th>
</tr>
</thead>
<tbody>
<tr>
<td>PC</td>
<td>151</td>
<td>-20</td>
<td>25</td>
<td>100</td>
<td>160</td>
</tr>
<tr>
<td>ABS</td>
<td>105</td>
<td>-20</td>
<td>25</td>
<td>50</td>
<td>110</td>
</tr>
<tr>
<td>PP</td>
<td>16</td>
<td>-20</td>
<td>25</td>
<td>70</td>
<td>120</td>
</tr>
</tbody>
</table>
2.2.1.2 High Strain Rate Compression Testing

The concept of high rate testing that led to the Split-Hopkinson Pressure Bar (SHPB) began with John Hopkinson experimenting with stress waves in iron wires [Hopkinson, 1872a,b]. Hopkinson [1905], Hopkinson [1914], Davies [1948], and Kolsky [1949] all contributed thereafter towards the advancement of the compression SHPB technique. For a historical review of the SHPB, see Gama et al. [2004].

As shown in Figure 2.3, the compression SHPB setup consists of a striker, incident, and transmitted bar. For all SHPB tests in this study, the three bars used were made of 7075 aluminum. The specimen geometry is the same as what was used in quasi-static testing. The aluminum bars have a diameter of 38.1 mm. The striker, incident, and transmitted bars are 0.46 m, 1.83 m, and 0.91 m in length, respectively. To begin the test, a compressed gas launches the striker bar into the incident bar. From the impact of the striker bar, a stress wave then propagates through the incident bar. The stress wave is purely elastic (assuming the velocity of the striker was slow enough to no induce plasticity in the aluminum bars) in the incident and transmitted

![Diagram of SHPB setup](image)

Figure 2.3 The layout of a compression Split Hopkinson Pressure Bar.
bars and therefore a theoretical solution exists for the propagation of the stress wave as well as the dispersion of the wave as it travels along the bars.

Next, a strain gage on the incident bar records the strain as the wave passes. The specimen is sandwiched between the incident and transmitted bar and held in place by a molybdenum disulfide lubricant on both side, which was the same lubricant used for quasi-static testing. When the stress wave reaches the interface between the incident bar and the specimen, part of the wave is transmitted into the specimen while part of the wave is reflected back towards the incident bar strain gage. The magnitudes of the reflected and transmitted waves are determined by the acoustic impedance difference between the specimen material compared to the incident and transmitted bar material. After traveling through the specimen, the wave continues into the transmitted bar where a second strain gage records the strain wave. To conclude the test, a momentum stop connected to the back end of the transmitted bar deadens the wave. The strains are recorded at a rate of 2 MHz for the duration of the test. Figure 2.4 shows the strain–time data output from the strain gages during a test. Stress–strain curves are then generated from knowledge of the specimen geometry, bar material properties, bar geometries, and the strain–time histories.

Using the SHPB compression testing method described above, specimens are not loaded at a constant strain rate. In contrast to quasi-static testing from this study, there is no load frame to continually apply a constant load or strain rate. Figure 2.5 shows how the strain rate of PC changes through its loading. The strain rate reported for each test was generally found by averaging the rate over the first half of the test.
For the test shown in Figure 2.5, the strain rate was averaged from about 3% to 30% 
true strain for a strain rate of approximately 1950/s.

### 2.2.2 Quasi-Static Strain Rate Compression Test Results

The quasi-static true stress–true strain behavior of PC is shown in Figures 2.6 and 2.7. Each curve is the average of three tests. PC exhibits the same four regions 
mentioned for ABS: an initial linear elastic response, a nonlinear transition to a 
yield stress, strain softening, and strain hardening. Figure 2.6 groups the PC true 
stress–true strain data by strain rate. As expected, as temperature decreases, the 
yield stress increases. In Figures 2.6(a), (b), and (c), when $T = -20^\circ C$ and $25^\circ C$, the 
strain softening and hardening trends are nearly parallel; however, when $T = 100^\circ C$,

![Strain–time history from a SHPB test on a polycarbonate specimen at a strain rate of 2800/s.](image)

Figure 2.4  Strain–time history from a SHPB test on a polycarbonate specimen at a strain rate of 2800/s.
the strain softening was more abrupt and less strain hardening occurred. For all temperatures and strain rates, as strain increased, the variability increased. Figure 2.7 groups the PC true stress–true strain data by temperature. In Figures 2.7(a), (b), and (c), minimal strain rate dependence is observed below $T_g$. As the strain rate increased, the yield stresses increased. The variability is large enough where the error bands overlap at strains above 60%. At each temperature below $T_g$, while the strain hardening behavior at $\dot{\varepsilon} = 0.001/s$ and $\dot{\varepsilon} = 0.01/s$ had nearly parallel slopes, the strain hardening behavior at $\dot{\varepsilon} = 0.1/s$ deviates from the pattern. Instead of the strain hardening increasing at increased strain rates, after a certain threshold ($\dot{\varepsilon} > 0.01/s$ in this case) the strain hardening decreases. This phenomena was also observed by Arruda et al. [1995] for Poly(methyl methacrylate) in which they theorized that the

![Figure 2.5](image)

Figure 2.5 Strain rate fluctuations during a SHPB test on a polycarbonate specimen.

The dashed line indicates the average strain rate reported at 1950/s.
lack of strain hardening at higher strain rates is due to internal heat generation. At temperatures above $T_g$, shown in Figure 2.7(d), PC behaved in a rubber-like nature. No yield stress is observed and the material only hardens.

The quasi-static true stress–true strain behavior of ABS is shown in Figures 2.8 and 2.9. Four distinct regions are observed for ABS when the temperature is below $T_g$ (see Table 2.2): an initial linear elastic response followed by a non-linear transition curve to yield stress. Next, strain softening occurs with subsequent strain hardening. The true stress–true strain data contained in Figures 2.8 and 2.9 are identical; however, Figure 2.8 groups four temperatures at a given strain rate per plot and Figure 2.9 groups three quasi-static strain rates at a given temperature per plot. Grouping the data in this manner enables trends to be easily established. Also, each true stress–true strain curve is the average of three tests and the error bars show the variation from the average to the minimum and maximum stress for individual data sets. In Figures 2.8(a), (b), and (c), the yield peaks increase in proportion to one another as temperature decreases. As the strain rate increases, the amount of strain softening increases. The amount of variation generally increases as the strain increases. As expected, from the true stress–true strain curves in Figures 2.9(a), (b), and (c), the yield peaks increase proportionally as the strain rate increases. The same $\dot{\varepsilon} = 0.1/s$ strain hardening phenomenon observed in PC is also present in ABS. In Figure 2.9(d), the true stress–true strain behavior of ABS at a temperature above $T_g$ is shown. The behavior is profoundly different compared to the compression tests below $T_g$. The yield stresses are much less distinct and are an order of magnitude less than those
below \( T_g \). No strain softening occurs and immediate strain hardening occurs after yielding.

The quasi-static true stress–true strain behavior of PP is shown in Figures 2.10 and 2.11. Each curve is the average of three tests. From Figure 2.10, it is shown that PP generally did not strain harden in compression, except at \( T = -20^\circ\text{C} \) when the strain rate was 0.1/s or 0.001/s. Given the variational error for these two exceptions, sometimes these two cases do not strain harden either. As expected, when temperature or strain rates increased, the yield stress increased. In Figure 2.11(b), the strain softening crossover for \( \dot{\varepsilon} = 0.1/\text{s} \) occurred in the same manner as ABS and PC. Although all tests were above \( T_g \) (except for \( T = -20 \)), the crystalline microstructure prohibited rubber-like behavior that was observed in PC and ABS at high temperatures.
Figure 2.6 Compressive true stress–true strain behavior for polycarbonate for varying temperatures.

Compressive true stress–true strain behavior for polycarbonate for $T = -20, 25, 100, \text{ and } 160{\degree}\text{C}$ at (a) $\dot{\varepsilon} = 0.1/s$, (b) $\dot{\varepsilon} = 0.01/s$, and (c) $\dot{\varepsilon} = 0.001/s$. 
Figure 2.7  Compressive true stress–true strain behavior for polycarbonate for varying strain rates.

Compressive true stress–true strain behavior for polycarbonate for $\dot{\varepsilon} = 0.1$, 0.01, and 0.001/s at (a) $T = -20^\circ$C, (b) $T = 25^\circ$C, (c) $T = 100^\circ$C, and (d) $T = 160^\circ$C.
Figure 2.8  Compressive true stress–true strain behavior for acrylonitrile butadiene styrene for varying temperatures.

Compressive true stress–true strain behavior for acrylonitrile butadiene styrene for $T = -20, 25, 50,$ and $110\, ^\circ C$ at (a) $\dot{\varepsilon} = 0.1/\text{s}$, (b) $\dot{\varepsilon} = 0.01/\text{s}$, and (c) $\dot{\varepsilon} = 0.001/\text{s}$.
Figure 2.9  Compressive true stress–true strain behavior for acrylonitrile butadiene styrene for varying strain rates.

Compressive true stress–true strain behavior for acrylonitrile butadiene styrene for $\dot{\varepsilon} = 0.1$, 0.01, and 0.001/s at (a) $T = -20^\circ\text{C}$, (b) $T = 25^\circ\text{C}$, (c) $T = 50^\circ\text{C}$, and (d) $T = 110^\circ\text{C}$. 
Figure 2.10  Compressive true stress–true strain behavior for polypropylene for varying temperatures.

Compressive true stress–true strain behavior for polypropylene for $T = -20, 25, 70,$ and $120\,^\circ C$ at (a) $\dot{\varepsilon} = 0.1$/s, (b) $\dot{\varepsilon} = 0.01$/s, and (c) $\dot{\varepsilon} = 0.001$/s.
Figure 2.11  Compressive true stress–true strain behavior for polypropylene for varying strain rates.

Compressive true stress–true strain behavior for polypropylene for $\dot{\varepsilon} = 0.1$, 0.01, and 0.001/s at (a) $T = -20^\circ$C, (b) $T = 25^\circ$C, (c) $T = 70^\circ$C, and (d) $T = 120^\circ$C.
2.2.3 High Strain Rate Compression Test Results

Mechanical and thermal high strain rate behavior of PC can be observed in Figure 2.12. In Figure 2.12(a), the true stress–true strain behavior of PC at three high strain rates obtained from the SHBP (\(\varepsilon = 1900, 1500,\) and 850/s) are compared to two tests at quasi-static strain rates from the previous section (\(\varepsilon = 0.1\) and 0.001/s). Each high rate curve is not the average of multiple tests because repeating exact strain rates was not possible on the SHPB. As the strain rate increased, the yield stress increased. Also, as strain rate increased, the amount of strain softening decreased. The high rate true stress–true strain curves in Figure 2.12(a) compare well to Siviour et al. [2005]. The post test specimen temperature is shown in Figure 2.12(b). At \(\varepsilon \approx 800/s\), the total amount of true strain was 18\% and the change in temperature was about 10°C. At \(\varepsilon \approx 2000/s\), the total amount of true strain was 50\% and the change in temperature was about 55°C. The yield stresses for all the PC SHPB tests are shown in Figures 2.12(c) and (d) as a function of the applied strain rate. The variability is large enough in Figure 2.12(c) to conclude that the yield stress linearly increased with strain rate. However, if the same data is place on a log plot along with the quasi-static compressive yield stresses, as shown in Figure 2.12(d), the linear relationship would not be adequate to fit all points. Typically, to fit this yield stress–strain rate trend, a two stage Ree–Eyring model [Ree and Eyring, 1958] is employed. This model assumes two separate relaxation modes called \(\alpha\) and \(\beta\). The \(\alpha\) mode fits the quasi-static data and the \(\beta\) mode fit the high rate data. The result of this model provides two linear
regions on log plot with an elbow connecting them. In the Ree–Erying model [Ree and Eyring, 1958], which follows,

\[
\frac{\sigma_y}{T} = A_\alpha \left( \ln \left( 2C_\alpha \dot{\varepsilon} + \frac{Q_\alpha}{RT} \right) \right) + A_\beta \sin^{-1} \left( \left( \frac{2C_\beta \dot{\varepsilon} \exp \left( \frac{Q_\beta}{RT} \right)}{RT} \right) \right)
\]  

(2.1)

where \( \sigma_y \) is the yield stress, \( T \) is the absolute temperature, \( Q_\alpha \) and \( Q_\beta \) are activation energies, and \( R \) is the universal gas constant. \( A_\alpha, A_\beta, C_\alpha, \) and \( C_\beta \) are material parameters. See Mulliken [2004] for a review of this model. While this model is commonly used in polymer modeling, this approach to fitting only the yield peaks will not be employed for any predictive simulations.

Mechanical and thermal high strain rate behavior of ABS can be observed in Figure 2.13. In Figure 2.13(a), the true stress–true strain behavior of three high strain rates obtained from the SHBP (\( \dot{\varepsilon} = 1900, 1500, \) and \( 600/s \)) are compared to two quasi-static strain rates from the previous section (\( \dot{\varepsilon} = 0.1 \) and 0.001/s when \( T = 25^\circ C \)). Each high rate curve is from a single tests because repeating exact strain rates was not possible on the SHPB. As expected, as the strain rate increased, the yield stress increased. The strain softening behavior is relatively similar between the high strain rates and quasi-static rates. At \( \dot{\varepsilon} = 1900/s \), ABS experienced larger strain hardening compared to \( \dot{\varepsilon} \leq 0.1/s \). The high rate true stress–true strain behavior in Figure 2.13(a) compared well to Mulliken and Boyce [2006]. At the end of each test, the specimen’s surface temperature was immediately measured using an infrared thermometer. The surface temperatures obtained are plotted in Figure 2.13(b). The ambient testing temperature was 25°C. The slowest strain rate obtained on the SHPB
of 600/s produced a total of 15% true strain and caused a 10 °C rise in specimen surface temperature. The fastest strain rates of approximately 2250/s produced a total of 55% true strain and caused a 75–80 °C rise in specimen surface temperature. The increase in specimen temperature in Figure 2.13(b) appears linear. The ABS yield stress–strain dependent rate behavior is shown in Figures 2.13(c) and (d). Two distinct slopes in Figure 2.13(d) can be observed for the quasi-static yield stresses and the high rate yield stresses resulting in an “elbow” around \( \dot{\varepsilon} = 10/s \).

Mechanical and thermal high strain rate behavior of PP can be observed in Figure 2.14. In Figure 2.14(a), the true stress–true strain behavior of PC at three high strain rates obtained from the SHBP (\( \dot{\varepsilon} = 1900, 1500, \) and 850/s) are compared to two tests at quasi-static strain rates from the previous section (\( \dot{\varepsilon} = 0.1 \) and 0.001/s). The high rate true stress–true strain curves in Figure 2.14(a) compare well to Okereke et al. [2012]. In the quasi-static compression tests, as the strain rate increased, the strain hardening decreased. From SHPB tests, minimal strain hardening is observed. The yield stress also increased as the strain rate increased. The post test specimen temperature in Figure 2.14(b) is similar to PC. When \( \dot{\varepsilon} \approx 800/s, \Delta T = 10^\circ C \) and the total true strain is 15%. When \( \dot{\varepsilon} \approx 2000/s, \Delta T = 55^\circ C \) and the total true strain is 55%. The “elbow” trend in Figure 2.14(d) is located around \( \dot{\varepsilon} = 30/s \).
Figure 2.12 Measurements of high rate and quasi-static compressive behavior for polycarbonate.

Measurements of high rate and quasi-static compressive behavior for polycarbonate for (a) true stress–true strain, (b) temperature as a function of strain rate, (c) yield stress as a function of strain rate, and (d) yield stress as a function of strain rate along with quasi-static data (logarithmic).
Figure 2.13 Measurements of high strain rate and quasi-static compressive behavior for acrylonitrile butadiene styrene.

Measurements of high strain rate and quasi-static compressive behavior for acrylonitrile butadiene styrene for (a) true stress–true strain, (b) temperature as a function of strain rate, (c) yield stress as a function of strain rate, and (d) yield stress as a function of strain rate along with quasi-static data (logarithmic).
Figure 2.14  Measurements of high rate and quasi-static compressive behavior for polypropylene.

Measurements of high rate and quasi-static compressive behavior for polypropylene for (a) true stress–true strain, (b) temperature as a function of strain rate, (c) yield stress as a function of strain rate, and (d) yield stress as a function of strain rate along with quasi-static data (logarithmic).
2.3 Tension Testing
2.3.1 Experimental Procedures

For uni-axial quasi-static tension testing, the “Standard Test Method for Tensile Properties of Plastics” from ASTM D638-03 was followed, using the “Type I” specimen geometry, which is illustrated in Figure 2.15. ABS, PC, and PP coupon specimens were tested in tension. The stress–strain behavior as well as the force–extension behavior are reported due to extensive necking in each material. Necking is a geometric phenomenon associated with strain localizations in thermoplastics. See Figure 2.16 for a visual representation of necking. At stages (a) and (b), in Figure 2.16, the material behaves elastically and no necking occurs. At stage (c), yielding has just occurred and the cross-sectional area of the gage section becomes non-uniform. The smaller cross-sectional area that forms is called a neck, which softens the material. As the neck stabilizes, the neck cross-section remains constant and more material is drawn into the neck (stages (d) and (e)). Therefore, because of profound necking, all plots of the true stress–true strain behavior in this study end at the beginning of the strain softening regime where necking begins. The overall stress–strain behavior is calculated from the total displacement and applied force over an assumed uniform cross-section; thus, stress and strain would not be an accurate description of the entire specimen. Force–extension curves are included in this section in order to relate fracture surface morphology (given in Section 2.5) to elongation to failure.
Figure 2.15  Specimen geometry of flat tensile specimens.

The thickness is 3.2 mm. All units above are in millimeters.

Figure 2.16  Necking progression in a ductile polymer.
2.3.2 Tension Test Results

The true stress–true strain quasi-static behavior of PC is shown in Figure 2.17. For the three strain rates (0.1, 0.01, and 0.001/s) reported in Figure 2.17(a), as the strain rate increased, the yield stress increased. Each curve is the average of three tests and little variation is observed at the yield stresses. The elastic modulus appears strain rate independent under quasi-static tensile strain rates. The true stress–true strain temperature dependent behavior at −20, 25, and 75°C for PC is shown in Figure 2.17(b). As expected, as the temperature decreased, the yield stress increased. Also, the yield peak and subsequent strain softening occurs at at lower strains as the temperature increases.

![Figure 2.17](image_url)

Figure 2.17  Tensile true stress–true strain behavior for polycarbonate.

Tensile true stress–true strain behavior for polycarbonate displaying (a) strain rate dependence at $T = 25\,^\circ\text{C}$ and (b) temperature dependence at $\dot{\varepsilon} = 0.01/\text{s}$. 

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The true stress–true strain quasi-static behavior of ABS is shown in Figure 2.18. Each curve is an average of three tests. From the three quasi-static strain rates (0.1, 0.01, and 0.001/s) in Figure 2.18(a), no rate dependence on the elastic modulus is observed. As the strain rate increases, the yield peaks slightly increase. The experimental error associated with each yield peak is large enough where yield peaks for individual tests at different strain rates overlapped. However, from the temperature dependent true stress–true strain curves ($T = -20, 25, 50^\circ C$) while $\dot{\varepsilon} = 0.01/s$ in Figure 2.18(b), as the temperature increases, the yield peak decreases. The elastic modulus was not affected at temperatures between 25 $^\circ C$ and 50 $^\circ C$. Below 25 $^\circ C$, the modulus increases. Sub-zero Celsius temperatures embrittles the material by decreasing chain mobility; hence, the elastic modulus and yield peak increases.
Figure 2.18  Tensile true stress–true strain behavior for acrylonitrile butadiene styrene.

Tensile true stress–true strain behavior for acrylonitrile butadiene styrene displaying (a) strain rate dependence at $T = 25^\circ C$ and (b) temperature dependence at $\dot{\varepsilon} = 0.01/s$.

The true stress–true strain quasi-static behavior of PP is shown in Figure 2.19. In Figure 2.19(a), for the three strain rates reported (0.05, 0.01, and 0.001/s), as the strain rate increases, the slope of the nonlinear region between the elastic region and yield increases. The yield stress also increases as the strain rate increases. Each curve reported is the average for three tests. The experimental scatter is large enough in Figure 2.19(a) where the true stress–true strain response at $\dot{\varepsilon} = 0.01$ and 0.001/s for individual tests overlapped. The true stress-true strain behavior as temperature varied ($-20$, $25$, and $75^\circ C$) is shown in Figure 2.19(a). When temperature increased, the elastic modulus and yield peak decreased. The strain softening regime and
yield peak also occurred at lower strain values as the temperature decreased. This trend is opposite of the PC behavior. While the exact reason for this opposing behavior is unknown to the author, perhaps PC’s amorphous microstructure and PP’s semi-crystalline microstructure cause this phenomenon.

Figure 2.19  Tensile true stress–true strain behavior for polypropylene.

Tensile true stress–true strain behavior for polypropylene displaying (a) strain rate dependence at $T = 25^\circ C$ and (b) temperature dependence at $\dot{\varepsilon} = 0.01/s$.

The force–extension curves provide a clearer post-yield picture than the stress–strain curves due to extensive necking. The each force–extension curve in the following three figures (2.21, 2.20, and 2.22) is the average of three tests. Two different types of errors are shown for each curve. Similar to the true stress–true strain data, vertical maximum and minimum errors bar show the experimental variation in the force. At
the end of each curve, a horizontal error bar stretching in the positive displacement direction shows the amount of scatter in the elongation to failure. The average curves ends at the first fractured test. The horizontal error stretches to the displacement value for the test with the largest elongation to failure.

The force–displacement behavior of PC is shown in Figure 2.20. Three quasi-static strain rates of 0.1, 0.01, and 0.001/s were tested. The strain rate of 0.1/s produced the greatest elongation to failure. Instead of the elongation to failure decreasing as the strain rate decreased, the specimens at $\dot{\varepsilon} = 0.01/s$ failed at shorter extensions than tests at $\dot{\varepsilon} = 0.001/s$. The mechanism causing this behavior is unknown. No temperature dependence tests are shown due to inaccuracies found later in the data.

![Figure 2.20](image)

**Figure 2.20** Tensile force–extension behavior for polycarbonate displaying strain rate dependence at $T = 25^\circ C$.

The force–displacement behavior of ABS is shown in Figure 2.21. Three quasi-static strain rates of 0.1, 0.01, and 0.001/s were tested and the results are shown
in Figure 2.21(a). The strain rate of 0.01/s produced the greatest elongation to failure. Even when considering the scatter in the elongation to failure, the largest elongations at \( \dot{\varepsilon} = 0.1 \) and 0.001/s are still less than the shortest elongation to failure at \( \dot{\varepsilon} = 0.01/s \). Also, the specimens tested at \( \dot{\varepsilon} = 0.1 \) and 0.001/s fractured around the same extension values. ABS specimens tested at temperatures of \(-20, 25,\) and \(50^\circ C\) are shown in Figure 2.21(b). As expected, the specimen at \(-20^\circ C\) failed at a lower strain compared to \(25^\circ C\). Surprisingly, specimens at \(50^\circ C\) produced shorter elongations to failure that the other two temperatures. One hypothesis to explain this phenomenon would point to the rubber butadiene inclusions. At room temperatures, the particles toughen the material by inducing millions of short crazes between particles. At higher temperatures, the rubber particles lose their toughening capabilities and instead behave like pores as they are unable to bear loads. Instead of crazes beginning and ending at particle–matrix interfaces, crazes/cracks move cut right through.
Figure 2.21  Tensile force–extension behavior for acrylonitrile butadiene styrene.

Tensile force–extension behavior for acrylonitrile butadiene styrene displaying (a) strain rate dependence at $T = 25^\circ C$ and (b) temperature dependence at $\dot{\varepsilon} = 0.01/s$.

The force–displacement behavior of PP is shown in Figure 2.22. Three quasi-static strain rates of 0.05, 0.01, and 0.001/s were tested and the results are shown in Figure 2.22(a). The strain rate of 0.001/s produced the greatest elongation to failure and as the strain rate increased the elongation to failure decreased. As the strain rate increases, the ability for chains and crystalline areas to move past one another becomes increasing difficult and failure occurs at lower strains. PP specimens tested at temperatures of $-20$, $25$, and $75^\circ C$ are shown in Figure 2.22(b). The same temperature–elongation to failure trend that was observed for ABS was also observed in PP. When $T = -20^\circ C$, the elongation to failure was much less than when $T = 25^\circ C$, which was expected due to cold temperature embrittlement. The
elongation to failure also decreased when the temperature changed from 25°C to 75°C. Since the PP microstructure is dominated with semi-crystalline regions and spherulites, these structures must aid in faster fracture at higher temperatures.

Figure 2.22  Tensile force–extension behavior for polypropylene.

Tensile force–extension behavior for polypropylene displaying (a) strain rate dependence at $T = 25^\circ$C and (b) temperature dependence at $\dot{\varepsilon} = 0.01$/s.
2.4 Torsion Testing

2.4.1 Experiment Procedures

Torsion tests were performed for PC, ABS, and PP at room temperature (25°C) for three different strain rates. The torsional rotation of the load test frame limited the specimen testing to a maximum of 270° rotation, which was short of the rotation needed to fail the specimens. To compare strain rates to uni-axial compression and tension testing, the effective shear strain rates (0.058, 0.0053, and 0.0005/s) are shown in Figure 2.24 as opposed to the shear strain rates, \( \dot{\gamma} \), which were approximately 0.1/s, 0.01/s, and 0.001/s. At each strain rate, three repeat tests were conducted and the averages are shown in Figure 2.24. The effective stresses/strains related to the shear stresses/strains for torsion by the following

\[
\sigma_{\text{eff}} = \sqrt{3} \tau, \quad \varepsilon_{\text{eff}} = \frac{1}{\sqrt{3}} \dot{\gamma}
\]  

(2.2)

The specimen geometry used for the torsion testing of the thermoplastic materials is shown in Figure 2.23. The specimen geometry was chosen from literature so as to provide a comparatively easy-to-machine specimen while preventing buckling [Govaert et al., 2000]. All specimens were cut from 25.4 mm thick sheet material and lathed to finished dimensions.

2.4.2 Torsion Testing Results

Figure 2.24 shows the mechanical behavior of PC, ABS, and PP in torsion at room temperature at different strain rates. Each curve shown is the average of at least three tests each for each strain rate. As observed in Figure 2.24, each material
Figure 2.23 Specimen geometry of torsion specimens from Govaert et al. [2000].

exhibits some degree of rate dependence. As the strain rate increased, the yield stress increased. For PC, in Figure 2.24(a), four main regimes can be observed: a linear elastic regime followed by a yield peak, some slight material softening and then a slight strain hardening. The strain softening increased as the strain rate increased. ABS, in Figure 2.24(b), showed three main regimes: a linear elastic region, yield point, and strain hardening. The strain hardening regions were linear and exhibited no rate dependence. The variability was very large between these tests also. PP has a very short linear elastic region, followed by a very gradual yielding and strain hardening. The elastic region for PP was not prominent when compared to PC and ABS.

Since the torsion specimens were solid and not thin-walled, comparing the stress–strain behavior to tension and compression would be misleading. Solid torsion specimens will experience a stress gradient in their cross-sectional area during loading. Assuming microstructural homogeneity, the material along the axis of rotation would experience no stress. Starting at the axis rotation and moving radially outwards, the stress increases and will reach a maximum value at the surface. Because of the stress gradient, these tests could be used in model validation instead of calibration.
Figure 2.24  Torsion equivalent true stress–strain response at room temperature.

Torsion equivalent true stress–strain response at room temperature for (a) polycarbonate, (b) acrylonitrile butadiene styrene, and (c) polypropylene.

2.5  Microstructural Analysis of PC, ABS, and PP

The following microstructural analysis compares the fracture surfaces of tensile tests for varying strain rates and temperatures for ABS. For PP and PC, the fracture
surface morphology will only be discussed for low temperate tensile experiments. All images were taken on a Zeiss EVO® 50 Series scanning electron microscope. Samples were prepared beforehand with a gold–palladium sputter coating process to enable conduction.

Each side of a fracture from one PC tensile specimen tested at a strain rate of 0.01/s at -20°C is shown in Figure 2.25. The river marks point towards fracture beginning at the inside lower corner. At above midway up the specimen, the fracture has ceased to grow from right to left and, therefore, uniformly grew upwards. Necking occurred in the PC tensile tests, even at cold temperatures, which can be seen on the fracture surface where the thickness is not constant. The overall smooth surface with river-like ridges is similar to work by Chiang and Hwung [1987] and Inberg [2001].

More details of the PC fracture morphology in Figure 2.25 are provided in Figures 2.26, 2.27, and 2.28. While the purchased PC was bought under the assumption that the PC was amorphous and free from defects, the inclusion-ridden fracture surface in Figure 2.26 proves otherwise. In fact, while these inclusions did not directly cause the fracture, pores have nucleated and grown around the inclusion–matrix interface. In the bottom left micrograph from Figure 2.26, two distinct regions can be observed—one light and the other dark. Figure 2.27 highlights the fracture morphology along the surface edge. Around 200 microns from the free surface, three micron wide tears developed. These tears are not only located around the edges, but were prominent there. Figure 2.28 shows the existence of microcracks, about one micron wide, scattered throughout the surface. Inside the cracks, fibrils are observed
suggesting that these cracks began as crazes. Generally, crazes grow perpendicular to
the direction of the maximum stress; however, these crazes did not grow perpendicular
to the maximum stress direction, which was the loading direction, but instead grew in
a plane parallel to the loading direction. A cause for this growth can be explained by
the tri-axial stresses produced when material is drawn into the neck. The stress state
at the necking transition region creates through-thickness tensile stress and strain.
These off-directional crazes and cracks did not contribute the final fracture, yet their
presence cannot be ignored when considering damage mechanisms for material models.
Figure 2.25  Both fracture surfaces from a polycarbonate specimen tested at a strain rate of 0.01/s at -20°C.
Figure 2.26  Fracture surface of polycarbonate from a tensile test at $-20^\circ$C and a strain rate of 0.01/s highlighting the pore growth from inclusions.

The complete fracture surfaces of ABS specimens are shown in Figure 2.29. At $-21^\circ$C, in Figure 2.29(a), the failure appears to have originated at the lower left-hand corner of the surface. Three distinct regions are observed: a smooth area (lower left), a dark transition morphology curved area, and a rough area. The crack grew at a slower rate, beginning at the lower left corner. Once the reduction in area, due to the crack, reached approximately one-eighth of the cross-section, the crack speed increased. The fast, unstable crack growth tore through the rest of the specimen creating a very rough upper right edge. Like metals, polymers generally behave in a
Figure 2.27  Fracture surface of polycarbonate from a tensile test at $-20^\circ$C and a strain rate of 0.01/s highlighting the morphology along edges.
Figure 2.28  Fracture surface of polycarbonate from a tensile test at \(-20^\circ\text{C}\) and a strain rate of 0.01/s highlighting the off-directional crazes.
more brittle manner at lower temperatures. The more rigid bonding among molecular chains due to the low temperature results in a highly textured fracture surface.

Two strong similarities exist between the fracture surfaces at –21°C and 25°C, Figures 2.29(a) and (b), respectively. Fracture began at a free surface and the crack transitioned to create two separate fracture surface textures. For 25°C, the fracture began along the long free edge on the right. A large inclusion is located on the fracture surface, but does not seem to affect crack growth or direction. Once the smoother area, which represents the beginning of the crack, covers approximately one-third of the area, the crack accelerates. The lower left edge in Figure 2.29(b) takes on rougher texture similar to the fast fracture region in Figure 2.29(a).

The fracture initiation location in Figure 2.29(c) for an ABS tensile test at 50°C is at the lower left-hand inclusion, not at the specimen edge. The river marks on the lower half of the fracture surface all point back to the inclusion. As ABS is comprised of rubber particles with diameters less than 1 micron, the inclusion is not likely to be rubber butadiene particle. Another important feature that set the 50°C test apart is multi-planar fracture. The crack jumps between fracture planes during the fracture process. The elevated temperatures also cause the material to curl at these jump interfaces.

Two whole ABS fracture surfaces, one at $\dot{\varepsilon} = 0.01$/s and one at $\dot{\varepsilon} = 0.1$/s, are shown in Figure 2.30. The surfaces are similar in that the cracks originate at free surfaces: at a long edge for 0.01/s and a corner for 0.1/s. For each test, the smooth thumbnail-like section takes up about one-fourth to one-third of the fracture surface.
At the higher rate of 0.1/s, the thumbnail takes on a smoother appearance. Also, at 0.1/s, the specimen undergoes bi-planar fracture. This particular aspect will be discussed further in relation to Figure 2.31.
Figure 2.29  Whole fracture surfaces of acrylonitrile butadiene styrene tensile specimens tested at a strain rate of 0.01/s.

Whole fracture surfaces of acrylonitrile butadiene styrene tensile specimens tested at a strain rate of 0.01/s with an environmental temperature of (a) -21°C, (b) 25°C, and (c) 50°C.
Figure 2.30  Whole fracture surfaces of acrylonitrile butadiene styrene tensile specimens tested at room temperature.

Whole fracture surfaces of acrylonitrile butadiene styrene tensile specimens tested at room temperature at strain rates of (a) 0.01/s and (b) 0.1/s.
More details of the ABS fracture morphology in Figure 2.30(b) are provided in Figures 2.31, 2.32, 2.33, and 2.34. Figures 2.31 and 2.32 are one side of the fracture surface while Figures 2.33 and 2.34 are the opposing side. In Figure 2.31, the rubber butadiene clearly affects the fracture of the surrounding matrix. The elevated “finger-like” area, in both Figures 2.31 and 2.33, is common on fracture surfaces. Hull and Owen [1973] attributed this geometry to bi-planar fracture. The direction of the “finger” also points to the bottom right edge as the initiation point of the fracture, which agrees with the thumbnail shape separating the two fracture zones. Also, Hull and Owen [1973] state this morphology is a result of crazing, where the step is a result of secondary fractures along the craze.

The porosity is not uniform on the fracture surface of the ABS specimen. As in both Figures 2.32 and 2.33, the porosity increases around the larger defects. Void nucleation, growth, and coalescence is important to understand in rubber-modified polymers. The nucleation has been documented [Xu and Xu, 2011] but, to the author’s knowledge, it has never been quantified in a way to model damage as has been done for metals [cf. Horstemeyer et al. [2003]].

Figure 2.34 shows connected ligaments between two edges. Lee et al. [2001] states that these ductile, fibrous stripes are created as a result of viscoplastic flow. Within the ligaments, the effects void nucleation, growth, and coalescence are plainly observed.

The complete fracture surface of two different PP tensile tests are shown in Figure 2.35. From the force–extension curves in Figure 2.22(b), the elongation to failure was on average seven times greater at room temperature compared to sub-zero
Figure 2.31 Fracture surface of acrylonitrile butadiene styrene from a tensile test at room temperature and a strain rate of 0.1/s highlighting the bi-planar fracture due to a butadiene particle.
Figure 2.32  Fracture surface of acrylonitrile butadiene styrene from a tensile test at room temperature and a strain rate of 0.1/s highlighting a multiple pore sizes within matrix.
Figure 2.33  Fracture surface of acrylonitrile butadiene styrene from a tensile test at room temperature and a strain rate of 0.1/s highlighting pore nucleation around bi-planar fracture due to a butadiene particle.
Figure 2.34  Fracture surface of acrylonitrile butadiene styrene from a tensile test at room temperature and a strain rate of 0.1/s highlighting unbroken crazes in the fast fracture regime.
degrees Celsius temperatures. At room temperature, the elongation primarily evolved through the material being drawn into an increasing necking region. The final fracture occurred in the necked region; however, the fracture surface cross-sectional area in Figure 2.35(a) is even smaller than the surrounding necking region, which can be observed in the dark left side background. Compared to Figure 2.35(b), the room temperature test fracture surface produced was less planar. In order to get the image in Figure 2.35(a), multiple images at different focus levels were stitched together to get a larger depth of field. In the room temperature tests, the sample fractured initiated at the smoother upper portion. The crack moved downward and became unstable toward the bottom edge resulting in violent tearing. The torn fracture surface puckered around the edges. The fractured surface in Figure 2.35(b) is not ductile like Figure 2.35(a). Instead, the surface is a very flat cleavage. The crack began at the smooth right edge then propagated to the left. Once the crack reached the center of the specimen, it jumped between planes, creating a highly textured, yet rather uniformly textured, surface. This highly textured surface is the result of fast fracture [Chen et al., 2002, van der Wal et al., 1998].

More details of the PP fracture morphology in Figure 2.35(a) are provided in Figures 2.36 and 2.37. Figure 2.36 shows that crazing is the dominant feature on the lower half of the fracture surface. The crazes do not appear parallel to the tensile direction, as they should; however, the crazes shown are on the puckered edge which is highly deformed. The craze fibrils are oriented in the same directions in the bottom left micrograph in Figures 2.36 meaning they likely grew perpendicular to the loading
direction as a result of the loading, unlike the crazes observed in PC in Figure 2.28. Details from the top edge of Figure 2.35(a) are shown in Figure 2.37. While the surface cannot be considered smooth, it is smoother compared to the lower section of the fracture surface. The texture is uniform and takes on a shape similar to tree bark. Small pores can be observed among the bark-like sections.

More details of the PP fracture morphology in Figure 2.35(b) are provided in Figures 2.38, 2.39, and 2.40. Figure 2.38 focuses on the top right edge of the fracture surface. The surface is very rough and has random fibers and debris on the surface. The fibers do not appear to result from crazing as they are not similarly oriented. Figure 2.39 focuses on the right edge of the specimen where the crack began. The crack is assumed to have begun here because of the smooth surface with parabola-like ridges pointing in that direction. The fracture surface in Figure 2.39 gives concluding evidences as to the role of crazing this PP material. Along this surface, crazes can be observed inside large voids. Craze fibrils, both broken and intact, can also been observed. As the fracture becomes unstable and the crack growth speed increases, organized craze structures are less likely to be observed, as is the case in both Figures 2.38 and 2.40. Figure 2.40 highlights the transition region between the slow and fast fracture regions. While fracture occurred on multiple planes, the planes were not as separated as they are on the far left edge of the specimen.
Figure 2.35  Whole fracture surfaces from polypropylene specimens.

Whole fracture surfaces from polypropylene specimens tested at (a) a strain rate of 0.1/s at 25°C and (b) a strain rate of 0.01/s at -21°C
Figure 2.36  Fracture surface of polypropylene from a tensile test at 25°C and a strain rate of 0.1/s highlighting massive crazing.
Figure 2.37 Fracture surface of polypropylene from a tensile test at 25°C and a strain rate of 0.1/s highlighting bark-like morphology.
Figure 2.38  Fracture surface of polypropylene from a tensile test at $-21^\circ$C and a strain rate of 0.01/s around surface edge.
Figure 2.39  Fracture surface of polypropylene from a tensile test at $-21^\circ$C and a strain rate of 0.01/s highlighting pores, crazes, and fibrils.
Figure 2.40  Fracture surface of polypropylene from a tensile test at $-21^\circ$C and a strain rate of 0.01/s around fracture transition region.
CHAPTER 3
THEORETICAL DEVELOPMENT OF THE ISV DAMAGE MODEL FOR
THERMOPLASTICS

3.1 Introduction to the Theoretical Development

The following chapter, an ISV damage framework for thermoplastics that includes three damage mechanisms—damage from pores, damage from particles, and crazing—is proposed. Crazing in the context is the organized fibrillar microstructure with lines of voids perpendicular to the principle tensile stress resulting from weak imperfections in the molecular composition. The damage evolution from particles and crazes will be defined by separate void nucleation, growth, and coalescence rate equations that are included in a modified inelastic amorphous glassy thermoplastic internal state variable (ISV) model Bouvard et al. [2013]. First, the kinematics will be prescribed beginning with a multiplicative decomposition of the deformation gradient. Next, the thermodynamic restrictions as given by Coleman and Gurtin [1967] are followed to determine temperature evolution. Finally, the kinetics and constitutive model is proposed. Within the section, the damage evolution equations are given, and a void nucleation evolution model is developed.

Gibb’s (direct) notation is used [Gurtin, 1981] for all tensor qualities and their mathematical operations. Tensors are denoted by boldface font while scalar values will
have the standard weight. Uppercase terms \( A \) are second-rank tensor and lowercase terms \( a \) are first-rank tensors (vectors). Second-rank tensor operations between the tensors \( A \) and \( B \) are indicated as \( AB \) for the inner product (a second-rank tensor) and \( A : B \) for the scalar product (a scalar). For first-rank tensors \( a \) and \( b \), the dyadic product is defined as \( a \otimes b \) (a second-rank tensor). Special care is given to specify configurations throughout the derivation by using accent marks where the tilde \( \tilde{B} \), circumflex \( \hat{B} \), and macron \( \bar{B} \) represent different intermediate configurations.

### 3.2 Kinematics

For a continuous three dimensional body in its initial state, any arbitrary point \( X \) can be mapped smoothly to a corresponding point, \( x \), in the current configuration using the deformation gradient tensor \( F \) along with a mapping function, \( x = \chi(X,t) \), where

\[
F(X,t) = \frac{\partial \chi(X,t)}{\partial X}
\]  

(3.1)

Both points \( X \) and \( x \) are located in the same coordinate system \( (X_1, X_2, X_3) \), where \( X \) is the location of the point when time = 0 and \( x \) in the location of the point when time = \( t \). The extended multiplicative decomposition of the deformation gradient tensor [Bilby et al. [1955], Kröner [1958], and Bammann et al. [1996]] will take the following form:

\[
F = F_e F_t F_d F_p
\]

(3.2)

In Eq. (3.2), each individual deformation gradient represents a physical deformation phenomenon. The elastic deformation gradient tensor, \( F_e \), represents chain rotations
and bond stretching that are reversible. The isotropic thermal deformation gradient tensor, $F_t$, represents deformation due to thermal expansion. The damage deformation gradient tensor, $F_d$, or volumetric inelastic deformation gradient, represents volumetric deformation due to increasing void volume. The plastic deformation gradient tensor, $F_p$, represents isochoric irreversible deformation.

There is no consensus on the placement of the thermal deformation gradient tensor, $F_t$; however, it is usually found either following the elastic deformation gradient (Weber and Boyce [1989], Boyce et al. [1992], Arruda et al. [1995]) or following the plastic deformation gradient (Bammann and Solanki [2010], Bouvard et al. [2010]). A physical basis for the latter can be made by considering a uniaxial tension test at room temperature interrupted prior to failure. The internal temperatures of thermoplastics generally rise during deformation. After unloading, the specimen is allowed to return to room temperature. The elastic deformation and the isotropic thermal expansion, is assumed to be negligible and the volumetric and deviatoric plastic deformation remains.

Decomposing the total deformation gradient tensor into four separate deformation gradient tensors creates three intermediate configurations between the reference configuration, $B_0$, and the current configuration, $\bar{B}$. The first intermediate configuration, $\bar{B}$, is defined by $F_p$. The second intermediate configuration, $\bar{B}$, is defined by $F_d F_p$. The third intermediate configuration, $\bar{B}$, is defined by $F_*$ where

$$F_* = F_t F_d F_p, \quad F = F_e F_*$$

(3.3)
Figure 3.1 Decomposition of the deformation gradient $F$.

Decomposition of the deformation gradient $F$ into four components: deviatoric plastic $F_p$, volumetric plastic (damage) $F_d$, thermal $F_t$, and elastic $F_e$. $F_*$ represents the plastic-damage-thermal deformation gradient.

The model is primarily expressed in the intermediate configuration of $\mathcal{B}$ following Weber and Boyce [1989]. The order of the deformation gradient tensors and configurations are visualized in Figure 3.1. Each intermediate deformation gradient tensor is mathematically defined as

$$ F_* = \frac{\partial \mathbf{x}}{\partial \mathbf{X}}, \quad F_p = \frac{\partial \mathbf{x}}{\partial \mathbf{X}}, \quad F_d = \frac{\partial \mathbf{x}}{\partial \mathbf{x}} \quad F_t = \frac{\partial \mathbf{x}}{\partial \mathbf{x}} \quad F_e = \frac{\partial \mathbf{x}}{\partial \mathbf{x}} $$

The Jacobian of the deformation gradient tensor is the ratio of volume change for the previous configuration to the following configuration. For the damage deformation gradient, the Jacobian takes the following form:

$$ J_d = \det F_d = \frac{\dot{V}}{V} $$

Because of void nucleation, growth, and coalescence, the relationship between the volumes at $\mathcal{B}$ and $\mathcal{B}$ are given by

$$ \dot{V} = V_V + \dot{V} $$

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where \( V_V \) is the volume of voids. Damage, \( \phi \), is defined as the ratio of the void volume to the total volume in \( \mathbf{\hat{B}} \).

\[
\phi = \frac{V_V}{V} \quad (3.7)
\]

Given Eqs. (3.5), (3.6) and (3.7), assuming isotropic damage, the damage deformation gradient can thus be written in terms of \( \phi \) as

\[
J_d = \frac{1}{1-\phi}, \quad \mathbf{F}_d = \frac{1}{(1-\phi)^{1/3}} \mathbf{1} \quad (3.8)
\]

where \( \mathbf{1} \) is a second rank identity tensor. The total Jacobian, which accounts for total volumetric change becomes

\[
J = \det \mathbf{F} = J_e J_t J_d J_p \quad (3.9)
\]

where

\[
J_e = \det \mathbf{F}_e, \quad J_t = \det \mathbf{F}_t = F_t^3, \quad J_p = \det \mathbf{F}_p = 1 \quad (3.10)
\]

As linear isotropic thermal expansion is assumed for the thermal deformation gradient tensor,

\[
\mathbf{F}_t = (1 + \alpha_{th} \Delta \theta) \mathbf{1} = F_t \mathbf{1} \quad (3.11)
\]

where \( \alpha_{th} \) is the linear coefficient of thermal expansion and \( \theta \) is the temperature.

Given the deformation gradients in Eqs. (3.2) and (3.3), the Cauchy-Green deformation tensors are defined as the following,

\[
\mathbf{C} = \mathbf{F}^T \mathbf{F}, \quad \mathbf{C}_p = \mathbf{F}_p^T \mathbf{F}_p, \quad \mathbf{C}_* = \mathbf{F}_*^T \mathbf{F}_*,
\]

\[
\bar{\mathbf{C}}_d = \mathbf{F}_d^T \mathbf{F}_d, \quad \bar{\mathbf{C}}_t = \mathbf{F}_t^T \mathbf{F}_t, \quad \bar{\mathbf{C}}_e = \mathbf{F}_e^T \mathbf{F}_e \quad (3.12)
\]

along with the corresponding Green-Lagrangian strain tensors
\[ E = \frac{1}{2} (C - 1), \quad E_p = \frac{1}{2} (C_p - 1), \quad E_\ast = \frac{1}{2} (C_\ast - 1), \quad (3.13) \]

Each Cauchy-Green deformation tensor in Eq. (3.12) can undergo a spectral decomposition of the form

\[ C = \sum_{i=1}^{3} \lambda_i^2 n_i \otimes n_i \quad (3.14) \]

where the stretch ratio, \( \lambda_i \), is the square root of each positive eigenvalue that corresponds to each orthonormal eigenvector, \( n_i \). Each deformation gradient tensor has a polar decomposition of the form

\[ F_\bullet = R_\bullet U_\bullet \quad (3.15) \]

where (\( \bullet \)) can be any of terms resulting from the deformation gradient decomposition \((p, d, t, e)\). The relationship between \( C \) and \( U \) is

\[ U = \sqrt{C} = \sum_{i=1}^{3} \lambda_i n_i \otimes n_i \quad (3.16) \]

where the directions (eigenvalues) remain unchanged, and the principal stretch ratios are used. The right stretch tensors associated with the damage in the \( \tilde{B} \) and \( \bar{B} \) configurations, which will be used in the Thermodynamics Section, are found as

\[ \tilde{U}_d = \tilde{C}_d^{1/2} = (F_d^T F_d)^{1/2} = (1 - \phi)^{-1/3} 1, \]

\[ \bar{U}_d = F_t^{-T} F_d^{-1} \tilde{U}_d F_d^{-1} = \frac{(1 - \phi)^{1/3}}{F_t^2} 1 \quad (3.17) \]

and in rate form, assuming constant temperature,

\[ \dot{U}_d^{-1} = -\frac{\phi}{3F_t^2 (1 - \phi)^{2/3}} 1 \quad (3.18) \]
A scalar form of the damage right stretch tensor affecting the scalar ISVs along with the scalar rate form is

\[ \dot{t}_d = \frac{1}{3} \text{tr} (\bar{U}_d) = \frac{(1 - \phi)^{1/3}}{F_t^2}, \quad \dot{\phi} = -\frac{\phi}{3F_t^2(1 - \phi)^{2/3}} \quad (3.19) \]

The velocity gradients \( \dot{\mathbf{l}} \) in the current configuration \( \mathbf{B} \) and \( \dot{\mathbf{L}}_\ast \) in the intermediate configuration \( \bar{\mathbf{B}} \) are

\[
\dot{\mathbf{l}} = \dot{\mathbf{F}} \mathbf{F}^{-1} = \dot{\mathbf{F}}_{\mathcal{L}} \mathbf{F}^{-1}_{\mathcal{L}} + \dot{\mathbf{F}}_{\mathcal{L}} \mathbf{L}_\ast \mathbf{F}^{-1}_{\mathcal{L}}, \\
\dot{\mathbf{L}}_\ast = \dot{\mathbf{F}} \mathbf{F}^{-1} = \dot{\mathbf{F}}_{\mathcal{L}} \mathbf{F}^{-1}_{\mathcal{L}} + \dot{\mathbf{F}}_{\mathcal{L}} \mathbf{L}_\ast \mathbf{F}^{-1}_{\mathcal{L}} + \dot{\mathbf{F}}_{\mathcal{L}} \dot{\mathbf{L}}_\ast \mathbf{F}^{-1}_{\mathcal{L}} \mathbf{F}^{-1}_{d} \mathbf{F}^{-1}_{t} \quad (3.20)
\]

where

\[
\dot{\mathbf{l}} = \mathbf{F}_{\mathcal{L}} \dot{\mathbf{L}}_\ast \mathbf{F}^{-1}_{\mathcal{L}} + \mathbf{F}_{\mathcal{L}} \mathbf{L}_\ast \mathbf{F}^{-1}_{\mathcal{L}} + \mathbf{F}_{\mathcal{L}} \mathbf{L}_\ast \mathbf{F}^{-1}_{\mathcal{L}} \quad (3.21)
\]

Because both the damage and thermal deformation gradients are isotropic, they can be further simplified.

\[
\dot{\mathbf{L}}_\mathcal{L} = \dot{\mathbf{F}}_\mathcal{L} \mathbf{F}^{-1}_\mathcal{L} = \dot{\mathbf{F}}_\mathcal{L} \mathbf{F}^{-1}_\mathcal{L} \mathbf{1} = \mathbf{F}^{-1}_\mathcal{L} \frac{\partial \mathbf{F}}{\partial \theta} \dot{\theta} \mathbf{1} = f_\theta \dot{\theta} \mathbf{1}, \quad \dot{\mathbf{L}}_d = \mathbf{F}_d \dot{\mathbf{L}}_d \mathbf{F}^{-1}_d = \frac{\dot{\phi}}{3(1 - \phi)} \mathbf{1}, \quad \dot{\mathbf{L}}_d = \mathbf{F}_d \dot{\mathbf{L}}_d \mathbf{F}^{-1}_d = \frac{\dot{\phi}}{3(1 - \phi)} \mathbf{1} \quad (3.22)
\]

where \( f_\theta \) is a temperature dependent variable describing the thermal expansion.

Pulling back the velocity gradient \( \dot{\mathbf{l}} \) to the intermediate configuration \( \bar{\mathbf{B}} \) creates the following relations:

\[
\dot{\mathbf{L}} = \mathbf{F}^{-1}_e \dot{\mathbf{F}}_e = \dot{\mathbf{L}}_e + \dot{\mathbf{L}}_\ast, \quad \dot{\mathbf{L}}_e = \mathbf{F}^{-1}_e \dot{\mathbf{F}}_e \quad (3.24)
\]
The velocity gradients can then be decomposed into their symmetric and skew parts as

\[ \bar{D} = \text{sym} (\bar{L}) = \bar{D}_e + \bar{D}_s, \quad \bar{D}_s = \bar{D}_t + \bar{D}_d + \bar{D}_p \]  

(3.25)

and

\[ \bar{W} = \text{skew} (\bar{L}) = \bar{W}_e + \bar{W}_s, \quad \bar{W}_s = \bar{W}_t + \bar{W}_d + \bar{W}_p, \]  

(3.26)

respectively. Due to the assumed isotropy in \( F_t \) and \( F_d \), \( \bar{W}_t = 0 \) and \( \bar{W}_d = 0 \). Also, the plastic flow is assumed as incompressible (\( \text{det} \bar{F}_p = 1 \) and \( \text{tr}(\bar{L}_p) = \text{tr}(\bar{D}_p) = \text{tr}(\bar{W}_p) = 0 \)).

The second-rank Cauchy stress, \( \sigma \), expressed as the following,

\[ \sigma = J_e^{-1} \tau = J_e^{-1} F_e S F_e^T \]  

(3.27)

where the Cauchy stress and Kirchhoff stress (\( \tau \)) are found in the current configuration, \( B \), and the second Piola-Kirchhoff stress (\( S \)) is located in the intermediate configuration \( \bar{B} \) [Holzapfel, 2000].

### 3.3 Thermodynamics

The thermodynamic approach proposed by Coleman and Gurtin [1967] is followed as it describes the underlying irreversible effects governing plastic deformation. Beginning with the local form of the first law (energy balance) and second law (entropy inequality) in the \( \bar{B} \) configuration,

\[ \dot{\varepsilon}_V + \bar{e}_V \text{tr} (\bar{L}_s) - \left( S : \dot{\bar{E}}_e + \bar{M} : \bar{D}_d + \bar{M} : \bar{L}_p + \bar{M} : \bar{D}_t \right) + \nabla \cdot \bar{Q} - \bar{R}_V = 0 \]  

(3.28)

\[ \dot{s}_V + \bar{s}_V \text{tr} (\bar{L}_s) \geq \frac{\bar{R}_V}{\theta} - \frac{1}{\theta} \nabla \cdot \bar{Q} + \frac{1}{\theta^2} \bar{Q} \cdot \nabla \theta \]  

(3.29)
$\bar{e}_V$ and $\dot{s}_V$ are the internal energy and entropy per unit volume, $\dot{Q}$ is the heat flux per area, $\bar{R}_V$ is the heat source per unit volume, and $\bar{M}$ is the Mandel stress where $\bar{M} = \bar{C}_M \bar{S}$. The dot (·) in Equations (3.28) and (3.29) is used to designate the gradient and divergence with the del ($\nabla$) operator. For a detailed treatment of the derivations of Eqs. (3.28) and (3.29), see Bouvard et al. [2013]. From Eqs. (3.20), (3.22), and (3.23), we find

$$\text{tr}(\bar{L}_*) = \text{tr}(\bar{L}_d + \bar{L}_n) = \frac{\dot{\phi}}{1 - \phi} + 3f_{\theta}\dot{\theta}$$  \hspace{1cm} (3.30)

which will be used to simplify Eqs. (3.28) and (3.29). The Helmholtz free energy per unit volume function $\bar{\psi}_V$ at the $\bar{B}$ configuration can be related to the internal energy and entropy by

$$\bar{\psi}_V = \bar{e}_V - \theta \bar{s}_V, \hspace{0.5cm} \dot{\bar{\psi}}_V = \dot{\bar{e}}_V - \dot{\theta} \bar{s}_V - \theta \dot{\bar{s}}_V$$  \hspace{1cm} (3.31)

The Clausius-Duhem inequality is then found by substituting Eq. (3.28) into (3.29) for $\bar{R}_V$ and also using the Helmholtz free energy function from Eq. (3.31).

$$- \bar{\psi}_V - \bar{\psi}_V \text{tr}(\bar{L}_*) - \dot{\theta} \bar{s}_V + \left( \bar{S} : \dot{\bar{E}}_e + \bar{M} : \dot{\bar{D}}_t + \bar{M} : \dot{\bar{D}}_d + \bar{M} : \bar{L}_p \right) - \frac{1}{\theta} \dot{\bar{Q}} \cdot \nabla \theta \geq 0$$  \hspace{1cm} (3.32)

The Helmholtz free energy is assumed here to be a function of the following independent state variables: the elastic strain/damage stretch product $\bar{E}_e \bar{U}_d$, a set of kinematic-like ISVs $\bar{\Pi}$ that are affected by damage, and temperature $\theta$ as

$$\bar{\psi}_V = \bar{\psi}_V \left( \bar{E}_e \bar{U}_d, \bar{\Pi}, \theta \right) = \bar{\psi}_V \left( \bar{E}_e \bar{U}_d, \xi_1 \bar{t}_d, \xi_2 \bar{t}_d, \alpha \bar{U}_d, \theta \right)$$  \hspace{1cm} (3.33)

In the past, the void volume fraction, $\phi$, has been used as an ISV. The approach shown in Equation (3.33) was motivated by Bammann and Solanki [2010]. The rationale for
using the elastic-strain/damage-stretch product, as opposed to simply the void volume fraction, follows: consider a single void among amorphous chains. The presence of the void may change the surface energy, but it does not affect the internal energy given that the material is under no loads, assuming no residual stresses. If the material is then loaded, the elastic strains are then concentrated by the void. If a void-free material is loaded, the elastic strains are not concentrated. The effect on the free energy can be described as

$$
\psi (E_e U_d) = \begin{cases} 
0 & \text{if } E_e = 0 \\
\tilde{\psi} (E_e) & \text{if } \phi = 0 
\end{cases}
$$

(3.34)

When a material is void-free, $\phi = 0$ and $U_d = 1$.

The set of kinematic-like ISVs, $\Pi$, will follow the three proposed by Bouvard et al. [2010], where the two scalar ISVs, $\xi_1$ and $\xi_2$, represent internal strain induced by entanglement points and large strain chain alignment/coiling, respectively. Chain motion is restricted as entanglement density increases and as shown by Hossain et al. [2010], as deformation increases, the number of entanglement points decreases. The ISV $\xi_1$ is used to capture this phenomenon. Also, as shown in Bouvard et al. [2010], chain alignment resulting from large strains increases strain hardening due to van der Waals interactions, which $\xi_2$ captures. Also a part of $\Pi$ is a symmetric tensorial variable $\alpha$ that accounts for direction-dependent hardening instigated by
chain stretching between entanglement points. Given these ISVs, the entropy rate is

\[
\dot{\psi}_V = \frac{\partial \tilde{\psi}_V}{\partial (E_e U_d)} : \dot{E}_e U_d + \frac{\partial \tilde{\psi}_V}{\partial (E_e U_d)} : \dot{E}_e \dot{U}_d + \frac{\partial \tilde{\psi}_V}{\partial (\xi_1 \dot{t}_d)} \xi_1 \dot{t}_d + \frac{\partial \tilde{\psi}_V}{\partial (\xi_1 \dot{t}_d)} \xi_1 \dot{t}_d
\]

\[
+ \frac{\partial \tilde{\psi}_V}{\partial (\xi_2 \dot{t}_d)} \xi_2 \dot{t}_d + \frac{\partial \tilde{\psi}_V}{\partial (\xi_2 \dot{t}_d)} \xi_2 \dot{t}_d + \frac{\partial \tilde{\psi}_V}{\partial (\alpha U_d)} : \dot{\alpha} U_d + \frac{\partial \tilde{\psi}_V}{\partial (\alpha U_d)} : \dot{\alpha} \dot{U}_d + \frac{\partial \tilde{\psi}_V}{\partial \theta} \dot{\theta}
\]

(3.35)

By substituting Eq. (3.35) into (3.32) and rearranging, we get the dissipation inequality.

\[
\dot{S} = \frac{\partial \tilde{\psi}_V}{\partial (E_e U_d)} : \dot{U}_d^T \left( \dot{E}_e - \frac{\partial \tilde{\psi}_V}{\partial (E_e U_d)} : \dot{E}_e \dot{U}_d - \frac{\phi}{3(1 - \phi)} (3 \tilde{\psi}_V + \dot{M} : 1) \right)
\]

\[
+ \dot{M} : \dot{L}_p - \dot{\theta} \left( \frac{\partial \tilde{\psi}_V}{\partial \theta} + 3 f_\theta \tilde{\psi}_V + \dot{s}_V - f_\theta \dot{M} : 1 \right) \left( \frac{\partial \tilde{\psi}_V}{\partial (\xi_1 \dot{t}_d)} \xi_1 \dot{t}_d - \frac{\partial \tilde{\psi}_V}{\partial (\xi_1 \dot{t}_d)} \xi_1 \dot{t}_d \right)
\]

\[
- \frac{\partial \tilde{\psi}_V}{\partial (\xi_2 \dot{t}_d)} \xi_2 \dot{t}_d - \frac{\partial \tilde{\psi}_V}{\partial (\xi_2 \dot{t}_d)} \xi_2 \dot{t}_d - \frac{\partial \tilde{\psi}_V}{\partial (\alpha U_d)} : \dot{\alpha} U_d - \frac{\partial \tilde{\psi}_V}{\partial (\alpha U_d)} : \dot{\alpha} \dot{U}_d - \frac{1}{\theta} \dot{Q} \cdot \nabla \theta \geq 0
\]

(3.36)

Corresponding to the three ISVs \((\tilde{\xi}_1 \dot{t}_d, \tilde{\xi}_2 \dot{t}_d, \text{ and } \dot{\alpha} U_d)\) are their stress-like thermodynamic conjugates \((\tilde{\kappa}_1, \tilde{\kappa}_2, \text{ and } \tilde{b})\) where

\[
\tilde{\kappa}_1 = \frac{\partial \tilde{\psi}_V}{\partial (\xi_1 \dot{t}_d)} \tilde{\xi}_1 \dot{t}_d, \quad \tilde{\kappa}_2 = \frac{\partial \tilde{\psi}_V}{\partial (\xi_2 \dot{t}_d)} \tilde{\xi}_2 \dot{t}_d, \quad \tilde{b} = \frac{\partial \tilde{\psi}_V}{\partial (\alpha U_d)} U_d^T = \frac{\partial \tilde{\psi}_V}{\partial (\alpha U_d)} U_d
\]

(3.37)

In the same way the ISVs represent physical phenomena, so do their thermodynamic conjugates. Following the standard Coleman and Gurtin [1967] rationale, from dissipation inequality, Eq. (3.36), the general constitutive equations for the Second Piola–Kirchoff stress, \(\bar{S}\), and the entropy, \(\bar{s}_V\), are

\[
\bar{S} = \frac{\partial \tilde{\psi}_V}{\partial (E_e U_d)} \bar{U}_d^T = \frac{\partial \tilde{\psi}_V}{\partial (E_e U_d)} \bar{U}_d, \quad \bar{s}_V = - \frac{\partial \tilde{\psi}_V}{\partial \theta} - 3 f_\theta \tilde{\psi}_V + f_\theta \dot{M} : 1
\]

(3.38)
The dissipation inequality, Eq. (3.36), can be reduced using Eqs. (3.17), (3.18), (3.19), (3.37), and (3.38) to

\[
\dot{M} : \dot{L}_p - \bar{\kappa}_1 \dot{\xi}_1 - \bar{\kappa}_2 \dot{\xi}_2 - \dot{b} : \dot{\alpha} - \frac{1}{\theta} \dot{Q} \cdot \nabla \theta
- \frac{\dot{\phi}}{3 (1 - \phi)} \left[ 3 \bar{\psi}_V + 3 \bar{S} : \bar{E}_e + \text{tr} (\bar{S}) + \bar{\kappa}_1 \bar{\xi}_1 + \bar{\kappa}_2 \bar{\xi}_2 + \bar{b} : \bar{\alpha} \right] \geq 0
\]  

(3.39)

The first term in the dissipation inequality, Eq. (3.39), relates to plastic dissipation. The next three terms relate to internal work resulting from defect induced residual microstresses (such as entanglement points or chain alignment). The fifth term relates to internal dissipative work due to void nucleation, growth, and coalescence.

The free energy rate, Eq. (3.35), can also be simplified using Eqs. (3.17), (3.18), (3.19), (3.37), and (3.38) as

\[
\dot{\psi}_V = \bar{S} : \dot{\bar{E}}_e + \bar{\kappa}_1 \dot{\xi}_1 + \bar{\kappa}_2 \dot{\xi}_2 + \bar{b} : \dot{\alpha} - \dot{\theta} \left( \bar{s}_V + 3 f \bar{\psi}_V - f_{\theta} \bar{S} : \bar{C}_e \right)
- \frac{\dot{\phi}}{3 (1 - \phi)} \left( \bar{S} : \bar{E}_e + \bar{\kappa}_1 \bar{\xi}_1 + \bar{\kappa}_2 \bar{\xi}_2 + \bar{b} : \bar{\alpha} \right)
\]  

(3.40)

After substituting the free energy rate, Eq. (3.40), into Eq. (3.31)_2 which is then inserted into the energy balance, Eq. (3.28), yields

\[
- \dot{M} : \dot{L}_p + \bar{\kappa}_1 \dot{\xi}_1 + \bar{\kappa}_2 \dot{\xi}_2 + \dot{b} : \dot{\alpha} + 3 f_{\theta} \bar{s}_V \dot{\theta} + \theta \dot{\bar{s}}_V
- \frac{\dot{\phi}}{3 (1 - \phi)} \left[ 3 \bar{S} : \bar{E}_e + \text{tr} (\bar{S}) + \bar{\kappa}_1 \bar{\xi}_1 + \bar{\kappa}_2 \bar{\xi}_2 + \bar{b} : \bar{\alpha} - 3 \bar{\bar{\psi}}_V \right] + \nabla \cdot \dot{\bar{Q}} - \bar{R}_V = 0
\]  

(3.41)

The time derivative of entropy can be obtained from (3.38)_2 after some algebra as
\[
\dot{s}_V = \frac{\partial \bar{s}_V}{\partial \theta} \dot{\theta} - \frac{\partial S}{\partial \theta} + 3f_\theta S - f_\theta \frac{\partial C_e \cdot S}{\partial (E_e U_a)} \dot{U}_d \left( \dot{E}_e + \left( \frac{\partial \bar{\kappa}_1}{\partial \theta} + 3f_\theta \bar{\kappa}_1 \right) \dot{\xi}_1 - \left( \frac{\partial \bar{\kappa}_2}{\partial \theta} + 3f_\theta \bar{\kappa}_2 \right) \dot{\xi}_2 - \left( \frac{\partial b}{\partial \theta} + 3f_\theta \bar{b} \right) : \dot{\alpha} \right)
\]
\[
+ \frac{\dot{\phi}}{3(1 - \phi)} \left( \frac{\partial S}{\partial \theta} + 3f_\theta S - f_\theta \frac{\partial C_e \cdot S}{\partial (E_e U_a)} \dot{U}_d \right) : \dot{E}_e 
\]
\[
+ \left( \frac{\partial \bar{\kappa}_1}{\partial \theta} + 3f_\theta \bar{\kappa}_1 \right) \dot{\xi}_1 + \left( \frac{\partial \bar{\kappa}_2}{\partial \theta} + 3f_\theta \bar{\kappa}_2 \right) \dot{\xi}_2 + \left( \frac{\partial b}{\partial \theta} + 3f_\theta \bar{b} \right) : \dot{\alpha} \right] \tag{3.42}
\]

Using the definition of heat capacity per unit volume \((\bar{C}_V)\), the first term of Eq. (3.42) is determined using Eqs. (3.31)\textsubscript{1} and (3.38)\textsubscript{2} as

\[
\bar{C}_V = \frac{\partial \bar{e}_V}{\partial \theta} = \frac{\partial}{\partial \theta} \left( \bar{\psi}_V + \theta \bar{s}_V \right), \quad \theta \frac{\partial \bar{s}_V}{\partial \theta} = \bar{C}_V + 3f_\theta \bar{\psi}_V - f_\theta \bar{M} : \bar{1} \tag{3.43}
\]

The temperature increase due to adiabatic heating, which follows, can be found by substituting the entropy rate, Eq. (3.42), into Eq. (3.41) and then simplifying the result using Eqs. (3.31)\textsubscript{1}, (3.37), (3.38), and (3.43)\textsubscript{2}. The result couples damage, mechanical, and thermal effects to give the temperature increase.
\[
\dot{\theta} = \frac{1}{C_V + 3 f_0 \bar{e}_V - f_0 \text{tr} (\bar{M})} \times \\
\theta \frac{\partial S}{\partial \theta} + 3 f_0 \theta S - f_0 \theta \left( \frac{\partial \bar{C}_e : \bar{S}}{\partial (\bar{E}_e \bar{U}_d)} \right) : \dot{\bar{E}}_e + \left( \theta \frac{\partial \bar{\kappa}_1}{\partial \theta} + \bar{\kappa}_1 (3 f_0 \theta - 1) \right) \dot{\xi}_1 \\
+ \left( \theta \frac{\partial \bar{\kappa}_2}{\partial \theta} + \bar{\kappa}_2 (3 f_0 \theta - 1) \right) \dot{\xi}_2 + \left( \theta \frac{\partial \bar{b}}{\partial \theta} + \bar{b} (3 f_0 \theta - 1) \right) \dot{\bar{\alpha}} + \bar{M} : \bar{L}_p - \bar{\nabla} \cdot \bar{Q} + \bar{R}_V \\
- \frac{\phi}{3 (1 - \phi)} \left[ \theta \frac{\partial S}{\partial \theta} + 3 S (\theta f_0 - 1) - f_0 \theta \frac{\partial \bar{C}_e : \bar{S}}{\partial (\bar{E}_e \bar{U}_d)} \right] : \dot{\bar{E}}_e + \left( \theta \frac{\partial \bar{\kappa}_1}{\partial \theta} + \bar{\kappa}_1 (3 f_0 \theta - 1) \right) \dot{\xi}_1 \\
+ \left( \theta \frac{\partial \bar{\kappa}_2}{\partial \theta} + \bar{\kappa}_2 (3 f_0 \theta - 1) \right) \dot{\xi}_2 + \left( \theta \frac{\partial \bar{b}}{\partial \theta} + \bar{b} (3 f_0 \theta - 1) \right) \left( \dot{\bar{\alpha}} - \text{tr} (\bar{S}) + 3 \bar{e}_V \right) \right]
\]
(3.44)
3.4 Constitutive Equations

All constitutive equations will be expressed in the intermediate configuration, $\bar{B}$. Following the temperature dependent inelastic ISV model proposed in Bouvard et al. [2013], the addition of damage will accomplish two main goals: degrade moduli and predict failure using the void volume fraction. These stress-like quantities ($\bar{S}, \bar{\kappa}_1, \bar{\kappa}_2, \bar{b}$) are related to strain-like variables ($\bar{E}_e \bar{U}_d, \bar{\xi}_1 \bar{t}_d, \bar{\xi}_2 \bar{t}_d, \bar{\alpha} \bar{U}_d$) via an explicit expression for the Helmholtz free energy.

3.4.1 Helmholtz Free Energy

The Helmholtz free energy is assumed to additively decompose, which follows

$$\tilde{\psi} (\bar{E}_e \bar{U}_d, \bar{\xi}_1 \bar{t}_d, \bar{\xi}_2 \bar{t}_d, \bar{\alpha} \bar{U}_d, \theta) = \tilde{\psi}_{E_e U_d} (\bar{E}_e \bar{U}_d, \theta) + \tilde{\psi}_{\bar{\xi}_1 \bar{t}_d} (\bar{\xi}_1 \bar{t}_d, \theta)$$
$$+ \tilde{\psi}_{\bar{\xi}_2 \bar{t}_d} (\bar{\xi}_2 \bar{t}_d, \theta) + \tilde{\psi}_{\bar{\alpha} U_d} (\bar{\alpha} \bar{U}_d, \theta)$$

(3.45)

A quadratic form is used to describe the thermodynamic state assuming small elastic strains where

$$\tilde{\psi} = \mu (\theta) \text{tr} (\bar{E}_e \bar{U}_d : \bar{E}_e \bar{U}_d) + \frac{\lambda (\theta)}{2} (\text{tr} (\bar{E}_e \bar{U}_d))^2$$
$$+ C_{\bar{\kappa}_1} \mu (\theta) (\bar{\xi}_1 \bar{t}_d)^2 + C_{\bar{\kappa}_2} \mu (\theta) (\bar{\xi}_2 \bar{t}_d)^2$$
$$+ C_b \mu R (\bar{\alpha} \bar{U}_d : \bar{\alpha} \bar{U}_d) + \tilde{\psi} (\theta)$$

(3.46)

where $\lambda (\theta) = K (\theta) + \frac{2}{3} \mu (\theta)$. $C_{\bar{\kappa}_1}, C_{\bar{\kappa}_2},$ and $C_b$ are stress state parameters that allow for each ISV to account for tension, compression, and torsion [Miller and McDowell, 1992]. Each stress state parameter takes the form

$$C_\bullet = a_\bullet \ b_\bullet \left[ \frac{4}{27} - \frac{J_3^2}{J_2^2} \right] \left( c_\bullet \ J_3 \frac{J_3}{J_2^{3/2}} + d_\bullet \left\| \frac{I_1}{\sqrt{J_2}} \right\| \right)$$

(3.47)
where the • is a placeholder for three stress-like ISVs identifiers \((\bar{\kappa}_1, \bar{\kappa}_2, \text{and } \bar{b})\). \(I_1\) is the first invariant of the Cauchy stress \((I_1 = \operatorname{tr}(\sigma))\). \(J_2\) is the second invariant of the deviatoric stress\(^1\) \((J_2 = \frac{1}{2}(\sigma':\sigma'))\) where \(\sigma' = \sigma - \frac{1}{3} \operatorname{tr}(\sigma) \mathbf{1}\). \(J_3\) is the third invariant of the deviatoric stress \((J_3 = \det(\sigma'))\). The Lamé constants \(\mu(\theta)\) and \(K(\theta)\) are elastic shear and bulk modulus defined as

\[
\mu(\theta) = \frac{E(\theta)}{2(1 + \nu_p)}, \quad K(\theta) = \frac{2\mu(\theta)(1 + \nu_p)}{3(1 - 2\nu_p)}
\]  

(3.48)

\(E(\theta)\) is a temperature dependent isotropic Young’s modulus, \(\nu_p\) is Poisson’s ratio assumed constant below the glass transition temperature, and \(\mu_R(\theta)\) is a temperature dependent hyperelastic modulus. The temperature dependent Young’s modulus is defined as

\[
E(\theta) = E_{\text{ref}} + E_1(\theta - \theta_{\text{ref}})
\]  

(3.49)

where \(E_{\text{ref}}\) and \(E_1\) are specified material parameters, and \(\theta_{\text{ref}}\) is a reference temperature.

### 3.4.2 Cauchy Stress Tensor

From the constitutive law for \(\mathbf{S}\) in Eq. (3.38) the Cauchy stress tensor in Eq. (3.27) becomes

\[
\sigma = J^{-1}_e F_e \frac{\partial \bar{\psi}_V}{\partial \left( E_e U_d \right)} \bar{U}_d^T \left( F_e^T \right)
\]  

(3.50)

\(^1\)\(J_2\) plasticity and the von Mises yield criterion form the cornerstone for much of the continuum approaches to modeling today. While \(J_2\) is commonly called the second invariant of the deviatoric stress, strictly speaking in the mathematical sense, it is not the second invariant. See Appendix A for a discussion on this misnomer.
From Eq. (3.46)

\[
\frac{\partial \tilde{\psi}}{\partial (\mathbf{E}_e \mathbf{U}_d)} = 2\mu(\theta) \mathbf{E}_e \mathbf{U}_d + \lambda(\theta) \text{ tr } (\mathbf{E}_e \mathbf{U}_d) \mathbf{1}
\]  
(3.51)

and the Second Piola–Kirchoff stress for the case of isotropic damage becomes

\[
\mathbf{S} = [2\mu(\theta) \mathbf{E}_e \mathbf{U}_d + \lambda(\theta) \text{ tr } (\mathbf{E}_e \mathbf{U}_d)] \left( \mathbf{U}_d^T \right)
\]

\[
= [2\mu(\theta) \mathbf{E}_e + \lambda(\theta) \text{ tr } (\mathbf{E}_e) \mathbf{1}] \left( \frac{1 - \phi}{F_t^4} \right)
\]  
(3.52)

The co-rotational Jaumann rate of the Cauchy stress is

\[
\dot{\sigma} = \dot{\sigma} - \mathbf{W}_e \sigma + \sigma \mathbf{W}_e
\]  
(3.53)

where the elastic spin is

\[
\mathbf{W}_e = \mathbf{W} - \mathbf{W}_p
\]  
(3.54)

The form of the plastic spin is motivated by Dafalias [1985] and modified by Bammann [1990] and takes the form of

\[
\mathbf{W}_p = -b_n^{-1} (\mathbf{bD}_p - \mathbf{D}_p \mathbf{b})
\]  
(3.55)

where, from Bammann [1990], the evolution of the scalar value \(b_n\) is

\[
\dot{b}_n = r_s(\theta) \|\mathbf{b}\| b_n
\]  
(3.56)

The plastic spin is used to capture anisotropic chain alignment at large strains.

### 3.4.3 Internal State Variables and Rate Equations

From Eq. (3.46), the thermodynamic force conjugates to each ISV are

\[
\kappa_1 = \frac{\partial \tilde{\psi}}{\partial (\xi_1 \bar{t}_d)} \bar{t}_d = 2C_{\kappa_1} \mu(\theta) \bar{\xi}_1 (\bar{t}_d)^2
\]  
(3.57)
\[
\bar{\kappa}_2 = \frac{\partial \bar{\psi}_V}{\partial (\bar{\xi}_2 \bar{t}_d)} \bar{t}_d = 2C_{\bar{\kappa}_2} \mu (\theta) \bar{\xi}_2 (\bar{t}_d)^2 \quad (3.58)
\]
\[
\bar{b} = \frac{\partial \bar{\psi}_V}{\partial (\bar{\alpha} \bar{U}_d)} \bar{U}_d = 2C_{\bar{\theta}_R} \mu (\theta) (\bar{\alpha} \bar{U}_d) \bar{U}_d \quad (3.59)
\]

In the case of isotropic damage, from Eqs. (3.17) and (3.19), the internal stresses become
\[
\bar{\kappa}_1 = 2C_{\bar{\kappa}_1} \mu (\theta) \bar{\xi}_1 \frac{(1 - \phi)^{2/3}}{F_t^4} \quad (3.60)
\]
\[
\bar{\kappa}_2 = 2C_{\bar{\kappa}_2} \mu (\theta) \bar{\xi}_2 \frac{(1 - \phi)^{2/3}}{F_t^4} \quad (3.61)
\]
\[
\bar{b} = 2C_{\bar{\theta}_R} \mu (\theta) \bar{\alpha} \frac{(1 - \phi)^{2/3}}{F_t^4} \quad (3.62)
\]

The two scalar ISVs, \(\bar{\xi}_1\) and \(\bar{\xi}_2\), are used to describe the entanglement density and large-strain chain alignment/coiling, respectively. The evolution equations for \(\bar{\xi}_1\) follows the work of Boyce et al. [1988], Anand and Gu [2000], Anand and Gurtin [2003], and Bouvard et al. [2013]. For \(\bar{\xi}_1\),
\[\bar{\xi}_1 (\mathbf{X}, 0) = 0, \quad \bar{\xi}^* (\mathbf{X}, 0) = \bar{\xi}_0^* (\theta)\]

The strain-like qualities for chain slip, \(\bar{\xi}^*\), and its saturation value, \(\bar{\xi}_{sat}^*\), are temperature dependent while the hardening modulus \((H_1)\) is temperature independent.
\[\bar{\xi}_0^* (\theta) = C_3 (\theta - \theta_{ref}) + C_4, \quad \bar{\xi}_{sat}^* (\theta) = C_5 (\theta - \theta_{ref}) + C_6, \quad (3.64)\]
\[g_0 (\theta) = C_7 (\theta - \theta_{ref}) + C_8\]

As pointed out by Bouvard et al. [2013], the trend shown in Figure 3.2 between the \(\bar{\xi}_1\) due to chain entanglement motivated from molecular dynamics simulations in Hossain et al. [2010] gives confidence to the evolution equation. The viscous shear strain, \(\dot{\gamma}_p\),
Evolution of $\bar{\xi}_1$ as true strain increases. The entanglement density decreases as deformation increases after 20% true strain. (from Bouvard et al. [2013])

follows a modified (Richeton et al. [2005, 2007]) cooperative model (Fotheringham et al. [1976], Fotheringham and Cherry [1978]) where

$$\dot{\gamma}_p = \dot{\gamma}_{0p} \exp \left( \frac{\Delta H_\beta}{k_B \theta} \right) \sinh^n \left( \frac{\bar{\tau}_{eq} V}{2k_B \theta} \right) \left( \bar{\tau}_{eq} = \bar{\tau} - (Y(\theta) + \bar{\kappa}_1 + \bar{\kappa}_2) \right) \quad (3.65)$$

In Eq. (3.65), $\dot{\gamma}_{0p}$ is a reference strain rate, $\Delta H_\beta$ is an activation energy, $V$ is an activation volume, $n$ is a parameter describing the molecular chain segments’ cooperative behavior, and $Y(\theta)$ is a temperature dependent yield surface given by

$$Y(\theta) = C_1 (\theta - \theta_{ref}) + C_2 \quad (3.66)$$

$\bar{\tau} = \left\| \mathbf{S}' - \mathbf{b}' \right\| / \sqrt{2}$ is the equivalent shear stress, where $\mathbf{S}'$ and $\mathbf{b}'$ are the deviatoric parts of the second Piola-Kirchhoff stress and back stress, respectively.
For $\bar{\xi}_2$, the evolution equation, from Ames et al. [2009], is given as

$$\dot{\bar{\xi}}_2 = H_2 \left[ (\bar{\lambda}_p - 1) \left( - \frac{\bar{\xi}_2}{\bar{\xi}_{2\text{sat}}(\theta)} \right) \dot{\bar{\lambda}}_p - R_s(\theta) \right],$$

(3.67)

where, the hardening modulus, $H_2$, is temperature independent. The saturation value, $\bar{\xi}_{2\text{sat}}$, and the static recovery, $R_s$, are temperature dependent of the forms

$$\bar{\xi}_{2\text{sat}}(\theta) = C_9(\theta - \theta_{\text{ref}}) + C_{10}, \quad R_s(\theta) = C_{11}(\theta - \theta_{\text{ref}}) + C_{12} \quad (3.68)$$

The static recovery term, $R_{s2}$, is scalar in nature and helps capture creep-like phenomena [Bammann, 1990]. The effective plastic stretch, $\bar{\lambda}_p$, is related to the square root of the left Cauchy-Green deformation tensor [Ames et al., 2009].

The second-rank tensorial strain-like ISV, $\bar{\alpha}$, is introduced to capture the large strain hardening behavior of thermoplastics known to be caused by chain stretching. The free energy due to hyperelasticity in Eq. (3.46) deviates from the classical hyperelastic rubber models (cf., Mooney [1940], Rivlin [1948, 1949], Treloar [1943a,b], Varga [1966], Ogden [1972], Arruda et al. [1993]) where stretch ratios, not strains, are used. However, Bouvard et al. [2010] compared a quadratic form of “hyperelastic” strain to a classical hyperelastic model [Gent, 1996] and showed nearly identical results.

The temperature rubbery modulus, $\mu_R(\theta)$, is defined as

$$\mu_R(\theta) = n_{ed} k_B \theta \quad (3.69)$$

where $n_{ed}$ is an entanglement density, and $k_B$ is the Boltzmann constant ($k_B = 1.38065 \times 10^{-23}$ J/K).
Guided by Bouvard et al. [2010], the evolution equation for $\dot{\alpha}$ is

$$
\dot{\alpha} = (C_{\alpha_1} (\theta) + C_{\alpha_2} (\theta) \|\dot{\alpha}\|^2) \dot{D}_p - r_s (\theta) \sqrt{\frac{2}{3}} \|\dot{\alpha}\| \dot{\alpha}, \quad \alpha (X, 0) = 0 \quad (3.70)
$$

where $C_{\alpha_1} (\theta)$ and $C_{\alpha_2} (\theta)$ are temperature dependent material parameters defined as

$$
C_{\alpha_1} (\theta) = C_{13} (\theta - \theta_{ref}) + C_{14}, \quad C_{\alpha_2} (\theta) = C_{15} (\theta - \theta_{ref}) + C_{16} \quad (3.71)
$$

The static recovery takes the form

$$
r_s (\theta) = C_{17} (\theta - \theta_{ref}) + C_{18} \quad (3.72)
$$

Similar to the classic hyperelastic approaches, the $\|\dot{\alpha}\|$ term in the evolution equation denotes a stretching of the chains, and the $\dot{D}_p$ term defines the rate of these stretches in the direction of the plastic flow as suggested by Hoy and Robbins [2008] and Robbins and Hoy [2009].

### 3.4.4 Plastic Flow Rule

The flow rule describing the plastic deformation is given as [Boyce et al., 1988]

$$
\dot{F}_p = \tilde{L}_p F_p \quad (3.73)
$$

where

$$
\tilde{L}_p = \dot{D}_p + \dot{W}_p, \quad \dot{D}_p = \frac{1}{\sqrt{2}} \dot{\gamma}_p N_p \quad (3.74)
$$

The direction of the flow, $\tilde{N}_p$, is

$$
N_p = \frac{\dot{S}' - \dot{b}'}{\|\dot{S}' - \dot{b}'\|} \quad (3.75)
$$
3.4.5 Damage Evolution

In the previous Kinematics Section, the void volume fraction, \( \phi \), is defined (Eq. (3.7)). In this section, both physically and phenomenologically motivated equations will be developed to define damage evolution. The evolution equation for the total void volume fraction is expressed as

\[
\dot{\phi}_{\text{total}} = \left( \dot{\phi}_{\text{particles}} + \dot{\phi}_{\text{pores}} + \dot{\phi}_{\text{crazing}} \right) c \\
+ \left( \dot{\phi}_{\text{particles}} + \dot{\phi}_{\text{pores}} + \dot{\phi}_{\text{crazing}} \right) \dot{c}
\]

(3.76)

where \( c \) is damage coalescence and \( \dot{c} \) is the damage coalescence rate. For amorphous glassy thermoplastics (PC), the damage due to particles and pre-existing voids are likely negligible. However, for rubber-modified thermoplastics (ABS) or semi-crystalline polymers (PP), particles and voids may influence damage behavior more. For the sake of completeness, void growth from particles and void growth from pre-existing voids are given below. These evolution equations have successfully modeled void growth within metals [Horstemeyer, 2012]. More study needs to confirm that these formulations accurately capture deformation damage mechanisms in polymers. Yet, following the particle and void damage equations, a new crazing damage evolution equation is given that is motivated from failure in glassy polymers.

Particle damage begins with the nucleation, \( \eta \), of a void between the particle or fiber and the matrix. Once the particle either cracks or debonds, the newly formed void then grows. The void volume is described by \( \nu \). The rate of damage due to the particle follows:

\[
\dot{\phi}_{\text{particles}} = \dot{\eta}_{\text{particle}} \nu + \eta_{\text{particle}} \dot{\nu}
\]

(3.77)
A nucleation model developed by Horstemeyer and Gokhale [1999], originally applied to metals, could be used,

\[
\dot{\eta}_{\text{particle}} = \eta_{\text{particle}} \frac{d^{1/2} \| D_p \|}{K_{1c} f^{1/3}} \exp\left(\frac{C_{\eta p} \theta}{\eta} \right) \times \left\{ a_{\eta} \left[ \frac{4}{27} - \frac{J_3^2}{J_2^3} \right] + b_{\eta} \left[ \frac{J_3}{J_2^{3/2}} \right] + c_{\eta} \| I_1 \| \right\} \tag{3.78}
\]

where the average particle size, \( d \), the initial volume fraction of particles, \( f \), and fracture toughness of the particles, \( K_{1c} \), are needed for this model.

The void growth equation developed by Budiansky et al. [1982] could be adopted for polymer usage. The original form follows:

\[
\dot{\nu} = \frac{3}{2} \nu \left[ \frac{I_1}{m \sqrt{12} J_2} + \frac{(m - 1)(m + 0.4319)}{m^2} \right] \| D_p \| \tag{3.79}
\]

This void growth model assumes a spherical cavity within a strain rate hardening matrix. Other void growth models such as Rice and Tracey [1969], who assume a spherical cavity in a perfectly plastic matrix, or McClintock [1968], who assumes a cylindrical cavity in a plastic strain hardening matrix, could possibly be used in future studies. Assuming a constant plastic strain rate, Equation (3.79) can be integrated to become

\[
\nu = C_{\text{BUD}} \exp \left\{ \frac{3 \| \bar{E}_p \|}{2} \left[ \frac{I_1}{m \sqrt{12} J_2} + \frac{(m - 1)(m + 0.4319)}{m^2} \right]^m \right\} \tag{3.80}
\]

During polymer fabrication, voids arising in the bulk material are not uncommon, so having a damage model to predict failure would be of engineering value. The growth rate of these voids could be captured by the Cocks and Ashby [1980] model.

\[
\dot{\phi}_{\text{pores}} = \chi \left[ \frac{1}{(1 - \phi_{\text{pores}})} - (1 - \phi_{\text{pores}}) \right] \| D_p \| \tag{3.81}
\]
where

\[ \chi = \sinh \left[ \frac{2(m - 0.5) \ p}{(m + 0.5) \ \sigma_e} \right] = \sinh \left[ \frac{2(2m - 1) \ I_1}{3\sqrt{3}(2m + 1) \ \sqrt{J_2}} \right] \] (3.82)

where \( p \) is the hydrostatic pressure, and \( \sigma_e \) is the von Mises equivalent stress. As this growth rate was developed for a power law plasticity for metals, one might doubt the appropriateness of using it for polymers. However, Figure 3.3 shows a comparison between the Cocks–Ashby model and micromechanical void growth data using a unit cell with a void in tension embedded in a polymer from Socrate and Boyce [2000] using a material model from Arruda and Boyce [1993] and Boyce et al. [1988].

The volumetric strain, \( E_V \), was determined from the micromechanical simulation by Socrate and Boyce [2000] but not the void volume fraction. The increase of void volume fraction as a function of volumetric strain is determined as

\[ \phi = 1 - \left[ \exp(E_V) \left( \frac{\phi_0}{1 - \phi_0} \right) \right]^{-1} \] (3.83)

where \( E_V = \ln(V/V_0) \). For the comparison in Figure 3.3, the strain rate sensitivity exponent \( m = 0.74 \) was assumed. Socrate and Boyce [2000] studied two different representative volume elements (RVE) micromechanical models: an antisymmetric Stacked Hexagonal Array (SHA) of voids [Tvergaard, 1982] and a Voronoi tessellation of a Body Centered Cubic array of voids (V–BCC) [Dib and Rodin, 1993]. Socrate and Boyce [2000] concluded that the V–BCC model was more accurate. The Cocks and Ashby [1980] void growth equation shows its ability to capture void growth at low strains in polymers. However, at higher stress triaxialities, the Cocks–Ashby void volume fraction evolution does not match micromechanical simulations well.
Steenbrink et al. [1997] ran similar micromechanical calculations with a SHA model and modified Gurson’s yield potential [Gurson, 1977] to fit results. A comparison of their simulated void growth is compared to Cocks–Ashby void growth [Cocks and Ashby, 1980] using $m = 1.21$ in Figure 3.4. The micromechanical simulations suggest a more linear void growth where the Cocks–Ashby model returns exponential void growth. At lower stress triaxialities, the Cocks–Ashby model exhibits a nearly linear behavior between $\varepsilon = 0 - 0.4$ matching the micromechanical results very well as shown in Figure 3.3(a). Other void growth models, such as Rice and Tracey [1969] or McClintock [1968], also include the triaxiality in an exponential or hyperbolic sine nature.

A single void growth model alone is not sufficient to capture the void volume fraction evolution from the the micromechanical results shown in Figures 3.3 and 3.4. In both micromechanical simulations, the RVE boundaries were close enough to the initial voids to impact their growth. Horstemeyer et al. [2000] showed that if the intervoid ligament distance (ILD) was less than six diameters, then coalescence occurred for metals. The ILD in Steenbrink et al. [1997] was two diameters so the rate of growth would be expected to be greater than a single void growing. The ILD varied in Socrate and Boyce [2000] from 2.0 when $\phi_0 = 10\%$ to 1.5 when $\phi_0 = 25\%$, so the rate of growth would be greater than a single void growing as well. In order to match the Steenbrink et al. [1997] results and Socrate and Boyce [2000] results, a single void growth model would need to incorporate coalescence to addressing the small ILDs. Due to the RVE boundaries affecting void growth, using a simplified coalescence
Figure 3.3 Comparison between the Cocks–Ashby void growth model and the unit cell representative volume element (V–BCC Model).

Comparison between the Cocks–Ashby void growth model and the unit cell representative volume element (V–BCC Model) while varying the (a) initial void volume fraction ($\phi_0$) when $T_\Sigma = 0.33$ and (b) triaxiality ($T_\Sigma$) when $\phi_0 = 25\%$. The dashed lines represent the Cocks–Ashby equation and the solid lines represent the micromechanical simulation results from Socrate and Boyce [2000].
Figure 3.4  Comparison between the Cocks–Ashby void growth model and the unit cell representative volume element (SHA).

Comparison between the Cocks–Ashby void growth model and the unit cell representative volume element (SHA) while varying the triaxality when $\phi_0 = 8.3\%$. The dashed lines represent the Cocks–Ashby equation and the solid lines represent the micromechanical simulation results from Steenbrink et al. [1997].
equation, from Eq. (3.84), along with the Cocks–Ashby void growth equation more accurately captures all of the interacting mechanisms. Table 3.1 lists the parameters used to capture the void growth and coalescence interactions for the micromechanical simulations from Steenbrink et al. [1997] and Socrate and Boyce [2000], and Figure 3.5 shows the damage evolution as a function of strain. In Steenbrink et al. [1997], the ILD was only reported for stress triaxialities of 0.33, 1, and 3. In Socrate and Boyce [2000], the ILD was only reported for initial void volume fractions ($\phi_0$) of 10% and 25%. Including the coalescence ILD effects improves the accuracy of the model fits in both sets of data as shown in Figure 3.5. However, the hyperbolic nature of the void growth’s triaxiality function in Equation (3.82) does not follow the more linear micromechanical simulation results observed in in Figure 3.5(a).

$$\dot{c} = C_{\text{coal}1} \dot{\phi}_{\text{pores}} + C_{\text{coal}2} \left( \frac{4d_0}{d_{NN}} \right)^z \exp \left( C_{\text{coal}1} \theta \right) \|D_p\| \quad (3.84)$$

Table 3.1 Parameters for void growth and coalescence in Figure 3.5.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Steenbrink et al. [1997]</th>
<th>Socrate and Boyce [2000]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$m$</td>
<td>0.8</td>
<td>0.55</td>
</tr>
<tr>
<td>$C_{\text{coal}1}$</td>
<td>7.0</td>
<td>1.4</td>
</tr>
<tr>
<td>$C_{\text{coal}2}$</td>
<td>0.6</td>
<td>4.0</td>
</tr>
<tr>
<td>$z$</td>
<td>1.5</td>
<td>-2</td>
</tr>
</tbody>
</table>

Relationships directly relating the void volume fraction to both craze nucleation and craze growth are presently sparse. From other micromechanical simulations, Socrate et al. [2001] developed a model to predict multiple crazing in high impact
Figure 3.5  Comparison between the combined Cocks–Ashby void growth model and coalescence to literature data.

Comparison between the combined Cocks–Ashby void growth model and coalescence to data from (a) Steenbrink et al. [1997] and (b) Socrate and Boyce [2000].
polystyrene. Sharma et al. [2008] continued that work by calculating the craze volume fraction in an RVE of polymeric microlaminates. Seelig and der Giessen [2009] used the maximum hydrostatic stress as a criterion for craze initiation, and then a cohesive model (Tijssens et al. [2000] and Estevez et al. [2000]) for craze growth. A few creep craze damage models have been formulated (Luo et al. [2008] and Luo and Liu [2007]), and creep damage mechanisms have also been postulated by Hamouda et al. [2001]. Bucknall [2012] used linearly elastic fracture mechanics to relate biaxial loading conditions to craze initiation, and Estevez et al. [2000] studied how the fracture toughness in an amorphous glassy polymer changes by crazing and shear yielding. A good review of craze initiation as well as a fracture mechanics based approaches to crazing can be found in Bucknall [2007]. Starting with fracture mechanics, in a manner similar to Horstemeyer and Gokhale [1999] for particle nucleation, a craze nucleation will be shown here. Crazes generally initiate at locations of high stress intensity. Irwin’s equation for the stress intensity factor is given by the following,

\[ K_1 = \sigma_y \sqrt{2\pi r_p Y(w)} \]  \hspace{1cm} (3.85)

where \( K_1 \) is the stress intensity factor, \( \sigma_y \) is the yield stress, \( r_p \) is the plastic zone size, and \( Y(w) \) is a dimensionless constant or function that depends on the geometry of the specimen. Irwin’s equation (Eq. (3.85)) can be generalized as

\[ K_{ic} = f(\sigma) g(\zeta) Y(w) h(\text{rate}) \zeta(\theta) \]  \hspace{1cm} (3.86)
where \( f(\sigma) \) is a function of the applied stress, \( g(z) \) is a length scale parameter that uses the most important microstructural feature that contributes to crazing, \( h(\text{rate}) \) is a function related to strain rate, and \( \zeta(\theta) \) is a function related to temperature.

Tijssens et al. [2000] showed the importance that temperature plays in the behavior of crazes. Therefore, a simple Arrhenius temperature dependence is used for Eq. (3.86).

\[
\zeta(\theta) = \exp\left(\frac{C_{\eta\epsilon\theta}}{\theta}\right)
\]

Crazing is a complex process. The ability to nucleate crazes tends to increase the fracture toughness of polymers [Donald and Kramer, 1982], which is why dispersed rubber particles toughen thermoplastics. The particles generate many small crazes helping to dissipate energy. However, in thermoplastics with no inclusions, crazes are much less plentiful and when crazes do form, they tend to induce failure quicker rather than toughening the material. Therefore, and increase in the craze nucleation rate decreases the fracture toughness.

\[
h(\text{rate}) = \frac{\eta \| D_p \|}{\dot{\eta}}
\]

As for the geometrical function \( T(w) \), a material constant, \( C_{\text{coeff}} \), will be introduced to capture this geometrical effects once the craze evolution equation is integrated. The length scale parameter, \( g(z) \), in Eq. (3.86) represents the most important microstructural feature, which could be either the molecular weight, \( M_w \), [Pitman and Ward, 1979, Kramer, 1979, Rottler et al., 2002], molar weight [De Focatiis et al., 2008], or particle diameter [Donald and Kramer, 1982], since these features influence craze
nucleation. As crazes nucleate and grow primarily under tension [Sharma et al., 2008], an applied stress function, \( f(\sigma) \), is needed to account for this stress state dependence.

\[
f(\sigma) = f(I_1, J_2, J_3) = d_\eta \left[ \frac{4}{27} - \frac{J_3^2}{J_2^2} \right] + e_\eta \frac{J_3}{J_2^{3/2}} + f_\eta \frac{I_1 + \|I_1\|}{2\sqrt{J_2}}
\]  

(3.89)

This particular form allows for crazes to nucleate in tension as well as compression [Bevan, 1978], and torsion.

The craze nucleation rate is found by substituting Eqs. (3.87), (3.88), and (3.89) into Eq. (3.86) and then solving for \( \dot{\eta}_{\text{craze}} \).

\[
\dot{\eta}_{\text{craze}} = \eta_{\text{craze}} \frac{M_w}{K_{IC}} \|D_p\| \exp \left( \frac{C_{\eta\theta}}{\theta} \right) \left( d_\eta \left[ \frac{4}{27} - \frac{J_3^2}{J_2^2} \right] + e_\eta \frac{J_3}{J_2^{3/2}} + f_\eta \frac{I_1 + \|I_1\|}{2\sqrt{J_2}} \right)
\]  

(3.90)

The molecular weight was chosen as the most important microstructural feature for this study due to the absence of particles in an amorphous glassy polymer like PC, which will be studied in the next chapter’s FE analysis. Assuming a constant plastic strain rate, molecular weight, critical fracture toughness, and temperature, the integrated evolution equation in Eq. (3.90) becomes

\[
\eta_{\text{craze}} = C_{\text{coeff}} \exp \left[ \frac{M_w}{K_{IC}} \|\bar{E}_p\| \exp \left( \frac{C_{\eta\theta}}{\theta} \right) \left( d_\eta \left[ \frac{4}{27} - \frac{J_3^2}{J_2^2} \right] + e_\eta \frac{J_3}{J_2^{3/2}} + f_\eta \frac{I_1 + \|I_1\|}{2\sqrt{J_2}} \right) \right]
\]  

(3.91)

The damage rate resulting from a single craze is

\[
\dot{\phi}_{\text{craze}} = \dot{\eta}_{\text{craze}} \nu + \eta_{\text{craze}} \dot{\nu}
\]  

(3.92)

To show the functionality of this particular damage evolution, the damage due to crazing from the work of G’Sell et al. [2002] to the craze evolution in Eq. (3.92)
follows. In G’Sell et al. [2002], they calculated the volumetric strain during tension tests. They also analyzed micrographs at approximately 50% strain to show crazing details. From the micrograph in G’Sell et al. [2002], the number of crazes as well as the percent of crazes were calculated using ImageJ [Schneider et al., 2012]. Due to the limited micrographs, the void growth and crazing cannot be treated separately, thus they are plotted together in Fig. 3.6(a). The nucleation and total damage are plotted separately in Figs. 3.6(b) and (c), respectively. The total damage is calculated from the volumetric strain using Eq. (3.83). Table 3.2 lists the material properties and constants used. The Budiansky et al. [1982] void growth equation, Eq. (3.79), is also used. The experimental point for \( \nu_c \) will be slightly greater than reality due to G’Sell et al. [2002] forcing open the crazes in an unquantifiable manner to highlight them.

Table 3.2  The parameters used for the comparison to G’Sell et al. [2002].

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Nominal Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Strain rate</td>
<td>0.1</td>
<td>1/s</td>
</tr>
<tr>
<td>( C_{BUD} )</td>
<td>1.2</td>
<td>1/ unit area</td>
</tr>
<tr>
<td>( C_{coefficient} )</td>
<td>0.75</td>
<td></td>
</tr>
<tr>
<td>( M_w )</td>
<td>26</td>
<td>kg/mol</td>
</tr>
<tr>
<td>( d_\eta )</td>
<td>0</td>
<td>MPa(^2) mol ( \sqrt{\text{m}/\text{kg}} )</td>
</tr>
<tr>
<td>( e_\eta )</td>
<td>0</td>
<td>MPa(^{3/2}) mol ( \sqrt{\text{m}/\text{kg}} )</td>
</tr>
<tr>
<td>( f_\eta )</td>
<td>( 0.21 \times 10^{-3} )</td>
<td>mol ( \sqrt{\text{MPa m/kg}} )</td>
</tr>
<tr>
<td>( C_{y_ctheta} )</td>
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<td>K</td>
</tr>
<tr>
<td>( K_Ic )</td>
<td>7</td>
<td>MPa( \sqrt{\text{m}} )</td>
</tr>
<tr>
<td>( m )</td>
<td>1.2</td>
<td></td>
</tr>
<tr>
<td>( C_{\text{coal}_1} )</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>( C_{\text{coal}_2} )</td>
<td>1.5</td>
<td></td>
</tr>
<tr>
<td>( C_{\text{coal}_3} )</td>
<td>0</td>
<td></td>
</tr>
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Figure 3.6 Comparison between experimental work from G’Sell et al. [2002] to the proposed theoretical damage framework.

Comparison between experimental work from G’Sell et al. [2002] to the proposed theoretical damage framework excluding pre-existing porosity, void impingement effects, and temperature effects due to the lack of data. The experimental points are designated with a diamond (♦) in (a) the void growth and coalescence, $\nu_c$, and (b) the nucleation evolution. The total void volume fractions from the theory and experiment are compared in (c). Since the experimental specimen was bent after the test to expose the pores, the overall $\nu_c$ values were greater than what was actually experienced by the material in G’Sell et al. [2002]. Hence, our theoretical comparison for $\nu_c$ would be in closer agreement, where the number density would be equivalent.
The coalescence term, $\dot{c}$, in Eq. (3.76), take the following form in a manner similar to Horstemeyer et al. [2000] and Allison [2009].

$$
\dot{c} = C_{\text{coal}1} \left( \dot{\eta}_{\text{particle}} \nu + i \dot{\eta}_{\text{particle}} \right) + C_{\text{coal}2} \left( \dot{\eta}_{\text{craze}} \nu + i \dot{\eta}_{\text{craze}} \right) + C_{\text{coal}3} \left( \frac{4d_0}{d_{\text{NN}}} \right)^z \exp \left( C_{c\theta} \theta \right) \| D_p \|
$$

\hspace{10cm} (3.93)

where $C_{\text{coal}1}$, $C_{\text{coal}2}$, and $C_{\text{coal}3}$ are coalescence dependent parameters. The lengths $d_0$ and $d_{\text{NN}}$ represent the average particle diameter and the nearest neighbor distance, respectively. $C_{c\theta}$ is a void coalescence temperature dependent parameter, and $z$ is a material constant. The impingement term in Eq. (3.93) would only be needed as particles are added into matrix. Impingement in this case refers to void nucleating at particles and those voids growing together without crazing. As crazing is a complicated mechanism, there are at least two ways crazes coalesce. When rubber particles are distributed to toughen a polymer, thousands if not millions of crazes are formed [Nielsen and Landel, 1994], which is what the first term in Eq. (3.93) captures. Crazes also coalesce with other crazes, which is what the middle term of Eq. (3.93) attempts to capture.

### 3.4.6 Temperature Evolution

As thermoplastic polymers are strongly temperature dependent, their material models require a robust approach in capturing two dependencies: first, how temperature affects the stress and stress-like ISVs and second, how the temperature changes due to deformation. Experimental works such as Garg et al. [2008] and Bjerke
et al. [2002] where temperature increase during deformation is studied are critical in understanding these effects at the macroscale. From the heat equation, Eq. 3.44, the rise in temperature is simplified as

$$\dot{\theta} = \frac{1}{C_v + 3f_0\dot{e}_V - f_0 \text{tr} (\dot{\bar{M}})} \left\{ \bar{G}_e : \dot{E}_e + \bar{G}_1 \dot{\xi}_1 + \bar{G}_2 \dot{\xi}_2 + \bar{G}_\alpha \dot{\bar{\alpha}} + \bar{M} : \dot{\bar{L}}_p - \nabla \cdot \bar{Q} + \bar{R}_V \right\} \times \left( \frac{f_0}{3(1-\phi)} \left[ (\bar{G}_e - 3\bar{S}) : \dot{E}_e + \bar{G}_1 \dot{\xi}_1 + \bar{G}_2 \dot{\xi}_2 \right] + \bar{G}_\alpha : \dot{\bar{\alpha}} - \text{tr} (\bar{S}) + 3\bar{e}_V \right)$$

(3.94)

by assuming isotropic damage

$$\bar{G}_e = \left( 2 \frac{\partial \mu (\theta)}{\partial \theta} E_1 + \frac{\partial \lambda (\theta)}{\partial \theta} \text{tr} (E_e) \bar{1} \right) \theta^2 (1-\phi)^{2/3} - f_0 \theta S$$

$$\bar{G}_1 = 2C_{g_1} \bar{\xi}_1 \left( \frac{\partial \mu (\theta)}{\partial \theta} + \mu (\theta) (3f_0\theta - 1) \right) (1-\phi)^{2/3}$$

(3.95)

$$\bar{G}_2 = 2C_{g_2} \bar{\xi}_2 \left( \frac{\partial \mu (\theta)}{\partial \theta} + \mu (\theta) (3f_0\theta - 1) \right) (1-\phi)^{2/3}$$

$$\bar{G}_\alpha = 6C_bf_0\mu_R (\theta) \bar{\alpha} (1-\phi)^{2/3}$$

where

$$\frac{\partial \mu (\theta)}{\partial \theta} = \frac{E_1}{2(1-\nu_p)}, \quad \frac{\partial \lambda (\theta)}{\partial \theta} = \frac{E_1\nu_p}{(1+\nu_p)(1-2\nu_p)}$$

(3.96)

3.4.7 Temperature Dependence of the Physical Properties

As physical properties in thermoplastics are temperature dependent, below $T_g$, the density, heat capacity per unit volume, and thermal conductivity, from van Krevelen and te Nijenhuis [2009] and Bicerano [2002], are given as

$$\rho (\theta) = \rho (298 \text{K}) \frac{1.42T_g + 44.7}{1.42T_g + 0.15\theta}$$

(3.97)
\[ \tilde{C}_V(\theta) = \tilde{C}_V(298 \text{ K}) \left[ 0.106 + 3 \times 10^{-3} \theta \right] \]  
\[ k(\theta) = k(T_g) \left( \frac{\theta}{T_g} \right)^{0.22} \]
CHAPTER 4

MODEL IMPLEMENTATION, CALIBRATION, AND COMPARISON

4.1 Implementation

To implement the three-dimensional constitutive model, an forward Euler (explicit) time integration scheme was developed for a user subroutine (vumat) in Abaqus/Explicit\(^1\). The vumat was written in FORTRAN. The forward Euler method solves ordinary differential equations using the formula

\[ y_{n+1} = y_n + hf(x_n, y_n) \]  (4.1)

which advances a solution from \( x_n \) to \( x_{n+1} = x_n + h \). The subscript \( n \) represents the beginning of the step and \( n + 1 \) represents the end of the step. A summary of the implementation follows\(^2\).

1. The total deformation gradient tensor at the beginning and end of the step is given from Abaqus \((F_n, F_{n+1})\). ISVs, plastic and thermal deformation gradient tensors, total plastic strain, total damage, damage from pores, and temperature at the beginning of the step is given from Abaqus

\[(F^p_n, F^\theta_n, \bar{\gamma}_n^p, \bar{\gamma}_n^\theta, \bar{\xi}_n^p, \bar{\xi}_n^\theta, \bar{\xi}_n^p, \bar{\xi}_n^\theta, \alpha_n, \phi_n, \phi_{\text{pores}_n}, \theta_n).\]

\(^1\)The implemented model uses a different backstress than presented in the previous section. Also, the plastic spin is assumed to be zero. See Appendix B for a summary of the implemented model.

\(^2\)The \( e, p, \) and \( \theta \) that were shown in the subscript in the theoretical section have been placed in the superscript location to avoid confusion with the \( ns \) and \((n + 1)s\).
2. The elastic deformation gradient at the beginning of the step is determined by rearranging Equation (3.2).\(^3\)

\[
\bar{F}_n^\rho = \bar{F}_n \bar{F}_n^{\rho - 1} \bar{F}_n^{\rho - 1}
\] (4.2)

3. The elastic right stretch tensor at the beginning of the step is determined using Equation (3.16) and the Jacobi eigenvalue algorithm [Jacobi, 1846], which finds the square root of a matrix.

\[
\bar{U}_n^\rho = \sqrt{\bar{C}_n} = \sqrt{\bar{F}_n \bar{F}_n^\top}
\] (4.3)

4. The true (logarithmic/Hencky) elastic strain at the beginning of the step is calculated.

\[
\bar{E}_n^\rho = \ln \bar{U}_n^\rho
\] (4.4)

5. The temperature and damage dependent moduli at the beginning of the step are determined from Equations (3.49) and (3.48). The damage function \((1 - \phi)^{2/3}\) that was on the stresses and thermodynamic force conjugates was moved to the Young’s modulus for simplicity and the mathematical result is unchanged.

\[
E_n = [E_{\text{ref}} + E_1 (\theta_n - \theta_{\text{ref}})] (1 - \phi_n)^{2/3}
\] (4.5)

\[
\mu_n = \frac{E_n}{2 (1 + \nu)}, \quad K_n = \frac{2\mu_n (1 + \nu)}{3 (1 - 2\nu)}
\] (4.6)

6. The rubbery modulus at the beginning of the step is calculated using Equation (B.14).

\[
\mu_{R_n} = C_1 (\theta_n - \theta_{\text{ref}}) + C_2
\] (4.7)

\(^3\)See future work Section 5.2.1 for an explanation of why the damage deformation gradient is not used.
7. The eigenvalues \((\lambda_{\alpha}^\alpha)\) of \(\boldsymbol{\alpha}_n\) are calculated using the Jacobi eigenvalue algorithm.

The modulus for the backstress at the beginning of the step is determined using Equation (B.13).

\[
\mu_{B_n} = \mu_{R_n} \left[ \left( -\frac{\lambda_{1_n}^\alpha + \lambda_{2_n}^\alpha + \lambda_{3_n}^\alpha - 3}{\lambda_L} \right)^{-1} (1 - \phi_n)^{2/3} \right] \quad (4.8)
\]

8. The Mandel stress at the beginning of the step, \(\bar{M}_n\), is determined using Equation (B.2).

\[
\bar{M}_n = 2\mu_n \bar{E}_n^\varepsilon + \left( K_n - \frac{2}{3}\mu_n \right) \text{tr} (\bar{E}_n^\varepsilon)\quad (4.9)
\]

9. The thermodynamic force conjugates at the beginning of the step \((\bar{\kappa}_1, \bar{\kappa}_2, \text{and } \bar{b}_n)\) are determined using Equations (B.17), (B.18), and (B.19).

\[
\bar{\kappa}_{1n} = C_{\bar{\kappa}_1} \mu_n \bar{\xi}_{1n}, \quad \bar{\kappa}_{2n} = C_{\bar{\kappa}_2} \mu_n \bar{\xi}_{2n}, \quad \bar{b}_n = \mu_B (\theta_n) \bar{\alpha}_n \quad (4.10)
\]

10. The effective stress at the beginning of the step \((\bar{\tau}_n)\), and the hydrostatic stress at the beginning of the step \((\bar{\pi}_n)\) will be used for the plastic shear strain rate in Equation (B.6).

\[
\bar{\tau}_n = \frac{1}{\sqrt{2}} \left\| \bar{M}_n - \bar{b}_n' \right\|, \quad \bar{\pi}_n = -\frac{1}{3} \text{tr} (\bar{M}_n) \quad (4.11)
\]

11. The temperature dependent yield surface at the beginning of the step is determined using Equation (3.66).

\[
Y_n = C_3 (\theta_n - \theta_{\text{ref}}) + C_4 \quad (4.12)
\]
12. The change in the plastic shear strain at the beginning of the step is determined from Equation (B.6).

\[ \Delta \gamma_p^n = \hat{\gamma}_0 \exp \left( \left( \frac{\Delta H_\beta}{k_B \theta_n} \right) \sinh^n \left( \frac{\tau_n - (Y_n + \kappa_1 + \kappa_2 + \alpha_p \pi_n)}{2k_B \theta_n} \right) \right) \Delta t \] (4.13)

13. The plastic rate of deformation at the beginning of the step is determined from Equation (B.5).

\[ D_n^p = \frac{1}{\Delta t \sqrt{2}} \Delta \gamma_p^n \tilde{N}_n^p, \quad \tilde{N}_n^p = \frac{\tilde{M}_n' - \tilde{b}_n'}{\|\tilde{M}_n' - \tilde{b}_n'\|} \] (4.14)

14. The temperature dependent variables for strain-like chain slip evolution equation in Equation (3.64) are calculated for the beginning of the step.

\[ \xi_0^n = C_5 (\theta_n - \theta_{\text{ref}}) + C_6, \quad \xi_{\text{sat}}^n = C_7 (\theta_n - \theta_{\text{ref}}) + C_8, \quad g_0^n = C_9 (\theta_n - \theta_{\text{ref}}) + C_{10} \] (4.15)

15. Using the forward Euler method, the strain-like chain slip evolution equation in Equation (3.63) is calculated at the end of the step.

\[ \tilde{\xi}_{n+1}^* = \tilde{\xi}_n^* + \left( \tilde{\xi}_{\text{sat}}^* - g_0 \tilde{\xi}_n^* \right) \Delta \gamma_p^n \] (4.16)

16. Using the forward Euler method, the ISV chain entanglement evolution equation in Equation (3.63) is calculated at the end of the step.

\[ \tilde{\xi}_{n+1} = H_1 \left( \frac{\tilde{\xi}_n}{\tilde{\xi}^*_n} \right) \Delta \gamma_p^n \] (4.17)
17. The saturation value for the ISV $\xi_2$ from Equation (3.68) and the effective plastic stretch from Equation (3.67) [Ames et al., 2009] is calculated at the beginning of the step.

$$\xi_{2\text{sat}} = C_{11} (\theta_n - \theta_{\text{ref}}) + C_{12}, \quad \bar{\lambda}_n^p = \sqrt{\frac{\text{tr} (F_n^p F_n)}{3}} \quad (4.18)$$

18. Using the forward Euler method, the ISV large-strain chain alignment/coiling evolution equation in Equation (3.67) is calculated at the end of the step.

$$\xi_{2n+1} = H_2 (\bar{\lambda}_n^p - 1) \left( \frac{\xi_{2n}}{\xi_{2\text{sat}}} \right) \Delta \bar{s}_n^p \quad (4.19)$$

19. The temperature dependent material parameter $R_{s1n}$ is calculated at the beginning of the step using Equation (B.16).

$$R_{s1n} = C_{13} (\theta_n - \theta_{\text{ref}}) + C_{14} \quad (4.20)$$

20. The direction-dependent hardening instigated by chain stretching between entanglement points second-rank tensor ISV from Equation (B.15) at the end of the step.

$$\bar{\alpha}_{n+1} = \bar{\alpha}_n + R_{s1n} (\bar{D}_n^p \bar{\alpha}_n - \bar{\alpha}_n \bar{D}_n^p) \Delta t \quad (4.21)$$

21. From the plastic flow rule in Equation (B.5), the plastic deformation gradient tensor at the end of the step is calculated.

$$\dot{F}_p = \bar{D}_p F_p \quad \Rightarrow \quad \frac{F_{n+1}^p - F_n^p}{\Delta t} = \bar{D}_n^p F_n^p \quad (4.22)$$

$$F_{n+1}^p = (\Delta t \bar{D}_n^p + 1) F_n^p \quad (4.23)$$

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22. The density and heat capacity from Equations (3.97) and (3.98), respectively, are determined at the beginning of the step.

\[ \rho_n = \rho(298 \text{ K}) \frac{1.42T_g + 44.7}{1.42T_g + 0.15\theta_n} \quad (4.24) \]

\[ \bar{C}_V_n = \bar{C}_V(298 \text{ K}) \left[ 0.106 + 3 \times 10^{-3}\theta_n \right] \quad (4.25) \]

23. The temperature at the end of the step is calculated using Equation (B.20).

\[ \theta_{n+1} = \theta_n + \frac{\Delta t}{\bar{C}_V_n \rho_n} \left( \omega \bar{M}_n : \bar{D}_n^p - \bar{\nabla} \cdot \bar{Q} + \bar{R}_V \right) \quad (4.26) \]

24. The temperature deformation gradient tensor at the end of the step is calculated from Equation (3.11).

\[ \bar{F}^{e}_{n+1} = [1 + \alpha_{\text{th}} (\theta_{n+1} - \theta)] \mathbf{1} \quad (4.27) \]

25. The plastic Lagrangian strain in the reference configuration at the beginning of the step is determined using Equation (3.13).

\[ \bar{E}^p_n = \frac{1}{2} \left( \bar{F}^o_n^{-T} \bar{F}^o_n - \mathbf{1} \right) \quad (4.28) \]

26. The plastic Lagrangian strain is pushed forward the the intermediate configuration \( \bar{B} \).

\[ \bar{E}^p_n = \bar{F}_n^{-T} \bar{F}_n^{d^{-T}} \bar{F}_n^{o^{-T}} \bar{E}^o_n \bar{F}_n^{o^{-1}} \bar{F}_n^{d^{-1}} \bar{F}_n^{-1} \quad (4.29) \]

27. The first invariant of the stress and the second invariant of the deviatoric stress is calculated at the beginning of the step.

\[ I_{1n} = \text{tr} \, \bar{M}_n, \quad J_{2n} = \frac{1}{2} \bar{M}_n : \bar{M}_n^\prime \quad (4.30) \]
28. The damage due to pre-existing pores (Cocks–Ashby) is calculated at the end of the step using Equation (3.81).

\[ \phi_{\text{pores}_{n+1}} = 1 - \left\{ 1 + \left[ (1 - \phi_{\text{pores}_n})^{1+m} - 1 \right] \exp \left[ \chi D_n^p \Delta t (1 + m) \right] \right\}^{1/(1+m)} \]  
\[ \chi = \sinh \left( \frac{2(2m - 1)I_1}{3(2m + 1)\sqrt{3J_2}} \right) \]  

29. The number of nucleated crazes are determined for the end of the step using Equation (3.91).

\[ \eta_{\text{craze}_{n+1}} = C_{\text{coeff}} \exp \left[ \frac{M_w}{K_{\text{ic}}} \| \vec{E}_n^p \| \exp \left( \frac{C_{\text{rep}}}{\theta} \right) \right. \]
\[ \times \left\{ d_\eta \left[ \frac{4}{27} \frac{J_3^n}{J_2^n} \right] + e_\eta \frac{J_3^n}{J_2^n} + f_\eta \frac{I_1^{1/3} + \| I_1^n \|}{2\sqrt{J_2^n}} \right\} \]  

30. The number of voids nucleated from particles are determined for the end of the step using Equation (3.78).

\[ \eta_{\text{particle}_{n+1}} = C_{\text{coeff}} \exp \left[ \left( \frac{d_1}{d_2} \right)^{1/3} \| \vec{E}_n^p \| \exp \left( \frac{C_{\text{rep}}}{\theta} \right) \right. \]
\[ \times \left\{ a_\eta \left[ \frac{4}{27} \frac{J_3^n}{J_2^n} \right] + b_\eta \frac{J_3^n}{J_2^n} + c_\eta \frac{I_1^n}{\sqrt{J_2^n}} \right\} \]  

31. The Budiansky void growth at the end of the step is determined using Equation (3.80).

\[ \nu_{n+1} = C_{\text{BUD}} \exp \left\{ \frac{3}{2} \frac{\| \vec{E}_n^p \|}{\sqrt{12J_2}} \left[ \left( \frac{I_1^n}{\sqrt{12J_2}} + \frac{(m - 1)(m + 0.4319)}{m^2} \right)^m \right] \right\} \]  

32. The total coalescence at the end of the step is determined using Equation (3.93).

\[ c_{n+1} = C_{\text{coal}_1} (\nu_{n+1} \eta_{\text{particle}_{n+1}}) + C_{\text{coal}_2} (\nu_{n+1} \eta_{\text{craze}_{n+1}}) \]
\[ + C_{\text{coal}_3} \left( \frac{4d_0}{d_{\text{NN}}} \right)^z \exp (C_{\text{cr}} \theta) \| \vec{E}_n^p \| \]
33. The total damage at the end of the step is determined using Equation (3.76).

$$\phi_{n+1} = \left( \nu_{n+1} \eta_{\text{particle}_{n+1}} + \phi_{\text{pores}_{n+1}} + \nu_{n+1} \eta_{\text{craze}_{n+1}} \right) c_{n+1}$$ (4.37)

34. The elastic deformation gradient at the end of the step is determined by rearranging Equation (3.2).

$$\bar{F}^e_{n+1} = \bar{F}^e_{n+1} \bar{F}^{\theta-1}_{n+1}$$ (4.38)

35. The elastic right stretch tensor at the end of the step is determined using Equation (3.16) and the Jacobi eigenvalue algorithm [Jacobi, 1846], which finds the square root of a matrix.

$$\bar{U}^e_{n+1} = \sqrt{\bar{C}^e_{n+1}} = \sqrt{\bar{F}^e_{n+1} \bar{F}^{eT}_{n+1}}$$ (4.39)

36. The true (logarithmic/Hencky) elastic strain at the end of the step is calculated.

$$\ell^e_{n+1} = \ln \bar{U}^e_{n+1}$$ (4.40)

37. The temperature and damage dependent moduli at the end of the step are determined from Equations (3.49) and (3.48).

$$E_{n+1} = \left[ E_{\text{ref}} + E_1 \left( \theta_{n+1} - \theta_{\text{ref}} \right) \right] \left( 1 - \phi_{n+1} \right)^{2/3}$$ (4.41)

$$\mu_n = \frac{E_n}{2(1+\nu)}, \quad K_n = \frac{2\mu_n (1+\nu)}{3(1-2\nu)}$$ (4.42)

38. The Mandel stress at the end of the step, $\bar{M}_{n+1}$, is determined using Equation (B.2).

$$\bar{M}_{n+1} = 2\mu_{n+1} \bar{E}^e_{n+1} + \left( K_{n+1} - \frac{2}{3} \mu_{n+1} \right) \text{tr} \left( \bar{E}^e_{n+1} \right) 1$$ (4.43)
39. The elastic rotation tensor, $\bar{R}_{n+1}^e$, is calculated at the end of the step from Equation (3.15).

$$\bar{R}_{n+1}^e = \bar{F}_{n+1}^e \bar{U}_{n+1}^{-1}$$  \hspace{1cm} (4.44)

40. The elastic Jacobian at the end of the step, $J_{n+1}^e$, is determined from Equation (3.10).

$$J_{n+1}^e = \det (\bar{F}_{n+1}^e)$$  \hspace{1cm} (4.45)

41. The Cauchy stress at the end of the step is calculated using Equation (3.27).

$$\sigma_{n+1} = J_{n+1}^{e^{-1}} \bar{R}_{n+1}^e \bar{M}_{n+1} \bar{R}_{n+1}^T$$  \hspace{1cm} (4.46)

42. ISVs, plastic and thermal deformation gradient tensors, total plastic strain, total damage, damage from pores, temperature, and stress at the end of the step is given to Abaqus

$$\left( F_{n+1}^p, F_{n+1}^\theta, \tilde{\xi}_{n+1}^p, \tilde{\xi}_{n+1}^s, \tilde{\xi}_{n+1}^t, \tilde{\xi}_{n+1}^\alpha, \tilde{\xi}_{n+1}^\phi, \tilde{\xi}_{n+1}^\theta, \xi_{n+1}^\alpha, \xi_{n+1}^\phi, \xi_{n+1}^\theta, \phi_{n+1}, \phi_{\text{pores}_{n+1}}, \theta_{n+1}, \sigma_{n+1} \right).$$

43. If the total damage at the end of the step is greater than a predefined threshold, the stress in the element becomes zero, which effectively means the element is removed from the simulation.

### 4.2 Calibration of Material Point Simulator to a Three Dimensional Single Element

The damage evolution equations (Section 3.4.5) that were implemented in a three-dimensional FORTRAN routine (Section 4.1) were compared against a simple one-dimensional formulation. The one-dimensional formulation, henceforth called a
Figure 4.1 Comparison between material point simulator and FE simulation.

(a) The stress–strain response of the three-dimensional tension simulation.
(b) The plastic strain from the material point simulator (1-D) and the Abaqus simulation (3-D).

The material point simulator, was written in Excel. The material point simulator uses a given stress state and plastic strain rate along with all the damage parameters. The evolution of each damage variable ($\phi_{\text{total}}$, $\phi_{\text{pore}}$, $\phi_{\text{particle}}$, $\phi_{\text{craze}}$, $\eta_{\text{particle}}$, $\eta_{\text{craze}}$, $\nu$, and $c$) is monitored. The material point simulator enables users to fit damage evolution. To check the accuracy of the material point simulator, one element was deformed in tension in a three-dimensional FE simulation. Each damage variable listed above was compared between the FE simulation and the material point simulator. Most damage parameters were given non-zero values; however, the values given, shown in Table 4.1, do not characterize any of the materials in this study.
Table 4.1  Material properties for only damage parameters to verify material point simulator and three-dimensional simulation.

<table>
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<tr>
<th>Parameters</th>
<th>Values</th>
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<tr>
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<td>1/s</td>
</tr>
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<td>$\theta$</td>
<td>256</td>
<td>K</td>
</tr>
<tr>
<td>Initial $\phi_{\text{pore}}$</td>
<td>0.001</td>
<td></td>
</tr>
<tr>
<td>Cocks–Ashby $m$</td>
<td>7</td>
<td></td>
</tr>
<tr>
<td>$a_\eta$</td>
<td>0</td>
<td>MPa</td>
</tr>
<tr>
<td>$b_\eta$</td>
<td>0</td>
<td>MPa</td>
</tr>
<tr>
<td>$c_\eta$</td>
<td>6</td>
<td>MPa</td>
</tr>
<tr>
<td>$C_{P\text{coeff}}$</td>
<td>0.2</td>
<td></td>
</tr>
<tr>
<td>$d$</td>
<td>0.1</td>
<td>mm</td>
</tr>
<tr>
<td>$K_{\text{ic particle}}$</td>
<td>5</td>
<td>MPa $\sqrt{\text{mm}}$</td>
</tr>
<tr>
<td>$f$</td>
<td>0.05</td>
<td></td>
</tr>
<tr>
<td>$C_{\eta\theta}$</td>
<td>34</td>
<td>K</td>
</tr>
<tr>
<td>$d_\eta$</td>
<td>0</td>
<td>MPa $^2$ mol $\sqrt{\text{m/kg}}$</td>
</tr>
<tr>
<td>$e_\eta$</td>
<td>0</td>
<td>MPa$^{3/2}$ mol $\sqrt{\text{m/kg}}$</td>
</tr>
<tr>
<td>$f_\eta$</td>
<td>2.5</td>
<td>mol $\sqrt{\text{MPa m/kg}}$</td>
</tr>
<tr>
<td>$M_w$</td>
<td>5</td>
<td>kg/mol</td>
</tr>
<tr>
<td>$C_{C\text{coeff}}$</td>
<td>0.1</td>
<td></td>
</tr>
<tr>
<td>$K_{\text{ic matrix}}$</td>
<td>7</td>
<td>MPa $\sqrt{\text{mm}}$</td>
</tr>
<tr>
<td>$C_{\eta\mu\theta}$</td>
<td>44</td>
<td>K</td>
</tr>
<tr>
<td>$C_{\text{BUD}}$</td>
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<td></td>
</tr>
<tr>
<td>$m_{\text{BUD}}$</td>
<td>2</td>
<td></td>
</tr>
<tr>
<td>$C_{\text{coal}_1}$</td>
<td>0.02</td>
<td></td>
</tr>
<tr>
<td>$C_{\text{coal}_2}$</td>
<td>0.3</td>
<td></td>
</tr>
<tr>
<td>$C_{\text{coal}_3}$</td>
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<td></td>
</tr>
<tr>
<td>$d_0$</td>
<td>0.001</td>
<td>µm</td>
</tr>
<tr>
<td>$d_{\text{NN}}$</td>
<td>0.4</td>
<td>µm</td>
</tr>
<tr>
<td>$z$</td>
<td>1.5</td>
<td></td>
</tr>
<tr>
<td>$C_{c\theta}$</td>
<td>0.001</td>
<td>1/K</td>
</tr>
</tbody>
</table>
The comparison between the material point simulator and the three-dimensional Abaqus simulation is shown in Figures 4.1 and 4.2. The true stress–true strain response of the single element is shown in Figure 4.1(a). Plasticity parameters for PC from Bouvard et al. [2013], listed in Table 4.2, were used to produce such a response. Figure 4.1(b) shows the plastic strain the during the FE simulation compared to the material point simulator. In the FE simulation, the plastic strain did not increase linearly. Instead, the plastic strain evolution in the FE simulation takes on a slightly sigmoidal shape. The material point simulator assumes a linear plastic strain rate. The plastic strain rate used for comparison was 0.625/s. Even with the slight variation in plastic strain rate, good agreement is seen between each function of damage, as shown in Figure 4.2. For the Cocks–Ashby and Budiansky void growth evolution in Figures 4.2(a) and 4.2(b), respectively, the material point simulator and FE simulation are less than 1% different at 50% plastic strain. The material point simulator slightly over predicts the particle and craze nucleation shown in Figures 4.2(c) and 4.2(c), respectively. The slight over prediction causes both the coalescence, shown in Figure 4.2(e), and the total damage, shown in Figure 4.2(f), in the material point simulator to deviate from the FE results. However, the percent difference in the total damage between the one-dimensional case and three-dimensional FE simulation at 50% plastic strain is approximately 4%.
Table 4.2  Non-damage model parameters for PC, from Bouvard et al. [2013].

<table>
<thead>
<tr>
<th>Regime</th>
<th>Parameter</th>
<th>Constants</th>
<th>Units</th>
<th>PC</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Elasticity</strong></td>
<td>$E$</td>
<td>$E_{\text{ref}}$</td>
<td>MPa</td>
<td>2250</td>
</tr>
<tr>
<td></td>
<td>$E$</td>
<td>$E_1$</td>
<td>MPa/K</td>
<td>-2.72</td>
</tr>
<tr>
<td></td>
<td>$E$</td>
<td>$\theta_{\text{ref}}$</td>
<td>K</td>
<td>298</td>
</tr>
<tr>
<td></td>
<td>$\nu_p$</td>
<td></td>
<td></td>
<td>0.36</td>
</tr>
<tr>
<td><strong>Viscoplasticity</strong></td>
<td>$\dot{\gamma}_p$</td>
<td>$\dot{\gamma}_{p0}$</td>
<td>1/s</td>
<td>$1.294 \times 10^{19}$</td>
</tr>
<tr>
<td></td>
<td>$\dot{\gamma}_p$</td>
<td>$\Delta H_{\beta}$</td>
<td>KJ/mol</td>
<td>57.7</td>
</tr>
<tr>
<td></td>
<td>$\dot{\gamma}_p$</td>
<td>$V$</td>
<td>m$^3$</td>
<td>$4.98 \times 10^{-29}$</td>
</tr>
<tr>
<td></td>
<td>$\dot{\gamma}_p$</td>
<td>$n$</td>
<td></td>
<td>7</td>
</tr>
<tr>
<td></td>
<td>$\dot{\gamma}_p$</td>
<td>$\alpha_p$</td>
<td></td>
<td>0.109</td>
</tr>
<tr>
<td></td>
<td>$Y$</td>
<td>$C_3$</td>
<td>MPa/K</td>
<td>-0.02</td>
</tr>
<tr>
<td></td>
<td>$Y$</td>
<td>$C_4$</td>
<td>MPa</td>
<td>19</td>
</tr>
<tr>
<td><strong>Softening ($\xi_1$)</strong></td>
<td>$\bar{\xi}_s$</td>
<td>$C_5$</td>
<td>1/K</td>
<td>-0.003</td>
</tr>
<tr>
<td></td>
<td>$\xi_0$</td>
<td>$C_6$</td>
<td></td>
<td>0.516</td>
</tr>
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<td></td>
<td>$\xi_0^*$</td>
<td>$C_7$</td>
<td>1/K</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>$\xi_{\text{sat}}$</td>
<td>$C_8$</td>
<td></td>
<td>0.05</td>
</tr>
<tr>
<td></td>
<td>$g_0$</td>
<td>$C_9$</td>
<td>1/K</td>
<td>0.05</td>
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<tr>
<td></td>
<td>$g_0$</td>
<td>$C_{10}$</td>
<td></td>
<td>5.96</td>
</tr>
<tr>
<td></td>
<td>$H_1$</td>
<td></td>
<td></td>
<td>30</td>
</tr>
<tr>
<td></td>
<td>$\xi_{10}$</td>
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<td></td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>$C_{\bar{\kappa}_1}$</td>
<td></td>
<td></td>
<td>$5 \times 10^{-2}$</td>
</tr>
<tr>
<td><strong>Hardening ($\xi_2$)</strong></td>
<td>$\bar{\xi}_{\text{sat}}$</td>
<td>$C_{11}$</td>
<td>1/K</td>
<td>-0.0015</td>
</tr>
<tr>
<td></td>
<td>$\bar{\xi}_{\text{sat}}$</td>
<td>$C_{12}$</td>
<td></td>
<td>0.6</td>
</tr>
<tr>
<td></td>
<td>$\bar{\xi}_{\text{sat}}$</td>
<td>$H_2$</td>
<td></td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>$\xi_{2s}$</td>
<td></td>
<td></td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>$C_{\bar{\kappa}_2}$</td>
<td></td>
<td></td>
<td>$5 \times 10^{-2}$</td>
</tr>
<tr>
<td><strong>Hardening ($\alpha$)</strong></td>
<td>$\lambda_L$</td>
<td></td>
<td></td>
<td>4</td>
</tr>
<tr>
<td></td>
<td>$\mu_R$</td>
<td>$C_1$</td>
<td>MPa/K</td>
<td>-0.15</td>
</tr>
<tr>
<td></td>
<td>$\mu_R$</td>
<td>$C_2$</td>
<td>1/K</td>
<td>15</td>
</tr>
<tr>
<td></td>
<td>$R_{s1}$</td>
<td>$C_{13}$</td>
<td>1/K</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>$R_{s1}$</td>
<td>$C_{14}$</td>
<td></td>
<td>0.99</td>
</tr>
<tr>
<td><strong>Thermal</strong></td>
<td>$\alpha_{\text{th}}$</td>
<td></td>
<td>1/K</td>
<td>$7.7 \times 10^{-5}$</td>
</tr>
<tr>
<td></td>
<td>$\omega$</td>
<td></td>
<td></td>
<td>0.6</td>
</tr>
</tbody>
</table>
Figure 4.2  Plots of certain functions of the damage model using the material properties from Table 4.1 as a function of the plastic strain.

Plots of the following functions of the damage model using the material properties from Table 4.1 as a function of the plastic strain: (a) Cocks–Ashby void growth, (b) Budiansky void growth, (c) particle nucleation, (d) craze nucleation, (e) total coalescence, and (f) total damage.
4.3 Comparison to PC Impact Experiment

To employ the damage evolution equations in a full-scale FE simulation, the numerical model is compared to PC impact tests [Bouvard et al., 2009]. The impact tests were performed by following ASTM test standard D 5628 using a disk with a diameter of 100.5 mm and a thickness of 3.1 mm. The tests were displacement controlled and three impact velocities were considered: 3 mm/s, 30 mm/s, and 300 mm/s. All tests were performed at room temperature. A servo-hydraulic machine setup at the University of Dayton Research Institute, shown in Figure 4.3, was used to impact disks. The upper test fixture is secured to the upper cross-head on the test frame. The top fixture holds the PC disk while the loading nose is fastened to the actuator that moves during the event. Sufficient pressure from the fixture is applied along the edge of the disk to prevent slippage of the PC disk during impact. The diameter of the loading nose is 12.7 mm. A load cell is located under the loading nose to measure the load on impact. The loading nose moves at constant velocity until complete penetration and failure of the disk. Three repeat tests were performed at each strain rate and the results (force–displacement) were averaged.

For numerical predictions, non-unique material properties for damage as no image analysis was performed on the fractured surface. Regardless, the damage evolution will behave in an exponential manner. The geometry, loading, and boundary conditions for the simulations are shown in Figure 4.4. No friction was assumed between the striker and specimen.
Figure 4.3  Impact testing setup using a servo-hydraulic machine.

Figure 4.4  The axisymmetric model for polycarbonate impact tests showing the geometry, loading, and boundary conditions.
Because the disks were circular, the FE simulations for each strain rate employed axisymmetric elements. The striker was assumed rigid using element type RAX2 and the specimen was assumed deformable using element type RAX4R. Due to large deformation around the impact area, an adaptive mesh was used to ensure accuracy. The mesh is shown in Figure 4.5.

![Mesh of the polycarbonate specimen used in the FE impact simulations highlighting the element types and adaptive mesh domain.](image)

Figure 4.5  Mesh of the polycarbonate specimen used in the FE impact simulations highlighting the element types and adaptive mesh domain.

Figure 4.6 shows the comparisons between the numerical simulations and the experimental data at the three impact velocities (3 mm/s, 30 mm/s, and 300 mm/s). Each plot in Figure 4.6 compares two simulations per experiment: a simulation with no damage and a simulation with damage. The material parameters for damage for these simulations are listed in Table 4.3. The PC disks were made of a different material
than the PC in Chapter 2. Because no inclusions, particles, or pre-existing voids were assumed in the PC, all damage parameters relating to damage from particles and pre-existing voids are zero. Also, the material parameters not relating to damage for PC are listed in Table 4.2.

Table 4.3 Material properties for polycarbonate impact simulation.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Nominal Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_{\text{BUD}}$</td>
<td>1.0</td>
<td>1/ unit area</td>
</tr>
<tr>
<td>$m_{\text{BUD}}$</td>
<td>2.0</td>
<td></td>
</tr>
<tr>
<td>$C_{\text{coeff}}$</td>
<td>2.0</td>
<td></td>
</tr>
<tr>
<td>$M_w$</td>
<td>5</td>
<td>kg/mol</td>
</tr>
<tr>
<td>$d_\eta$</td>
<td>0</td>
<td>MPa$^2$ mol $\sqrt{\text{m}}$/kg</td>
</tr>
<tr>
<td>$e_\eta$</td>
<td>0</td>
<td>MPa$^{3/2}$ mol $\sqrt{\text{m}}$/kg</td>
</tr>
<tr>
<td>$f_\eta$</td>
<td>$4.0 \times 10^{-2}$</td>
<td>mol $\sqrt{\text{MPa m/kg}}$</td>
</tr>
<tr>
<td>$C_{\eta\theta}$</td>
<td>44</td>
<td>K</td>
</tr>
<tr>
<td>Matrix $K_{\text{Ic}}$</td>
<td>7</td>
<td>MPa$\sqrt{\text{m}}$</td>
</tr>
<tr>
<td>$C_{\text{coal}}$</td>
<td>1.5</td>
<td></td>
</tr>
<tr>
<td>Initial $\phi_{\text{pore}}$</td>
<td>$\times 10^{-5}$</td>
<td></td>
</tr>
<tr>
<td>$m_{\text{C-A}}$</td>
<td>7.0</td>
<td></td>
</tr>
</tbody>
</table>

To monitor craze nucleation and growth, values were taken from the element which first failed in the simulation. This element was the far element in the bottom left-hand side of Figure 4.5. The craze nucleation, growth, and total damage for all three simulations are shown in Figures 4.7, 4.8, and 4.9. Also, Figure 4.10 shows two deformed geometries mid-loading and post fracture in the FE simulation at 300 mm/s.
Figure 4.6  Force–displacement comparison between model prediction with and without damage to the experimental data for polycarbonate impact tests.

Force–displacement comparison between model prediction with and without damage to the experimental data for polycarbonate impact tests at impact velocities of (a) 3 mm/s, (b) 30 mm/s, and (c) 300 mm/s.
The craze damage evolution for the first failed element in the polycarbonate impact simulation at an impact velocity of 300 mm/s is decomposed into (a) the total damage evolution, (b) the craze nucleation evolution, and (c) the craze growth.

Figure 4.7  Craze damage evolution at an impact velocity of 300 mm/s.
Figure 4.8 Craze damage evolution at an impact velocity of 30 mm/s.

The craze damage evolution for the first failed element in the polycarbonate impact simulation at an impact velocity of 30 mm/s is decomposed into (a) the total damage evolution, (b) the craze nucleation evolution, and (c) the craze growth.
Figure 4.9 Craze damage evolution at an impact velocity of 3 mm/s.

The craze damage evolution for the first failed element in the polycarbonate impact simulation at an impact velocity of 3 mm/s is decomposed into (a) the total damage evolution, (b) the craze nucleation evolution, and (c) the craze growth.
Figure 4.10  Deformed geometries of polycarbonate impact simulations.

Deformed geometries of polycarbonate impact simulations at 300 mm/s: (a) Mid-loading and (b) post-fracture.
CHAPTER 5
SUMMARY AND FUTURE WORK

5.1 Summary

An experimental, theoretical, and computational study on the damage of thermo-plastics was conducted. Experimentally, material properties for PC, ABS, and PP were shown to be dependent upon strain rate, temperature, and stress state. These properties included the elastic modulus, yield stress, strain softening, strain hardening, and elongation to failure. The fracture surface morphology was also dependent on temperature and strain rate. A new theoretical continuum material model was developed in the intermediate configuration through the large deformation of kinematics and the thermodynamics related to ISVs. This model builds upon the work proposed by Bouvard et al. [2013] by including damage. Isotropic damage was included in the thermodynamics is such a way to naturally result in degrading the elastic modulus. A new craze-damage evolution equation was developed and implemented along with damage resulting from particles [Horstemeyer and Gokhale, 1999] and pre-existing voids [Cocks and Ashby, 1980]. The damage model was compared to micromechanical models from the literature (Socrate and Boyce [2000] and Steenbrink et al. [1997]). The full inelastic model was implemented into an FE code. A material point simulator
for damage was compared to a three-dimensional one element FE simulation. Finally, the model was used to predict failure in polycarbonate impact testing.

5.2 Future Work

5.2.1 Full Implementation of ISV Model

In Chapter 3, the kinematics, thermodynamics, and kinetics were developed for an inelastic thermoplastic ISV model. The full damage evolution equations were implemented in Chapter 4, but with the rest of the ISV material model presented in Appendix B, which is based upon Bouvard et al. [2013]. Further work is needed to implement the full model in Chapter 3. While many similarities exist between the two models, the plastic spin, static recovery, and dynamic recovery set them apart. How these three differences impact the numerical response would be the subject of further research.

All simulations in this study were implemented in Abaqus/Explicit (vumat), which is generally used for dynamic events. Further work is needed to implement the model into Abaqus/Standard (umat), which is better suited for static and lower-speed dynamic simulations.

Currently, the damage deformation gradient tensor, $F_d$, is not implemented in the kinematics section of this work. When the damage deformation gradient with an initial porosity is included in the kinematics implementation, the elastic strain is forced into a state of compression. To the author's knowledge, rarely are kinematics used to determine the elastic strain in material models (e.g., Bammann [1990], Marin et al. [2006], Horstemeyer et al. [2003]). However, for this study, both the thermal
and plastic deformation gradients are used to find the elastic strain. This issue needs further attention to be resolved.

5.2.2 Void Growth Simulation

Micromechanical void growth simulations are needed to further explore the unique behavior of thermoplastics. The void growth models implemented in this study (Cocks and Ashby [1980] and Budiansky et al. [1982]) were developed for power law hardening material. While that assumption might work well for some thermoplastics, it would not capture the unique stress softening behavior exhibited by many thermoplastics (e.g., all material in Chapter 2: ABS, PC, and PP).

The literature is replete with micromechanical simulations of thermoplastics with voids (Chen and Mai [1998]; Socrate and Boyce [2000]; Tzika et al. [2000]; Danielsson et al. [2002]; Steenbrink et al. [1997]). However, in these works, voids are closely grouped together in an attempt to capture realistic void growth. These authors have crazing in mind as single voids growing independent of other voids are not common in thermoplastic deformation. In those cases, simulated void growth is strongly affected by the RVE boundaries. In order to define damage as three processes—nucleation, growth, and coalescence—it is necessary to setup micromechanical simulations in such a way where the boundaries do not contribute to the void growth. A parametric study to determine the factors influencing void growth in polymer, in a manner similar to Horstemeyer and Ramaswamy [2000], would be the next step in formulating a void growth theory for thermoplastics.
5.2.3 Uncertainty Analysis

In order to compare experimental results to numerical predictions, error in experimental results and approximations in numerical simulations need to be accounted for. In Chapter 2, the experimental variation on the true stress–true strain behavior and the elongation to failure were given. However, uncertainties arise from numerous areas. No thermoplastic specimens are identical to one another, nor are any heterogeneous. Therefore, variability will be present when analyzing the initial microstructure as well as deformed/fractured microstructure. All experiments have underlying assumptions as well as data acquisition errors. Simulations also work under necessary assumptions, use error-prone data extracted from experiments, and are subject to numerical approximations. Figure 5.1 gives a visual representation of where errors arise in experimental and computational environments. See Solanki et al. [2010] for a detailed example of uncertainty propagation in these fields. An uncertainty analysis is necessary because it takes all of the errors, correlates them, and then provides bounds for realistic expectations of computational predictability.

5.2.4 Damage Progression Quantification

In order to develop more accurate theories in regard to damage accumulation in thermoplastics, experiments tailored to such data need to be performed. There are a few different methods that could be used to achieve this: In situ SEM tensile testing, X-ray computed tomography (CT) imaging of interrupted mechanical testing, acoustical methods, or light scattering methods. Each has been used to calculate
Figure 5.1  An uncertainty flow chart to show the many sources of uncertainty in both experiments and computations.
damage progression in metals; however, thermoplastics create new challenges to each technique.

*In situ* SEM mechanical testing required very small specimens. Two obstacles to this method are machining a small thermoplastic specimen and acquiring high resolution SEM imaging on a non-conductive surface. With metals, these specimens can be cut with a wire electric discharge machining. As this method generally requires the material to be conductive, polymers are not a good candidate. Other methods of machining commonly build up heat which alters the material properties, especially along cut edges. Finally, water-jet cutting can leave a rough surface finish thus creating many points of stress concentrations. The second obstacle is related to how to get high quality, thus useful, images from an SEM when sputter coating the surface could create problems. The sputter coat might impede the view to distinguish when and how void nucleate, grow, and coalesce. To bypass sputter coating, a variable pressure SEM (or environmental SEM) allowing for non-conductive specimens to be viewed in their natural state should be used.

While the *in situ* SEM approach would render two dimensional data, X-ray CT imaging could be used to acquire the third dimension. This approach was used by Horstemeyer et al. [2003]. Both void nucleation and growth could be monitored by interrupting monotonic loading experiments and then examining specimens in the X-ray. Figure 5.2, from Horstemeyer et al. [2003], shows the results of such an experimental method. Many polymers are considered “x-ray transparent;” thus this method would not be useful.
Figure 5.2 Comparison of nucleation density between numerical model and experimental results for a cast A356 aluminum for three stress states from Horstemeyer et al. [2003].

Acoustical methods have been used to count nucleation events in thermoplastics, thermosets, and composites [Grabec and Peterlin, 1976, Koenczoel et al., 1986, Giordano et al., 1998]. The drawback to this method is that no distinction could be made between what is causing the acoustical emission event—craze nucleation, fibril breakdown, or particle/fiber debonding. However, this method coupled with the SEM [Siegmann and Kander, 1991] or X-ray CT techniques described above would give extra confidence to counting total nucleation.

Finally, light scattering techniques have been used to correlate the total void volume fraction to light intensity [Schirrer et al., 1997, Dijkstra et al., 1994]. This technique can return a total void volume fraction by light diffraction but cannot distinguish between damage mechanisms.
REFERENCES


APPENDIX A

DISCUSSION ON STRESS INVARIANT MISNOMERS
In the solid mechanics field, the concept of stress invariants is widely used. Invariants are scalar and will not “vary” if the stress undergoes a coordinate transformation, meaning they are also frame indifferent. Due to their ability to remain indifferent, invariants are commonly employed in yield functions and void growth equations. A review of the use of stress invariants in yield functions and damage evolution equations can be found in Horstemeyer [1995].

Invariants are commonly calculated from the Cauchy stress and the deviatoric Cauchy stress; however, for generalization, the following discussion will just consider a symmetric second order stress tensor, $\sigma$, and its deviatoric part, $\sigma'$. The deviatoric stress is calculated as

$$\sigma' = \sigma - \text{tr}(\sigma) \mathbf{1}$$

(A.1)

where $\mathbf{1}$ is a second order identity tensor. From the stress, the following relationship is true

$$\det(\sigma - \lambda \mathbf{1}) = -\lambda^3 + I_1(\sigma) \lambda^2 - I_2(\sigma) \lambda + I_3(\sigma)$$

(A.2)

The stress’s invariants are generally labeled $I_1$, $I_2$, and $I_3$ while the deviatoric stress’s are $J_1$, $J_2$, and $J_3$. If $\det(\sigma - \lambda \mathbf{1}) = 0$ then $\lambda$ is an eigenvalue.

The Cayley–Hamilton Theorem can also be used for these tensors which states that the each tensor will satisfy its own characteristic equation:

$$\sigma^3 - I_1(\sigma)\sigma^2 + I_2(\sigma)\sigma - I_3(\sigma) \mathbf{1} = 0$$

(A.3)
There is generally no confusion when it comes to defining \( I_1, I_2, \) and \( I_3 \):

\[
I_1 = \text{tr} (\sigma) \tag{A.4}
\]
\[
I_2 = \frac{1}{2} \left[ (\text{tr} \sigma)^2 - \text{tr} (\sigma^2) \right] \tag{A.5}
\]
\[
I_3 = \text{det} (\sigma) \tag{A.6}
\]

These invariants satisfy the Cayley–Hamilton Theorem. However, the widely used deviatoric stress invariants do not satisfy the theorem. The deviatoric stress invariants, \( J_1, J_2, \) and \( J_3 \), are usually defined (in summation and index notation) as:

\[
J_1 = \text{tr} (\sigma') = 0 \tag{A.7}
\]
\[
J_2 = \frac{1}{2} \text{tr} (\sigma'^2) = \frac{1}{2} \sigma'_{ij} \sigma'_{ij} \tag{A.8}
\]
\[
J_3 = \frac{1}{3} \text{tr} (\sigma'^3) = \frac{1}{3} \sigma'_{ij} \sigma'_{ij} \sigma'_{ij} \tag{A.9}
\]

Since \( J_1 = 0 \), it is generally unused. If these deviatoric “invariants” were defined in such a way to satisfy the Cayley–Hamilton Theorem, the \( J_2 \) and \( J_3 \) would be

\[
J_2 = \frac{1}{2} \left[ (\text{tr} \sigma')^2 - \text{tr} (\sigma'^2) \right] \tag{A.10}
\]
\[
J_3 = \text{det} (\sigma') \tag{A.11}
\]

It so happens that in the Eringen [1967] (Eq. A.9) definition of \( J_3 \)

\[
J_3 = \frac{1}{3} \text{tr} (\sigma'^3) \tag{A.12}
\]

However, partial derivatives of the invariants with respect to the deviatoric stress will not be equivalent. Partial derivatives of \( J_1, J_2, \) and \( J_3 \) with respect to the deviatoric stress and the differences between them are shown in Equations (A.13), (A.14), and...
(A.15). Simplifications are made on the transpose as the Cauchy stress is always symmetric. However, not all stresses used are symmetric (e.g. First Piola–Kirchoff Stress).

\[
\frac{\partial J_1}{\partial \sigma'} = \frac{\partial \text{tr} (\sigma')}{\partial \sigma'} = 1 \tag{A.13}
\]

\[
\frac{\partial J_2}{\partial \sigma'} = \begin{cases} 
\frac{\partial}{\partial \sigma'} \left[ \frac{1}{2} \text{tr} (\sigma'^2) \right] = \sigma'^T = \sigma' \\
\frac{\partial}{\partial \sigma'} \left[ \text{tr} (\sigma')^2 - \text{tr} (\sigma'^2) \right] = \text{tr} (\sigma') \mathbf{1} - \sigma' 
\end{cases} \tag{A.14}
\]

\[
\frac{\partial J_3}{\partial \sigma'} = \begin{cases} 
\frac{\partial}{\partial \sigma'} \left[ \text{tr} (\sigma'^3) \right] = \left( \sigma'^2 \right)^T = \sigma'^2 \\
\frac{\partial}{\partial \sigma'} \det (\sigma') = \det (\sigma') \sigma'^{-T} = \det (\sigma') \sigma'^{-1} 
\end{cases} \tag{A.15}
\]

The relationship between the “true” invariant \( J_{2true} \) and the one widely used \( (J_2) \) is

\[
J_{2true} = \frac{1}{2} \left[ (\text{tr} \sigma')^2 - \text{tr} (\sigma'^2) \right] = -\frac{1}{2} \text{tr} (\sigma'^2) = -J_2 \tag{A.16}
\]
APPENDIX B

MODIFIED BOUVARD 2013 MODEL TO INCLUDE DAMAGE
The material model developed by Bouvard et al. [2013] and modified by Francis et al. [Submitted] to include damage follows. Details and explanations of each variable and equation are given in Chapter 3. The Cauchy stress, \( \sigma \), is determined from pushing forward the Mandel stress, \( \bar{M} \), which follows,

\[
\sigma = J_e^{-1} \tau = J_e^{-1} R_e \bar{M} R_e^T
\]

The Mandel stress is defined as

\[
\bar{M} = C_e \bar{S} = 2\mu(\theta) \bar{E}_e + \left( k(\theta) - \frac{2}{3} \mu(\theta) \right) \text{tr}(\bar{E}_e) \mathbf{1}
\]

The model is set in the intermediate configuration of \( \bar{B} \), which is shown in Figure 3.1. In Chapter 3.2, the void volume fraction was introduced in such a way that the kinematic and thermodynamic derivations naturally resulted in the elastic modulus’s, \( E(\theta) \), degradation.

\[
E(\theta) = [E_{ref} + E_1(\theta - \theta_{ref})](1 - \phi)^{2/3}
\]

This degradation in Equation (B.3), also naturally degrades the shear modulus, \( \mu(\theta) \), and the bulk modulus, \( K(\theta) \).

\[
\mu(\theta) = \frac{E(\theta)}{2(1 + \nu_p)}, \quad K(\theta) = \frac{2\mu(\theta)(1 + \nu_p)}{3(1 - 2\nu_p)}
\]

The plastic flow rule, where

\[
\hat{F}_p = D_p F_p, \quad D_p = \frac{1}{\sqrt{2}} \hat{\gamma}_p N_p, \quad N_p = \frac{M - \bar{b}'}{\|M - \bar{b}'\|}
\]

is a function of the plastic shear strain rate, \( \hat{\gamma}_p \), where

\[
\hat{\gamma}_p = \hat{\gamma}_0 \exp \left( \frac{\Delta H_\beta}{k_B \theta} \right) \sinh^n \left( \frac{L_2}{k_B \theta} \left( \frac{1}{2} \frac{M - \bar{b}'}{\|M - \bar{b}'\|} - (Y(\theta) + \bar{k}_1 + \bar{k}_2 + \alpha_p \bar{n}) V \right) \right)
\]

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The plastic shear rate from Richeton et al. [2005, 2007] in Equation (B.6) is a function of several variables: $\dot{\gamma}_{0p}$ is a reference strain rate, $\Delta H_{\beta}$ is an activation energy, $k_B$ is the Boltzmann constant, $V$ is an activation volume, $n$ is a parameter describing the molecular chain segments’ cooperative behavior, and $Y(\theta)$ is a temperature dependent temperature dependent yield surface where

$$Y(\theta) = C_3 (\theta - \theta_{ref}) + C_4$$

(B.7)

$\alpha_p$ is a pressure sensitivity parameter from Boyce et al. [1988] and $\bar{\pi} = -(1/3) \text{tr} \bar{M}$ where $\bar{\pi}$ is an effective pressure. $\bar{M}'$ and $\bar{b}'$ are the deviatoric parts of the Mandel stress and backstress, respectively. $\bar{\kappa}_1$ and $\bar{\kappa}_2$ are scalar stress-like terms related to the internal state variables $\bar{\xi}_1$ and $\bar{\xi}_2$, respectively.

The evolution equations for $\bar{\xi}_1$ and $\bar{\xi}_2$ are the same as those presented in Chapter 3. $\bar{\xi}_1$ and $\bar{\xi}_2$ are two scalar internal state variables that relate to entanglement density and large-strain chain alignment/coiling, respectively. The evolution equation for $\bar{\xi}_1$ is given as

$$\dot{\bar{\xi}}_1 = H_1 \left( \left( \frac{-\bar{\xi}_1}{\bar{\xi}^*} \right) \dot{\gamma}_{0p} \right)$$

(B.8)

and the evolution equation related to chain slippage follows, where

$$\dot{\bar{\xi}}^*(\theta) = \left( \bar{\xi}^*_{\text{sat}}(\theta) - g_0(\theta) \bar{\xi}^* \right) \dot{\gamma}_{0p}$$

(B.9)

The temperature dependent variable for $\bar{\xi}_1$ is

$$\bar{\xi}^*_0(\theta) = C_5 (\theta - \theta_{ref}) + C_6, \quad \bar{\xi}^*_{\text{sat}}(\theta) = C_7 (\theta - \theta_{ref}) + C_8, \quad g_0(\theta) = C_9 (\theta - \theta_{ref}) + C_{10}$$

(B.10)
The evolution equation from Boyce et al. [1988], Anand and Gu [2000], and Anand and Gurtin [2003] are used for the entanglement density ISV in Equations (B.8) and (B.9). The evolution equation from Ames et al. [2009] is used for the large-strain chain alignment/coiling ISV \( \bar{\xi}_2 \).

\[
\dot{\bar{\xi}}_2 = H_2 (\bar{\lambda}_p - 1) \left( \frac{- \bar{\xi}_2}{\bar{\xi}_{2\text{sat}} (\theta)} \right) \dot{\bar{\gamma}}_p, \quad \bar{\lambda}_p = \sqrt{\frac{\text{tr} B_p}{3}}, \quad \text{where} \quad B_p = F_p F_p^T \quad (B.11)
\]

The temperature dependent saturation for \( \bar{\xi}_2 \) is

\[
\bar{\xi}_{2\text{sat}} (\theta) = C_{11} (\theta - \theta_{\text{ref}}) + C_{12} \quad (B.12)
\]

The modulus for the backstress comes from Gent [1996] where \( \mu_R (\theta) \) is the rubbery modulus, \( \mu_R (\theta) \) is the modulus for the backstress, and \( \lambda_L \) is the network locking stretch. \( \lambda_1^\alpha, \lambda_2^\alpha, \text{and} \lambda_3^\alpha \) are eigenvalues of \( \bar{\alpha} \).

\[
\mu_B (\theta) = \mu_R (\theta) \left[ \frac{- \lambda_1^\alpha + \lambda_2^\alpha + \lambda_3^\alpha - 3}{\lambda_L} \right]^{-1} \quad (B.13)
\]

\[
\mu_R (\theta) = C_1 (\theta - \theta_{\text{ref}}) + C_2 \quad (B.14)
\]

The evolution equation for the ISV \( \bar{\alpha} \) is taken originally from the second-order structure tensor developed by Prantil et al. [1993]. Both Ames et al. [2009] and Bouvard et al. [2010] showed its application for polymers.

\[
\dot{\bar{\alpha}} = R_{s_1} (\theta) (\bar{D}_p \bar{\alpha} + \bar{\alpha} \bar{D}_p), \quad \bar{\alpha} (X, 0) = 1 \quad (B.15)
\]

The temperature dependent variable for \( \dot{\bar{\alpha}} \) is

\[
R_{s_1} = C_{13} (\theta - \theta_{\text{ref}}) + C_{14} \quad (B.16)
\]
The reader is referred to Chapter 3.3 for the complete thermodynamic derivations, but it would suffice to say that each thermodynamic conjugate pair \((\bar{\kappa}_1, \bar{\kappa}_2, \bar{b})\) is the derivative of the free energy with respect to their respective ISV \((\bar{\xi}_1, \bar{\xi}_2, \bar{\alpha})\).

\[
\bar{\kappa}_1 = C_{\bar{\kappa}_1} \mu (\theta) \bar{\xi}_1 \quad \text{(B.17)} \\
\bar{\kappa}_2 = C_{\bar{\kappa}_2} \mu (\theta) \bar{\xi}_2 \quad \text{(B.18)} \\
\bar{b} = \mu_B (\theta) \bar{\alpha} \quad \text{(B.19)}
\]

A simple temperature evolution is used which assumes that the majority of temperature change is attributed to plastic work. The ratio of the plastic work that is transferred into temperature change is given as \(\omega\).

\[
\bar{C}_V \dot{\theta} = \omega \bar{M} : \bar{D}_p - \nabla \cdot \bar{Q} + \bar{R}_V \quad \text{(B.20)}
\]

The void volume fraction (damage) is composed of three types of interacting phenomena: damage from the growth of pre-existent voids, \(\phi_{\text{pores}}\); damage from void nucleating at growing from particles, \(\phi_{\text{particles}}\); and damage from nucleating and growing crazes, \(\phi_{\text{crazing}}\). The three processes do not happen independently of one another in applications; therefore, an interacting coalescence term, \(c\), is used as well.

\[
\phi_{\text{total}} = (\phi_{\text{particles}} + \phi_{\text{pores}} + \phi_{\text{crazing}}) c
\]

\[
\phi_{\text{particles}} = \eta_{\text{particle}} v \\
\phi_{\text{crazing}} = \eta_{\text{crazing}} v \\
\]

Damage from the growth of pre-existent voids is modeled with the Cocks–Ashby model [Cocks and Ashby, 1980] which follows,

\[
\dot{\phi}_{\text{pores}} = \chi \left[ \left( \frac{1}{1 - \phi_{\text{pores}}} \right)^m - (1 - \phi_{\text{pores}}) \right] \| \bar{D}_p \| \quad \text{(B.22)}
\]
where

\[
\chi = \sinh \left[ \frac{2(m - 0.5) p}{(m + 0.5) \sigma_e} \right] = \sinh \left[ \frac{2(2m - 1) I_1}{3\sqrt{3}(2m + 1) \sqrt{J_2}} \right]
\]  

(B.23)

\( m \) is a strain rate sensitivity parameter, \( I_1 \) is the first invariant of the Cauchy stress, and \( J_2 \) is half of the scalar product of the deviatoric Cauchy stress. Damage arising from particles is modeled by void nucleation and growth. The particle-void nucleation from Horstemeyer and Gokhale [1999] is used where

\[
\dot{\nu}_{\text{particle}} = \| \mathbf{D}_p \| \frac{d^{1/2}}{K_c f^{1/2}} \eta_{\text{particle}} \left\{ a_\eta \left[ \frac{4}{27} - \frac{J_3^2}{J_2^3} \right] + b_\eta \frac{J_3}{J_2^{3/2}} + c_\eta \left\| \frac{I_1}{\sqrt{J_2}} \right\| \right\} \exp \left( \frac{C_{\eta \theta}}{\theta} \right)
\]  

(B.24)

For the void growth created by particles, the void growth model developed by Budiansky et al. [1982] is used where

\[
\dot{\nu} = \frac{3}{2} \nu \left[ \frac{I_1}{\eta \sqrt{12J_2}} + \frac{[m - 1] [m + 0.4319]}{m^2} \right]^m \| \mathbf{D}_p \|
\]  

(B.25)

For crazing nucleation, the model developed in Chapter 3 is used where

\[
\dot{\eta}_{\text{craze}} = \eta_{\text{craze}} \frac{M_w}{K_c} \left\{ d_\eta \left[ \frac{4}{27} - \frac{J_3^2}{J_2^3} \right] + e_\eta \frac{J_3}{J_2^{3/2}} + f_\eta \left\| \frac{I_1 + \| I_1 \|}{2\sqrt{J_2}} \right\| \right\} \| \mathbf{D}_p \| \exp \left( \frac{C_{\eta \theta}}{\theta} \right)
\]  

(B.26)

Equation (B.25) is used for craze growth also. The coalescence term from Chapter 3, which modifies Horstemeyer et al. [2000] and Allison [2009], follows where

\[
c = C_{\text{coal}_1} \phi_{\text{particle}} + C_{\text{coal}_2} \phi_{\text{crazing}} + C_{\text{coal}_3} \left( \frac{4d_0}{d_{\text{NN}}} \right)^z \exp (C_{e \theta}) \| \mathbf{E}_p \|
\]  

(B.27)

where \( C_{\text{coal}_1}, C_{\text{coal}_2}, \) and \( C_{\text{coal}_3} \) are coalescence dependent parameters. \( d_0 \) is the average particle diameter and \( d_{\text{NN}} \) is the nearest neighbor distance. \( C_{e \theta} \) is a void coalescence temperature dependent parameter, and \( z \) is a material parameter.