CHARACTERIZATION OF DELAMINATION IN 2099-T861 ALUMINUM-LITHIUM

BY

RUSSELL J. MCDONALD

DISSERTATION

Submitted in partial fulfillment of requirements
for the degree of Doctor of Philosophy in Mechanical Engineering
in the Graduate College of the
University of Illinois at Urbana-Champaign, 2009

Urbana, Illinois

Doctoral Committee:

Adjunct Associate Professor Peter Kurath, Chair and Director of Research
Professor Armand J. Beaudoin, Contingent Chair
Professor Daniel A. Tortorelli
Professor Claude Fressengeas, University of Metz, France
Professor Nikolaos Aravas, University of Thessaly, Greece
Abstract

Aluminum-lithium alloys provide a lower density and higher stiffness alternative to other high strength aluminum alloys. However, many Al-Li alloys exhibit a non-traditional failure mechanism, delamination. Delamination refers to the failure along the grain boundary interface. The delamination phenomenon is often observed from fracture toughness testing as cracking along grain boundaries perpendicular to the mode I primary crack. In this investigation, delaminations were also observed after cyclic deformation of both uniaxial and torsion experiments. Many of the experimental observations, such as rate insensitivity and crystallographic orientation, were incorporated into a cyclically stable crystal plasticity framework with rate independent kinematic hardening. It was hypothesized that texture lead to interface stresses that could not be obtained by a continuum approach. Local grain boundary interface stresses were estimated using the uniform deformation and bi-crystal models. These models were computationally amenable to provide both orientation dependence and the statistical nature of the grain boundary stresses for a given bulk texture and nominal loading. A coupled shear-normal damage parameter was formulated to quantitatively characterize the nucleation of delamination. The damage estimated for a wide range of simulations (uniaxial, torsion, fracture) correlated well with the experimental trends.
Acknowledgements

Both this work and the completion of graduate studies would not have been possible without the contribution of others. In my case, I was most fortunate to be blessed with two doctoral advisors: Peter Kurath and Armand J. Beaudoin. Peter Kurath has been guiding my development since I was an undergrad. He taught me countless things about experiments, communication, and life. His insatiable curiosity and insightful “thoughts for the day” truly improved this work at every stage. Armand Beaudoin’s patience and careful guidance supplied some freedom to make the most of my experience as a graduate student. His talent for modeling was pivotal throughout this project. Furthermore, he taught me the importance of linking to the “bigger picture” and always recognizing the direction the research is heading. Both my advisors provided me with a unique nurturing working environment. Their connections lead me to meet many of the other talented individuals that provided many essential components of this research.

The NASA Marshall Space Flight Center provided some of the support for the work through Grant NNM04AA37G (MSFC, Mr. D. N. Wells, Technical Monitor). Mr. D. N. Wells also generously provide the Al-Li 2099-T61 plate utilized throughout the experimental investigation. Several others from related to the project provided valuable insights during several reoccurring discussions, including M. Adler, P. Allen, P. Chen, R. Crooks, M. Domack, S. Kalyanam, D. Lambert, K. Morgan, P. McGill, R. H. Dodds, C. Sam, S. Shah, W. Tayon, and J. Wagner. The topics of discussion presented at these meetings certainly impacted the direction of this investigation.

Many of the experiments discussed throughout Chapter 2 were completed with assistance. For instance, the Material Research Laboratory (MRL) provided the equipment and necessary guidance used for X-ray Diffraction, Election Backscatter Diffraction, and Auger Spectroscopy. These components of the work was supported by the U.S. Department of Energy, Division of Materials Sciences under Award No. DEFG02-91ER45439, through the Frederick Seitz Materials Research Laboratory at the University of Illinois at Urbana-Champaign. Specifically, Dr. Mauro R. Sardela, Jr. trained me to run a successful X-ray diffraction texture scan and use the X’pert XRD
software. Dr. Jim Mabon taught me several things about specimen preparation, ran the
Electron Backscatter diffraction experiments, and provided many beneficial insights on
the results. Dr. Nancy Finnegan patiently ran the Auger Spectroscopy experiments,
including both chemical composition makes and point measurements during sputtering,
and provided many useful references on the Auger process.

The mechanical experiments would not have been possible without the careful
and accurate specimen machining provided by Kent Elam, David Foley, and Greg
Milner. Similarly, the LabVIEW software and mechanical equipment would not have
worked properly without the efforts of Rick Rottet and Dr. Gavin Horn. Dr. Horn also
provided guidance and interpretation of the Lock-In Thermography experiments. The
Split Hopkinson Bar experiments were conducted through the guidance and assistance of
Dr. Henry Padilla. Finally the tension tests were made possible through collaboration
with Prof. Claude Fressengeas and Prof. Dennis Entemeyer at LPMM in Metz, France.
Much of the specimen polishing and optical micrographs were completed by the efforts
of Ernie Timmons.

A variety of invaluable information was passed on to me by a number of sources.
For example, the successful implementation of Rodrigues space would not have been
possible without the DPLAB software provided by Prof. Donald E. Boyce and Prof. Paul
R. Dawson. Necessary implementation modifications to display stress on orientation
space was expedited through the guidance of Prof. Matthew P. Miller. The choice of
integration for the implementation of the finite deformation material model was a
consequence of the guidance of Prof. Nikolaos Aravas. A FEM stress solution of the
interface shear test was provided by Dr. Suresh Kalyanam. Most recently, the ultimate
fracture toughness estimates were considered based on experiments conducted by Mr.
Mark Hernquist.
To my friends and family
# Table of Contents

<table>
<thead>
<tr>
<th>Chapter</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Introduction and Background</td>
<td>1</td>
</tr>
<tr>
<td>Experimental Investigation</td>
<td>8</td>
</tr>
<tr>
<td>2.1 Initial Plate Properties</td>
<td>8</td>
</tr>
<tr>
<td>2.1.1 X-ray Diffraction (XRD)</td>
<td>10</td>
</tr>
<tr>
<td>2.1.2 Electron Back-Scatter Diffraction (EBSD)</td>
<td>24</td>
</tr>
<tr>
<td>2.1.3 Auger Electron Spectroscopy (AES)</td>
<td>26</td>
</tr>
<tr>
<td>2.2 Small Strain Deformation</td>
<td>32</td>
</tr>
<tr>
<td>2.2.1 Incremental Step Test</td>
<td>33</td>
</tr>
<tr>
<td>2.2.2 Lock-in Thermography (LIT)</td>
<td>48</td>
</tr>
<tr>
<td>2.2.3 Cyclic Torsion</td>
<td>52</td>
</tr>
<tr>
<td>2.2.4 Small Strain Compression</td>
<td>57</td>
</tr>
<tr>
<td>2.3 Large Strain Deformation</td>
<td>60</td>
</tr>
<tr>
<td>2.3.1 Large Strain Compression</td>
<td>61</td>
</tr>
<tr>
<td>2.3.2 Split Hopkinson Bar</td>
<td>74</td>
</tr>
<tr>
<td>2.3.3 Tension Testing</td>
<td>77</td>
</tr>
<tr>
<td>2.3.4 Shear Interface Strength</td>
<td>82</td>
</tr>
<tr>
<td>2.4 Experimental Summary</td>
<td>84</td>
</tr>
<tr>
<td>Modeling Material Behavior</td>
<td>86</td>
</tr>
<tr>
<td>3.1 Modeling Background</td>
<td>86</td>
</tr>
<tr>
<td>3.2 Finite Deformation</td>
<td>94</td>
</tr>
<tr>
<td>3.3 Elasticity</td>
<td>96</td>
</tr>
<tr>
<td>3.4 Plasticity</td>
<td>99</td>
</tr>
<tr>
<td>3.5 General Solution Implementation</td>
<td>103</td>
</tr>
<tr>
<td>3.6 Uniform Deformation Model</td>
<td>109</td>
</tr>
<tr>
<td>3.7 Bi-Crystal Model</td>
<td>112</td>
</tr>
<tr>
<td>3.8 Modeling Summary</td>
<td>116</td>
</tr>
<tr>
<td>Results and Discussion</td>
<td>117</td>
</tr>
<tr>
<td>4.1 Modeling Parameters</td>
<td>117</td>
</tr>
<tr>
<td>4.1.1 Anisotropic Elasticity</td>
<td>117</td>
</tr>
<tr>
<td>4.1.2 Independent Slip-System Plasticity</td>
<td>120</td>
</tr>
<tr>
<td>4.2 Single Crystal Behavior</td>
<td>122</td>
</tr>
<tr>
<td>4.3 Uniform Deformation Model</td>
<td>123</td>
</tr>
<tr>
<td>4.4 Bi-Crystal Deformation Model</td>
<td>134</td>
</tr>
<tr>
<td>4.5 Bulk Texture and Loading Direction</td>
<td>142</td>
</tr>
<tr>
<td>4.6 Shear Deformation</td>
<td>149</td>
</tr>
<tr>
<td>4.7 Plane Strain Cyclic Deformation</td>
<td>154</td>
</tr>
<tr>
<td>4.8 Deformation near a crack-tip</td>
<td>157</td>
</tr>
<tr>
<td>4.9 Summary of Results</td>
<td>166</td>
</tr>
<tr>
<td>Conclusions and Recommendations</td>
<td>170</td>
</tr>
<tr>
<td>5.1 Conclusions</td>
<td>170</td>
</tr>
<tr>
<td>5.2 Recommendations</td>
<td>174</td>
</tr>
</tbody>
</table>
List of References .................................................................................................................. 176

Appendices .............................................................................................................................. 185
A. True Stress Conversion ...................................................................................................... 185
B. Machine Stiffness .............................................................................................................. 187
C. Coordinate Rotations ........................................................................................................ 189
D. Elastic Anisotropy .............................................................................................................. 191
   D.1 Elastic Strain Energy Density ...................................................................................... 191
   D.2 Elastic Stress Dependence .......................................................................................... 191
   D.3 Sensitivity to Elasticity Assumption .......................................................................... 192
E. Sensitivity to Plasticity Parameters .................................................................................. 194

Author's Biography ............................................................................................................... 198
List of Figures

Figure 1.1: KIC fracture specimen pulled in the L-direction with the crack oriented on the T-N plane, illustrating (a) the fracture surface and (b) a cross-section with Chevron v-notches [3]. .................................................. 2

Figure 1.2: Failure surfaces illustrating delamination after cyclic deformation .......... 5

Figure 2.1: Initial plate microstructure at the edge of the plate (t/10) ....................... 10

Figure 2.2: Typical specimen orientation in the XRD and defined machine angles. ................................................................. 11

Figure 2.3: 2θ scans of the undeformed Al-Li plate at various thicknesses with an N-normal polished surface. ......................................................... 12

Figure 2.4: [111], [100], and [110] pole figures for the 3 texture regimes of the Al-Li plate relative to an L-T-N reference frame ................................. 13

Figure 2.5: Schematic illustrating a) the poles of a crystal extended to a unit sphere and b) the projection scheme for a stereographic pole figure [36]. ................................................................. 14

Figure 2.6: Bunge angle illustration (φ1=30°, Φ=45°, and φ2=60°) ............................ 15

Figure 2.7: Rodrigues space illustrating axes of rotation and magnitude of angles ................................................................. 18

Figure 2.8: Common texture components displayed in Rodrigues space .................. 19

Figure 2.9: Undeformed [111] pole-figures measured at the a) center (t/2) and b) edge textures of the Al-Li plate illustrating L, T, and N-normal measurements and the corresponding L-T-N reference frame. ............. 22

Figure 2.10: Initial plate texture measurement illustrated in Rodrigues space for the three plate regions ................................................................. 23

Figure 2.11: EBSD texture maps and SEM images for L, T, and N planes near the edge of the plate (t/10) ................................................................. 25

Figure 2.12: EBSD texture maps representing the three Rodrigues vectors for the L, T, and N planes of the Edge (t/10) texture ........................................ 26

Figure 2.13: Auger specimen geometry implemented with the notch centered at t/2, t/3, and t/6. ................................................................. 27

Figure 2.14: SEM images illustrating the fracture surface at (a) the edge (t/6) of the plate and (b) at the center (t/2) of the plate ........................................ 27

Figure 2.15: (a) Counts versus kinetic energy and (b) derivative versus kinetic energy for a survey at the grain boundary in the transition (t/3) region ................................................................. 28

Figure 2.16: (a) SEM image of mapped region at t/6 indicated in Figure 2.14a (b) the corresponding copper concentration (black is positive) map ........ 29

Figure 2.17: (a) Depth profile near the edge (t/6) of the plate illustrating the copper atomic composition at the points indicated in Figure 2.16 (b) Map of the copper content after sputtering of the same region in Figure 2.16 ................................................................. 30

Figure 2.18: (a) SEM image of mapped region at t/2 indicated in Figure 2.14b (b) the corresponding chemical composition (Cu[green], Mn[red]) map ................................. 31

Figure 2.19: (a) Depth profile near the center (t/2) of the plate illustrating the Cu and Mn atomic compositions at the points indicated (b) Map of
the chemical composition (\(\text{Cu}^{\text{(green)}}\), \(\text{Mn}^{\text{(red)}}\)) after sputtering of the same region in Figure 2.18

Figure 2.20: Cyclic test setup of a) the environmental chamber and b) the high temperature frame, with an extensometer and thermocouple attached

Figure 2.21: (a) Incremental step test control at 0.01%/s (b) Typical stress vs. strain for 1 block of the incremental test

Figure 2.22: Incremental step test specimen geometry for a) low temperature tests b) high temperature tests

Figure 2.23: Elastic regions of an incremental step test conducted at \(T=100^\circ \text{C}\), \(\dot{\varepsilon}=0.1%/\text{s}\)

Figure 2.24: (a) modulus vs. stress for the elastic regions (b) the Stress vs. plastic strain with removed linear and stress dependent elastic behavior; both plots are for an incremental step block \((T=100^\circ \text{C}, \dot{\varepsilon}=0.1%/\text{s})\)

Figure 2.25: Linear elastic modulus vs. temperature for L-direction loading of the Edge texture illustrating modified Varshni temperature dependence

Figure 2.26: (a) Elastic and (b) the stress dependent modulus vs. temperature for loading in the L and T-directions of the Edge, Transition, and Center textures

Figure 2.27: Transverse strain vs. axial strain for the strain gage specimen illustrating Poisson’s ratio = 0.30

Figure 2.28: (a) Plastic hysteresis loops and (b) the corresponding Masing loops displaying the ‘going tension’ curve

Figure 2.29: Effective tensile stress versus plastic strain at a) -20^\circ \text{C} and b) 100^\circ \text{C} for L-direction incremental step tests illustrating the first cycle and subsequent stabilized cycles are each strain rate

Figure 2.30: L-direction (Edge) incremental step test (a) normalized flow stress vs. temperature/strain-rate parameter for various hardening levels (b) fracture surfaces illustrating delamination trends with temperature

Figure 2.31: L-direction (Transition) incremental step test (a) normalized flow stress vs. temperature/strain-rate parameter for various hardening levels (b) fracture surfaces illustrating delamination trends with temperature

Figure 2.32: L-direction (Center) incremental step test (a) normalized flow stress vs. temperature/strain-rate parameter for various hardening levels (b) fracture surfaces illustrating delamination trends with temperature

Figure 2.33: (a) SEM image and (b) EBSD texture map of a small delamination cyclically loaded in the L-direction for the Transition texture

Figure 2.34: (a) SEM image and (b) EBSD texture map of a large delamination cyclically loaded in the L-direction for the Transition texture

Figure 2.35: Rodrigues vector coordinates of two delaminations observed for the Transition \((3t/8)\) plate regime
Figure 2.36: Lock-in Thermography specimens (a) straight at t/3 and t/2 (b) notched at t/4 with $K_t = 1.26$ [67] ............................................ 50
Figure 2.37: Straight specimen in-phase data illustrating localized plasticity .......... 51
Figure 2.38: Thermal Stress cyclic test at t/4, $T=20^\circ$C with $\Delta \sigma = 340$ MPa (R=0) @ 5Hz for (a) In-Phase data and (b) Out-of-Phase data progressions. .......................................................... 52
Figure 2.39: Solid bar torsion test specimen geometry oriented in the L-direction. .......................................................... 53
Figure 2.40: Shear stress vs. shear strain for torsion (long life fatigue) including linear curve-fits estimating the shear modulus. .......................................................... 54
Figure 2.41: (a) Short life fatigue cycles illustrating decreasing compliance with growing delaminations. (b) Final delaminated state after 1059 cycles. .......................................................... 55
Figure 2.42: Shear stress vs. shear strain at various strain rates at (a) t/2 and (b) t/6 .......................................................... 56
Figure 2.43: Small strain compression (a) specimen geometry and (b) Experimental setup .......................................................... 57
Figure 2.44: Small strain compression in the L-Direction for Edge, Center and Transition textures, illustrating the stress-strain response at various temperatures and the flow stress vs. temperature/strain-rate at various hardening slopes. .......................................................... 58
Figure 2.45: (a) Stress relaxation versus time for small strain compression tests in the L-direction at the edge of the plate and (b) estimated creep rate versus stress .......................................................... 60
Figure 2.46: Large strain compression (a) specimen geometry and (b) images of undeformed and deformed specimens. .......................................................... 61
Figure 2.47: (a) Small strain compression and (b) corresponding large strain compression test illustrating the threshold and offset points. .......................................................... 64
Figure 2.48: Large strain compression of the Edge texture in the L, T, and N-directions illustrating the stress-strain at various temperatures and the flow stress vs. temperature/strain-rate at various hardening slopes. .......................................................... 66
Figure 2.49: Large strain compression of the Transition texture in the L, T, and N-directions illustrating the stress-strain at various temperatures and the flow stress vs. temperature/strain-rate at various hardening slopes. .......................................................... 67
Figure 2.50: Large strain compression of the Center texture in the L, T, and N-directions illustrating the stress-strain at various temperatures and the flow stress vs. temperature/strain-rate at various hardening slopes. .......................................................... 68
Figure 2.51: N-direction compression for center (t/2), transition (3t/10) and edge (t/10) plate regimes .......................................................... 70
Figure 2.52: T-direction compression for center (t/2), transition (3t/10) and edge (t/10) plate regimes .......................................................... 70
Figure 2.53: L-direction compression for center (t/2), transition (3t/10) and edge (t/10) plate regimes .......................................................... 71
Figure 2.54: An optical micrograph of a large strain compression specimen in the L-direction at the edge of the plate illustrating heavy deformation between edge cracks or grain delaminations..........................72

Figure 2.55: Large strain compression in the L-Direction in the plate transition region illustrating localized slip bands in (a) SEM image and (b) EBSD Texture map ....................................................................72

Figure 2.56: Large strain compression in the N-direction at the center of the plate illustrating macroscopic slip localization for (a) image sequence of strain levels, (b) stress-strain, and (c) an optical micrograph showing localized deformation .................................................73

Figure 2.57: (a) Specimen geometry (b) Schematic of the experimental setup ..........74

Figure 2.58: (a) Typical split Hopkinson bar raw data for t/10 illustrating the incident, transmitted and reflected wave components. (b) Resulting stress and strain-rate magnitudes versus time for the homogeneous deformation assumption ........................................75

Figure 2.59: Split Hopkinson bar compression in the L-direction illustrating (a) stress vs. strain and (b) normalized flow stress versus x for each texture..........................................................76

Figure 2.60: Tension tests of 2099-T861 from Alcoa ......................................................................78

Figure 2.61: (a) Specimen geometry (b) L-Direction and (c) N-Direction failure locations.................................................................................................................................79

Figure 2.62: Stress-displacement curves for (a) L-direction and (b) N-direction ......79

Figure 2.63: ‘Zoomed’ stress-displacement curves for (a) L-direction and (b) N-direction illustrating stress serrations.............................................................80

Figure 2.64: Stress-strain curves illustrating the (a) all, (b) 0.5%, (c) 0.75%, and (d) 3.0% strain slow-fast and fast-slow jump tests. ......................................................81

Figure 2.65: (a) Shear test specimen geometry (b) ASTM D695 [76] support fixture .................................................................................................................................82

Figure 2.66: (a) Shear Test illustrating three ligament failures (b) Summary of the grain boundary shear strength at t/10, 3t/10, and t/2. .........................83

Figure 2.67: FEM simulation presenting the shear stress field in the interface strength specimen [77]. ............................................................84

Figure 3.1: Multiplicative decomposition of the deformation gradient for an arbitrary time increment .................................................................95

Figure 3.2: Independent slip system hardening model illustrating changes in slope..........................................................................................................................101

Figure 3.3: Typical residual convergence for plastic strain-rates .......................107

Figure 3.4: Typical residual convergence for the uniform deformation model ......109

Figure 3.5: Potential deformation modes of the bi-crystal model .........................112

Figure 4.1: Temperature dependence of the a) shear b) bulk c) anisotropic and d) stress-dependent moduli. .................................................................119

Figure 4.2: Representative shear stress vs. plastic strain behavior on an independent slip system.................................................................121

Figure 4.3: The effect of texture on stress vs. strain for (a) monotonic and cyclic experimental results and (b) material model simulations ..........122

Figure 4.4: Single crystal stress vs. strain for common texture orientations ........123
Figure 4.5: Uniaxial cyclic simulation in the L-direction of the edge texture illustrating (a) strain components versus time, (b) stress components versus time, and (c) axial stress versus strain..............124
Figure 4.6: Axial stress in Rodrigues space of the L-direction cyclic simulation for the edge texture demarking points A-J...........................................126
Figure 4.7: (a) Cumulative probability and (b) Histogram of the axial stress of the L-direction simulation for the edge texture, demarking points A-J........................................................................127
Figure 4.8: Grain-boundary normal stress of the L-direction cyclic simulation for the edge texture illustrating Rodrigues space (points D and G), the cumulative probability and histogram with demarcated points A-J........................................................................128
Figure 4.9: Grain-boundary shear stress of the L-direction cyclic simulation for the edge texture illustrating Rodrigues space (points D and G), the cumulative probability and histogram with demarcated points A-J........................................................................129
Figure 4.10: Shear-normal stress histogram of the L-direction cyclic simulation for the edge texture illustrating points D and G.............................130
Figure 4.11: Findley based damage parameter for symmetric L-direction cyclic loading reversed at Points B, C, and D for the edge texture................133
Figure 4.12: Damage at various percentages versus axial strain for L-direction fully-reversed cyclic loading using the uniform deformation model......134
Figure 4.13: Bi-crystal results for uniaxial cyclic loading of the Edge texture in the T-direction illustrating the normal stress, $\sigma_{nn}$, with Cube, Shear1, and Brass pairs in Rodrigues space and a comparison of the statistical results with the uniform deformation model ................136
Figure 4.14: Bi-crystal results for uniaxial cyclic loading of the Edge texture in the T-direction illustrating the resolved shear stress, $\tau$, with Cube, Shear1, and Brass pairs in Rodrigues space and a comparison of the statistical results with the uniform deformation model .................137
Figure 4.15: Bi-crystal results for uniaxial cyclic loading of the Edge texture in the T-direction illustrating the damage parameter, $D_f$, with Cube, Shear1, and Brass pairs in Rodrigues space and a comparison of the statistical results with the uniform deformation model ................138
Figure 4.16: Damage at various percentages versus axial strain for L-direction fully-reversed cyclic loading using the bi-crystal model ...............139
Figure 4.17: The 1% most damaging Bi-crystal pairs (100 pairs) presented in Rodrigues space for cyclic loading of the Edge texture in the T-direction.............................................140
Figure 4.18: Cumulative probability vs. the damage parameter for L-Direction uniaxial cycling of the transition texture (1% max), with grain pairs corresponding to the EBSD investigation (Figure 2.35)...............141
Figure 4.19: Nominal stress-strain behavior of each texture and loading direction............................................................................144
Figure 4.20: Texture and Direction dependence of uniaxial cyclic loading (peak at 1% strain) of the normal stress, $\sigma_{NN}$, illustrating the Rodrigues space and statistics .......................................................... 145

Figure 4.21: Texture and Direction dependence of uniaxial cyclic loading (peak at 1% strain) of the resolved shear stress, $\tau$, illustrating the Rodrigues space and statistical representation .................................................. 147

Figure 4.22: Texture and Direction dependence of uniaxial cyclic loading (peak at 1% strain) of the damage parameter, $D_f$, illustrating the Rodrigues space and statistical representation ................................................. 148

Figure 4.23: Macroscopic shear stress versus shear strain for each shear direction for the Edge texture ........................................................................................................... 150

Figure 4.24: Shear direction effect for cyclic loading of the Edge texture (peak at $\gamma=1\%$) of the normal stress, $\sigma_{NN}$, illustrating the Rodrigues space and statistics .................................................. 151

Figure 4.25: Cyclic shear deformation of the Edge texture (peak at $\gamma=1\%$), illustrating the orientation and statistical dependence of the shear stress, $\tau$ ............................................................................................................. 152

Figure 4.26: Cyclic shear deformation of the Edge texture (peak at $\gamma=1\%$), illustrating the orientation and statistical dependence of the damage, $D_f$ ................................................................................................................... 153

Figure 4.27: Macroscopic axial stress-strain response for L-direction loading of the Edge texture for uniaxial and plane strain boundary conditions .... 154

Figure 4.28: Uniaxial versus plane strain boundary conditions for L-direction cyclic loading of the Edge texture (peak at 1% strain) of the normal stress, $\sigma_{NN}$, illustrating the Rodrigues space and statistics ............... 155

Figure 4.29: Uniaxial versus plane strain boundary conditions for L-direction cyclic loading of the Edge texture (peak at 1% strain) of the resolved shear stress, $\tau$, illustrating the Rodrigues space and statistics .................................................................................. 156

Figure 4.30: Uniaxial versus plane strain boundary conditions for L-direction cyclic loading of the Edge texture (peak at 1% strain) of the damage, $D_f$, illustrating the Rodrigues space and statistics ................................................................. 157

Figure 4.31: The HRR solution for the crack-divider and crack-turner configurations for a hardening exponent of $n = 8$ .............................................................. 158

Figure 4.32: L-direction mode I loading near a crack-tip based on the HRR solution for the normal stress, $\sigma_{NN}$, illustrating the Rodrigues space and statistics ........................................................................................................ 159

Figure 4.33: L-direction mode I loading near a crack-tip based on the HRR solution for the shear stress, $\tau$, illustrating the Rodrigues space and statistics ........................................................................................................ 160

Figure 4.34: L-direction mode I loading near a crack-tip based on the HRR solution for the damage, $D_f$, illustrating the Rodrigues space and statistics ........................................................................................................ 161

Figure A.1: Reversal point of a typical incremental step test illustrating the difference of engineering stress, true stress with elasticity, and typical true stress .............................................................................. 187
Figure B.1:  (a) 2024 aluminum strain gage specimen (b) Machine stiffness vs. load at room temperature for temperature chamber test frame............. 189
Figure C.1: Coordinate rotation between various reference frames......................... 190
Figure D.1: Macroscopic stress-strain response of four elastic assumptions .......... 193
Figure D.2: Sensitivity of the normal and shear stress histograms for uniaxial loading of the Edge texture in the L-direction to elasticity assumptions: large strain elasticity vs. small strain elasticity and anisotropic vs. isotropic.................................................................................. 194
Figure E.1: Sensitivity of L-direction uniaxial loading to a 10 MPa drop in pseudo-saturation stress through a sample of plastic slip parameters..... 195
Figure E.2: Sensitivity of L-direction uniaxial loading to a hardening shift through a sample of plastic slip parameter pairs................................................. 197
List of Tables

Table 2.1: Chemical composition of the 2099-T861 plate under investigation [25] ........................................................................................................................................8
Table 2.2: Initial grain size summary (based on micrographs [27]) ................................. 9
Table 2.3: Pole figure orientation vs. measured 2θ angles for pure aluminum [29] .......................................................................................................................................12
Table 2.4: Common texture components and their orientation descriptions ........ 19
Table 2.5: Split Hopkinson bar summary ........................................................................ 77
Table 3.1: Primary slip systems for an FCC crystal structure [55] ............................. 100
Table 4.1: Stress and strain determined from the HRR solution for the crack-divider and crack-turner configurations at half the fracture load ........ 160
### Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>2nd order zero tensor</td>
</tr>
<tr>
<td>a</td>
<td>Indice typically specifying the hardening term</td>
</tr>
<tr>
<td>b&lt;sub&gt;(s)&lt;/sub&gt;</td>
<td>Slip direction for slip system, s</td>
</tr>
<tr>
<td>c&lt;sub&gt;bar&lt;/sub&gt;</td>
<td>Wave speed of Split Hopkinson bar</td>
</tr>
<tr>
<td>f</td>
<td>Unspecified function</td>
</tr>
<tr>
<td>g</td>
<td>Orientation matrix</td>
</tr>
<tr>
<td>i</td>
<td>Free indice specifying a particular component</td>
</tr>
<tr>
<td>k</td>
<td>Unit-less constant</td>
</tr>
<tr>
<td>m</td>
<td>Generic vector</td>
</tr>
<tr>
<td>m&lt;sub&gt;(x)&lt;/sub&gt;</td>
<td>Uniaxial Hardening slope</td>
</tr>
<tr>
<td>n</td>
<td>Power law hardening exponent</td>
</tr>
<tr>
<td>n</td>
<td>Axis vector in axis-angle orientation description</td>
</tr>
<tr>
<td>n&lt;sub&gt;(s)&lt;/sub&gt;</td>
<td>Normal vector of the slip plane for slip system, s</td>
</tr>
<tr>
<td>q&lt;sub&gt;(s)&lt;/sub&gt;</td>
<td>Plastic state variables for slip system, s</td>
</tr>
<tr>
<td>q&lt;sub&gt;(s)(a)&lt;/sub&gt;</td>
<td>Plastic state variables for slip system, s, hardening term, a</td>
</tr>
<tr>
<td>r</td>
<td>Radius</td>
</tr>
<tr>
<td>r&lt;sub&gt;(a)&lt;/sub&gt;</td>
<td>Plastic barrier strength associated with hardening term, a</td>
</tr>
<tr>
<td>s</td>
<td>Indice typically specifying a slip system</td>
</tr>
<tr>
<td>t</td>
<td>Time</td>
</tr>
<tr>
<td>t&lt;sub&gt;o&lt;/sub&gt;</td>
<td>Reference time</td>
</tr>
<tr>
<td>x</td>
<td>Temperature / plastic strain-rate coupling parameter</td>
</tr>
<tr>
<td>X</td>
<td>Vector in the current Cauchy-frame</td>
</tr>
<tr>
<td>A</td>
<td>Generic 2nd order tensor</td>
</tr>
<tr>
<td>A&lt;sub&gt;bar&lt;/sub&gt;</td>
<td>Cross-sectional area of Split Hopkinson bar</td>
</tr>
<tr>
<td>A&lt;sub&gt;i&lt;/sub&gt;</td>
<td>Initial specimen’s cross-sectional area</td>
</tr>
<tr>
<td>A&lt;sub&gt;LSC&lt;/sub&gt;</td>
<td>Cross-sectional area for large strain compression test</td>
</tr>
<tr>
<td>C&lt;sub&gt;i&lt;/sub&gt;</td>
<td>Varshni model fit parameters with units of temperature</td>
</tr>
<tr>
<td>C&lt;sub&gt;Ge&lt;/sub&gt;</td>
<td>Cauchy-Green strain tensor</td>
</tr>
<tr>
<td>D&lt;sub&gt;f&lt;/sub&gt;</td>
<td>Findley-based damage parameter</td>
</tr>
<tr>
<td>D&lt;sup&gt;p&lt;/sup&gt;</td>
<td>Symmetric velocity gradient</td>
</tr>
<tr>
<td>E</td>
<td>Elastic modulus</td>
</tr>
<tr>
<td>E&lt;sub&gt;bar&lt;/sub&gt;</td>
<td>Linear elastic modulus of Split Hopkinson bar</td>
</tr>
<tr>
<td>E&lt;sub&gt;i&lt;/sub&gt;</td>
<td>Varshni model fit parameters with units of stress</td>
</tr>
<tr>
<td>E&lt;sub&gt;σ&lt;/sub&gt;</td>
<td>Stress dependent elastic modulus</td>
</tr>
<tr>
<td>E&lt;sup&gt;Ge&lt;/sup&gt;</td>
<td>Elastic Green strain</td>
</tr>
<tr>
<td>F</td>
<td>Deformation gradient</td>
</tr>
<tr>
<td>F&lt;sup&gt;e&lt;/sup&gt;</td>
<td>Elastic deformation gradient</td>
</tr>
<tr>
<td>F&lt;sup&gt;e&lt;/sup&gt;&lt;sub&gt;(i)&lt;/sub&gt;</td>
<td>Elastic deformation gradient at previous time</td>
</tr>
<tr>
<td>F&lt;sup&gt;e&lt;/sup&gt;&lt;sub&gt;(i+1)&lt;/sub&gt;</td>
<td>Elastic deformation gradient at current time</td>
</tr>
<tr>
<td>F&lt;sup&gt;e&lt;/sup&gt;&lt;sub&gt;guess&lt;/sub&gt;</td>
<td>Solution guess of the elastic deformation gradient</td>
</tr>
<tr>
<td>F&lt;sup&gt;p&lt;/sup&gt;</td>
<td>Plastic deformation gradient</td>
</tr>
<tr>
<td>Symbol</td>
<td>Definition</td>
</tr>
<tr>
<td>----------</td>
<td>---------------------------------------------------------------------------</td>
</tr>
<tr>
<td>$F^{(i)}$</td>
<td>Plastic deformation gradient at previous time</td>
</tr>
<tr>
<td>$F^{(i+1)}$</td>
<td>Plastic deformation gradient at current time</td>
</tr>
<tr>
<td>$F^{(i)}$</td>
<td>Deformation gradient at previous time-step</td>
</tr>
<tr>
<td>$F^{(i+1)}$</td>
<td>Deformation gradient at current time-step</td>
</tr>
<tr>
<td>$G_a$</td>
<td>Amplifier gain</td>
</tr>
<tr>
<td>$G_f$</td>
<td>Strain gage gain factor</td>
</tr>
<tr>
<td>$I$</td>
<td>2nd order identity matrix</td>
</tr>
<tr>
<td>$I^\text{max}$</td>
<td>Infrared intensity at maximum stress</td>
</tr>
<tr>
<td>$I^\text{min}$</td>
<td>Infrared intensity at minimum stress</td>
</tr>
<tr>
<td>$I^\frac{\sigma^\text{max}-\sigma^\text{min}}{2}$</td>
<td>Infrared intensity at midpoint of going tension cycle</td>
</tr>
<tr>
<td>$I^\frac{\sigma^\text{max}-\sigma^\text{min}}{2}$</td>
<td>Infrared intensity at midpoint of going compression cycle</td>
</tr>
<tr>
<td>$J^e$</td>
<td>Elastic Jacobian (determinate of $F^e$)</td>
</tr>
<tr>
<td>$K_{\text{mach}}$</td>
<td>Machine stiffness</td>
</tr>
<tr>
<td>$K_{\text{LVDT}}$</td>
<td>LVDT stiffness</td>
</tr>
<tr>
<td>$K_{\text{Spec}}$</td>
<td>Specimen stiffness</td>
</tr>
<tr>
<td>$L$</td>
<td>Current specimen length</td>
</tr>
<tr>
<td>$L$</td>
<td>Velocity gradient</td>
</tr>
<tr>
<td>$L_o$</td>
<td>Initial specimen length</td>
</tr>
<tr>
<td>$L^A$</td>
<td>Velocity gradient in grain $A$ with interface in the 3-direction</td>
</tr>
<tr>
<td>$L^p$</td>
<td>Plastic velocity gradient</td>
</tr>
<tr>
<td>$L^A$</td>
<td>Velocity gradient in grain $A$</td>
</tr>
<tr>
<td>$L^B$</td>
<td>Velocity gradient in grain $B$</td>
</tr>
<tr>
<td>$M$</td>
<td>Number of plastic hardening terms</td>
</tr>
<tr>
<td>$M_x$</td>
<td>Taylor factor (Generic)</td>
</tr>
<tr>
<td>$M_{\text{LSC}}$</td>
<td>Taylor factor for large strain compression test</td>
</tr>
<tr>
<td>$M_{\text{SSC}}$</td>
<td>Taylor factor for small strain compression test</td>
</tr>
<tr>
<td>$N$</td>
<td>Number of orientations</td>
</tr>
<tr>
<td>$P$</td>
<td>Load</td>
</tr>
<tr>
<td>$P^\text{thresh}$</td>
<td>Load threshold</td>
</tr>
<tr>
<td>$P^L$</td>
<td>Linearly distributed random number</td>
</tr>
<tr>
<td>$P^U$</td>
<td>Uniformly distributed random number</td>
</tr>
<tr>
<td>$Q$</td>
<td>Quaternion orientation vector</td>
</tr>
<tr>
<td>$Q$</td>
<td>Average probability density of 8-node Bunge angle space</td>
</tr>
<tr>
<td>$R^{3m}$</td>
<td>Rotation matrix rotating axis $\mathbf{m}$ to the 3-axis</td>
</tr>
<tr>
<td>$R^F$</td>
<td>Rodrigues-Frank orientation vector</td>
</tr>
<tr>
<td>$R^\Phi$</td>
<td>Second Bunge angle rotation matrix</td>
</tr>
<tr>
<td>$R^\Phi_1$</td>
<td>First Bunge angle rotation matrix</td>
</tr>
<tr>
<td>$R^\Phi_2$</td>
<td>Third Bunge angle rotation matrix</td>
</tr>
<tr>
<td>$R^e$</td>
<td>Rigid rotation that relates the crystal lattice to the current Cauchy-frame</td>
</tr>
<tr>
<td>$S_{11}$</td>
<td>Common anisotropic elasticity parameter</td>
</tr>
<tr>
<td>$S_{12}$</td>
<td>Common anisotropic elasticity parameter</td>
</tr>
</tbody>
</table>
Common anisotropic elasticity parameter
Engineering strain (2\textsuperscript{nd} Piola-Kirchoff stress)
Temperature
Elastic stretch
Current specimen volume
Initial specimen volume
Voltage of a generic wave
Vector in the reference lab-frame
Excitation voltage
Shear-normal coupling for Findley-based damage
Backstress-like term associated with slip system, \( s \)
Generic indice
Kronecker delta
Strain tensor (for small elastic strains)
Strain from the reflected wave
Strain from the transmitted wave
Dynamic total strain of a generic wave
Uniaxial elastic strain
Elastic uniaxial strain offset
Engineering uniaxial strain
Elastic uniaxial engineering strain
Uniaxial plastic strain
Plastic strain at latest reversal
Plastic uniaxial strain offset
Tensile plastic strain determined using Masing behavior
Reference plastic uniaxial strain offset
True total uniaxial strain
Elastic uniaxial true strain
Uniaxial total strain
Total uniaxial strain offset
First Bunge angle
Third Bunge angle
Shear strain
Maximum shear strain
Plastic strain-rate for slip system, \( s \)
Bulk modulus
Flag specifying direction of cyclic loading
Stress dependent bulk modulus
Elastic shear modulus
Poisson’s ratio
Set of random angles on face \( i \)
\( \theta \) Hardening slope for hyperbolic tangent model
\( \theta_{(a)} \) Hardening slope associated with hardening term, \( a \)
\( \theta^{(i)} \) Reference angle associated with \( \theta \)
\( \rho \) Density
\( \rho_{\text{bar}} \) Density of Split Hopkinson bar
\( \sigma \) Uniaxial stress
\( \sigma \) Cauchy stress tensor
\( \sigma_{\text{asym}} \) Average stress range
\( \sigma_{\text{eq}} \) Equivalent or von Mises stress
\( \sigma_{\text{max}} \) Maximum cyclic stress
\( \sigma_{\text{min}} \) Minimum cyclic stress
\( \sigma_{\text{o}} \) Reference stress
\( \sigma_{\text{sat}} \) Uniaxial saturation stress
\( \sigma_{\text{ten}} \) Tensile stress determined using Masing behavior
\( \sigma_{\text{A}}^{(3)} \) Cauchy stress in grain \( A \) with interface in the 3-direction
\( \sigma^{\text{avg}} \) Stress averaged for a set of crystallographic orientations
\( \sigma_{\text{max}}^{(n)} \) Maximum normal stress
\( \sigma^{\text{true}} \) Uniaxial true stress
\( \sigma^{\text{thres}} \) Threshold uniaxial stress
\( \sigma^{(i)} \) \( i \)th Cauchy stress tensor
\( \sigma^{(BC)} \) Stress boundary conditions
\( \hat{\sigma} \) Rotated Cauchy stress
\( \tau_{(s)} \) Shear stress resolved onto slip system, \( s \)
\( \tau_{(s)}^{(3A)} \) Shear stress resolved in grain \( A \) with the interface in the 3-direction
\( \tau_{(s)}^{(s)} \) Shear stress on slip system, \( s \), determined from plasticity
\( \omega \) Angle in axis-angle orientation description
\( \zeta \) Anisotropic modulus
\( \Delta \) Displacement
\( \Delta_{\text{thres}} \) Displacement threshold
\( \Delta t \) Time increment
\( \Delta \mathbf{F} \) Deformation gradient increment
\( \Delta \mathbf{F}^{(\text{guess})} \) Solution increment of the elastic deformation gradient
\( \Delta \mathbf{F}^{(p)} \) Plastic deformation gradient increment
\( \Delta L \) Change in specimen length
\( \Delta L \) Solution increment of the velocity gradient
\( \Delta T_{\text{in}} \) In-phase change in temperature
\( \Delta T_{\text{out}} \) Out-of-phase change in temperature
\( \Delta Q_{i} \) Difference in probability density of opposing faces in the \( i \) direction
\( \Delta V \) Change in specimen volume
\( \Delta \epsilon^{e} \) Elastic strain change
\( \Delta \gamma^{(p)}_{(s)} \) Solution increment of the slip system plastic strain-rate
\( \Delta \theta_i \)  
Angle range associated with \( \theta_i \)

\( \Delta \tau \)  
Resolved shear stress range

\( \phi \)  
Second Bunge angle

\( \Theta \)  
Unit Twist

\( \Sigma^e \)  
Mandel stress

\( T \)  
Torque

\( \Xi^{tr} \)  
Solution residual associated with the elastic deformation gradient

\( \Xi^r \)  
Solution residual associated with stress boundary conditions

\( \Xi^i \)  
Solution residual associated with the slip system shear stress

\( \Psi^e \)  
Elastic strain energy density

\( \Psi^p \)  
Rate of change of the plastic strain energy density

\( \mathcal{O} \)  
4th order zero tensor

\( \mathcal{A} \)  
Generic 4th order tensor

\( \mathcal{B} \)  
Generic 4th order tensor

\( \mathcal{C}^\varepsilon \)  
4th order elastic stiffness tensor

\( \mathcal{J} \)  
4th order spherical tensor

\( \mathcal{K} \)  
4th order deviatoric tensor

\( \mathcal{X} \)  
4th order anisotropic tensor

**Other Mathematical Conventions:**

\( A^T \)  
Transpose of tensor \( A \)

\( A^{-1} \)  
Inverse of tensor \( A \)

\( A \cdot B \)  
Dot product of tensors \( A \) and \( B \)

\( A \otimes B \)  
Alternate dot product of tensors \( A \) and \( B \)

\( A : B \)  
Inner product of tensors \( A \) and \( B \)

\( x \otimes y \)  
Tensor product of vectors \( x \) and \( y \)

\( x \times y \)  
Cross product of vectors \( x \) and \( y \)

\( \frac{dA}{dx} \)  
Derivative of \( A \) with respect to \( x \)

\( \frac{\partial A}{\partial x} \)  
Partial derivative of \( A \) with respect to \( x \)

\( \dot{x} \)  
Derivative of \( x \) with respect to time
1 Introduction and Background

Aluminum-lithium alloys have been the subject of multiple investigations over the past 30 years due to its lower density, increased elastic stiffness, and high strength when compared to other aluminum alloys. The significance of adding lithium to aluminum is often quantified by the relationship that every 1 wt% of lithium added increases the elastic modulus by 6% and lowers the density by 3% [1], both of which are advantageous in the aerospace industry. However, this material remains underutilized due to its propensity for localized deformation and grain boundary delamination. Delamination in polycrystalline metals has some resemblance to those in laminate composites, but is a distinct phenomenon despite similar nomenclature. This moniker was not initiated by the author, but has been used frequently in the literature.

Delamination in aluminum-lithium alloys often refers to the observed secondary cracking normal to the mode I crack during the fracture process. Delamination may give artificially high fracture toughness in certain crack orientations, but may lower toughness when cracks are oriented along elongated grain boundaries. This grain shape is a result of the rolling operation utilized during production of most wrought aluminum products.

As an introduction to the delamination process, consider the fracture of a $K_{IC}$ specimen in a variety of orientations. In the orientation when the mode I crack is aligned with the elongated grains, specimens failed in a traditional manner, displaying lower fracture toughnesses than other orientations [2]. In contrast, when the primary crack is not aligned with the elongated grains (take the T-N plane for instance), then the mode I crack propagates in the assumed direction with delaminated sub-cracks decorating the crack front (Figure 1.1, [2-4]). As shown trans-granular fracture occurs out-of-plane with the traditional $K_{IC}$ fracture expected during such an experiment. Previous investigations have shown that in a Mode I crack field, the driving force to propagate an existing delamination is inherent [5, 6]. This increased tendency to delaminate after initiation is a result of the geometry, loading, and relative strength of the grain boundary interface relative to the primary crack front. Instead of characterizing delamination growth, the task of understanding the onset (initiation) of the delamination phenomenon is the goal of this investigation.
Delamination in polycrystal metals is a form of localized deformation that manifests itself with failure along grain boundaries. Before the onset of delamination, other forms of localization may occur that initiate the delamination process. Many Al-Li alloys, similar to the 2099-T861 alloy under investigation, exhibit localized phenomena, such as serrated flow, deformation banding, and crack splitting [1-23]. These observed localizations are explained with a variety of mechanisms, which include precipitate shearing, negative strain-rate sensitivity, the Portevin-Le Châtelier effect (PLC), modulus dislocation interactions, reduced friction stress, precipitate free zones, and lithium segregation [7-23].

Perhaps the most obvious association to localized deformation is serrated plastic flow. Serrated flow refers to stress drops during a displacement/strain control experiment. Serrated flow is most commonly observed in single crystals and relatively small polycrystal specimens of Al-Li alloys under certain aging conditions, temperatures, and strain rates [7-12]. The onset of serrated flow is typically described by some critical strain, which varies with temperature and strain rate [10], and it may subside at a higher strain level. In some circumstances, serrated flow may restart after arrest because of a change in localization mechanism [7]. The magnitude and frequency of stress-drops (in
strain or displacement control) can be measured for various loading conditions to assist in identification of plausible mechanisms. Macroscopic observation of serrated flow is limited to situations where a dominant volume fraction of the material is experiencing localized phenomena. This is easily observed for single crystals and specimens with a limited number of grains. For typical polycrystal specimens, localized deformation may occur without observing serrations in the macroscopic stress-strain response. This is explained by the constraint and dampening effect of non-localized crystals in polycrystal materials. Additionally, this dampening effect makes observing serrations at very small strains exceptionally difficult.

The most common microstructural observation related to localization is deformation banding. Deformation banding refers to localized slip concentrated along a specific orientation (or band) in the material. These regions resemble persistent slip bands observed in fatigue, in the sense that there are localized differences in mobile dislocation densities at a dimension smaller than the grain size. Although deformation banding is typically observed on the scale of a single grain, larger bands (macro-slip) may develop at large (>3%) strains. Deformation banding is typically observed using optical microscopy, SEM, or bulk visual inspection after mechanical testing. Alternatively, a series of strain gauges or image correlation techniques could be implemented during mechanical loading to observe banding phenomenon. In the case of Al-Li alloys, deformation banding has been independently reported by several authors [11-16]. Slip band localization and its relation to observed load drops in displacement (or strain) control were isolated from the effect of micro-crack development via permutations of surface polishing, aging and reloading [15]. They concluded that localized deformation banding is a distinct microstructural mechanism, rather than a result of existing micro-cracks.

The observation of crack turning or delamination is commonly observed for fatigue loading of many Al-Li alloys. The texture, heat treatment, and loading direction affect this phenomenon, but the literature attributes crack turning to an embrittled grain boundary or slip band cracking [1, 14, 15, 17-19]. Takahasi et. al. [22] correlated a resolved stress normal to the elongated grain boundaries in a 2091-T8 alloy with the onset of delamination cracking using ultrasonic wave measurements. Delamination has
been reported as being prevalent at lower temperatures including the cryogenic regime. In a recent investigation, delamination in 8090 Al-Li was attributed to lithium segregation at grain boundaries [23]. Although this contrasts the localization postulate, direct evidence of lithium segregation was not presented and its argument is based on elimination of other plausible explanations. Additionally, only under-aged conditions were considered and other mechanisms could be driving delaminations in peak-aged alloys. Despite the apparent conflict, localization before the onset of micro-cracking may accelerate the crack turning and delamination process [13].

A variety of explanations on localization are available in the literature, but the most common mechanism stipulated forwards the notion that small shearable precipitates may locally soften the material [9-15, 18-20]. Most Al-Li alloys with sufficient lithium content (>1.3wt%) contain small metastable spherical δ’ (Al3Li) precipitates that are amenable to shear failure under certain heat treatments, temperatures, and loading conditions [11]. When a precipitate shears, it results in sudden deformation that causes localized material disorder, which in turn softens the material because the prior ordered structure is lost [15]. This shearing mechanism is often related Portevin-Le Châtelier effect [8] with the phenomena exhibiting negative strain-rate sensitivity [11]. At very large strains these shearable obstacles are expected to contribute to a decreasing friction stress, resulting in the development of a macro-slip bands [12]. The most convincing aspect of this hypothesis is the correlation of unique microscopic features for various permutations of loading rates, temperatures and heat treatments where delamination does or does not occur. One of the finer points under contention in the literature concerns behavior at small plastic strains. For instance, some accounts explain the small strain localization by invoking a modulus dislocation coupling [21]. Because of lithium’s significant effect on the elastic modulus of aluminum, it’s not unreasonable for modulus dislocation coupling to occur. It should be emphasized that particularly for fatigue loading (Figure 1.2), the plastic strain level for delamination is on the order of the nominal elastic deformation and is also temperature and strain-rate dependent.
In 2099-T861 and other similar materials, shearable δ’ precipitates are expected to drive localization in its peak-aged condition. If aging were to continue to some over-aged regime, precipitates may increase in size enough to become unshearable, thus hypothetically homogenizing deformation. However, for this over-aged condition, the increased precipitate spacing could result in precipitate free zones in the material, which may provide local regions of ‘softer’ material for localizations to develop [11]. Along with the δ’ (Al₃Li) phase previously associated with localizations, 2099-T861 also exhibits a needlelike T₁ (Al₂CuLi) and θ’ (Al₂Cu) phases that directly influence strain hardening [13]. The θ’ precipitate phase is preferentially oriented along the <100> direction, which contributes significantly to the anisotropy in the material [24]. The T₁ phase was found in higher concentrations along grain boundaries particularly for peak-aged and over-aged heat treatments [4]. These precipitate phases at material interfaces, such as grain boundaries may result in locally higher stresses, which drive the delamination phenomenon.

Extensive research [11-24] has been conducted that focus on metallurgical and localization aspects of the aluminum alloys. Rather than examine the delamination phenomenon with a metallurgical approach, a mechanical framework is forwarded that examines the state of stress at potential delamination sites. The current investigation proceeds through four additional chapters: Experimental Investigation (Chapter 2), Modeling Material Behavior (Chapter 3), Results and Discussion (Chapter 4), and
Conclusions (Chapter 5). A brief overview of each of these chapters is provided below to guide the subsequent discussion.

Most of the existing experimental work where delamination was observed involved fracture toughness testing. The experimental investigation (Chapter 2) is subdivided into three sections: Initial plate properties, small strain deformation, and large strain deformation. Each section provides additional observations that are relevant to formulating a model for the delamination phenomenon. The initial plate properties that are anticipated to contribute to delamination include: grain characteristics and crystallographic texture. The small strain deformation is primarily comprised of cyclic deformation, which was found to cause delamination under the right conditions (sufficient loads and moderate temperature and strain-rate). Finally, large strain deformation provides an avenue toward obtaining the critical loads leading to failure along the elongated grain boundaries, through both N-direction tensile and interface shear loading.

The material model framework (Chapter 3) is developed to incorporate many of the experimental observations. Most notably, a cyclic crystal plasticity model was developed that reproduces stable kinematic hardening for a rate independent material, as was the case in the temperature / strain-rate regime where delamination was observed. Finite strain and anisotropic elasticity were included to accommodate potential localizations (for a spatially discretized applications) and to be sufficiently accurate in the small strain regime where cyclic deformations are appropriate. A uniform deformation model is utilized this framework to provide an upper bound estimate of the local stress behavior on the elongated grain boundary interface. To obtain an improved estimate on the interface of specific orientation pairs, a bi-crystal model was formulated.

The Results and Discussion chapter (Chapter 4) presents the results of modeling simulations and relates them to experimental observations. It begins by considering the uniaxial cyclic loading, which dominated the experimental investigation. First the uniform deformation model is presented to highlight the orientation dependence and statistical character of the uniaxial loading case. Significant shear and normal components were predicted on elongated grain boundaries, which lead to the hypothesis
that a Findley-based shear-normal coupled damage parameter is appropriate for cyclic deformation. The results from the uniform deformation model are compared to the Bi-crystal model simulations. The damage parameter is shown to mirror the experimental observations for the initiation of delamination. Finally, other loading cases including: shear, plane strain tension, and deformation near a crack-tip are modeled and the results are related to potential delamination.

The Conclusions and Recommendations chapter (Chapter 5) summarizes the most important observations of the previous chapters and offers observations that are only apparent with hindsight. The successful components and limitations of the modeling effort are highlighted. Finally, future recommendations are included to provoke further study on the delamination phenomenon.
2 Experimental Investigation

At the onset of this investigation on the delamination of 2099-T861 aluminum-lithium, a broad range of experiments were preformed to obtain material properties, observe localization phenomenon, and provide a robust foundation for characterization of delamination. For convenience, the experimental findings are presented in the following three subsections, including initial plate properties, small strain deformations, and large strain deformations. The sections were chosen to represent properties and characteristics found in the material as received, after or during relatively small deformations (< 1% strain), and after or during relatively large deformation (> 1% strain).

2.1 Initial Plate Properties

Alcoa™ manufactured the 2099-T861 (also called C458-T8 during alloy development) rolled plate employed in this investigation. The bulk chemical composition of the plate is summarized in Table 2.1, where the most notable characteristics are the 1.73 wt% Li and the 2.58 wt% Cu. After rolling, the plate experienced a 6% stretch in the rolling direction and 24 hours aging at 150°C [25]. This heat treatment corresponds to a T861 condition, which is close to peak-aged (though slightly under-aged as it exhibits some hardening with further aging). The undeformed characteristics of the 2099-T861 plate (63.5 mm thick), were initially investigated using a variety of techniques including optical microscopy, X-ray Diffraction (XRD), Electron Back-Scatter Diffraction (EBSD), and Auger Electron Spectroscopy (AES). Each technique provides a unique perspective and helps quantify the initial plate properties.

Table 2.1: Chemical composition of the 2099-T861 plate under investigation [25]

<table>
<thead>
<tr>
<th>Comp</th>
<th>Cu</th>
<th>Li</th>
<th>Zn</th>
<th>Mg</th>
<th>Mn</th>
<th>Zr</th>
<th>Si</th>
<th>Fe</th>
<th>Ti</th>
<th>Al</th>
</tr>
</thead>
</table>
| wt%  | 2.58| 1.73| 0.60| 0.26| 0.25| 0.09| 0.03| 0.03| 0.01| Bal.
| at%  | 1.06| 6.53| 0.24| 0.28| 0.12| 0.26| 0.03| 0.01| 0.005| Bal.

For brevity, innate plate directions will be referred to by the following notation: L – Longitudinal or rolling direction, T – Transverse direction, and N – Normal or through thickness direction. Since there was a variation of microstructures and textures in the N-direction, the thickness location is specified relative to the total plate thickness in a fractional form. For instance a location denoted as t/2 is at the center of the plate, and t/10 refers to a location only one tenth of the total thickness from the outer edge of the
plate. Three distinct symmetric plate thickness regions were identified: edge (0 to t/5), transition (t/5 to 2t/5), and center (2t/5 to t/2). The as received plate thickness is 63.5 mm, which is large enough for a gradient of properties to be anticipated and provide representative volumes for measuring bulk material properties.

To ascertain the grain size and bulk micro-structural characteristics, optical micrograph specimens were prepared from the as received plate within each distinct region. Each specimen was polished mechanically up to a 0.05 µm using an alumina solution. To achieve optimal polishing quality, a final vibrational polish was conducted in a 0.02 µm colloidal silica solution. To emphasize the grain structure for optical microscopy, samples were etched using Kellers Reagent \[26\] (0.5% HF, 1.5%HCl, 2.5% HNO\(_3\), and 95.5% H\(_2\)O) for approximately 15 seconds.

**Table 2.2: Initial grain size summary (based on micrographs [27])**

<table>
<thead>
<tr>
<th></th>
<th>L (mm)</th>
<th>T (mm)</th>
<th>N (mm)</th>
<th>Aspect Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Edge (t/6)</strong></td>
<td>1.20</td>
<td>0.90</td>
<td>0.086</td>
<td>14.0</td>
</tr>
<tr>
<td><strong>Transition (t/3)</strong></td>
<td>1.20</td>
<td>0.75</td>
<td>0.088</td>
<td>13.9</td>
</tr>
<tr>
<td><strong>Center (t/2)</strong></td>
<td>1.05</td>
<td>0.81</td>
<td>0.11</td>
<td>9.6</td>
</tr>
</tbody>
</table>

A representative three-dimensional optical micrograph at thickness location t/10 is presented in Figure 2.1. As illustrated, a pancake structure of elongated grains is observed with an average grain size of approximately 1.2 x 0.9 x 0.09 mm in the L x T x N directions respectively. At these magnifications, it is difficult to see significant differences in the grain structure throughout the plate. An elongated grain structure is typical of the rolling process and has been reported to be an essential feature of the delamination phenomenon [2-4]. The compilation of micrographs at various plate thicknesses indicates the grain aspect ratio is most pronounced at the edge of the plate. However, throughout the entire plate a significant elongated grain structure is evident. For each plate region, the average grain size was obtained by employing the intersection counting method for non-equiaxed grains [27]. A summary of these results is presented in Table 2.2. As brief observation suggested, the grain sizes are very similar throughout the plate with slightly shorter and thicker grains near the plate center.
2.1.1 X-ray Diffraction (XRD)

Since 1912, when Bragg [28] showed that a diffraction pattern could be used to determine the crystallographic orientation of a crystal lattice, X-ray Diffraction (XRD) has been employed in conjunction with crystal-based modeling. A variety of physical measurements are possible with XRD, including: crystallography (crystal structure determination), statistical crystallographic orientation (texture), and lattice distortion (residual stresses). For 2099-T861, XRD provides an ideal avenue to statistically characterize crystallographic orientations at various thicknesses of the rolled plate.

2.1.1.1 Experimental Procedure

To explore the bulk texture of the undeformed plate at various locations through the thickness, XRD measurements were conducted. Specifically, the plate of Al-Li was sectioned into 3 mm thick pieces to investigate the texture at various thicknesses (t/8, t/6, t/4, t/3, t/2, 2t/3, 3t/4, 5t/6, and 7t/8) by measuring on the N-face. Additional samples were also evaluated after deformation at thicknesses (t/10, 3t/10 and t/2) from the L, T, and N-faces after both large and small strain deformation. Each sample was mechanically polished up to 0.05 µm using an alumina solution. Etching and vibrational polishing were not necessary for X-ray specimens. To measure the texture of the specimens, a Philip’s X’pert MRD Goniometer with monochromatic Cu-K radiation was used. The X-ray source was set to a 2 mm x 2 mm configuration using a crossed-slit collimator and a nickel filter to eliminate secondary peaks. N-face specimens were mounted in the XRD such that the rolling direction (L) was aligned with the X-ray source.
and detector when the machine angles are set to $2\theta = 0^\circ$, $\psi = 90^\circ$, and $\phi = 0^\circ$ (Figure 2.2). A 2 mm x 2 mm region corresponds to approximately 100 grains, accounting for typical X-ray penetration in aluminum. To ensure that the region was statistically sufficient, the measurements were repeated at various locations on several specimens. These specimens were also tested using an oscillatory pattern spanning an 8 mm x 2 mm area. These tests verified that a 2 mm x 2 mm region was statistically sufficient to obtain representative bulk texture measurements.

**Figure 2.2: Typical specimen orientation in the XRD and defined machine angles.**

With the specimen properly mounted and aligned, the peaks corresponding to various pole figures could be measured using a 2\(\theta\)-scan. A 2\(\theta\)-scan holds the angles $\psi$ and $\phi$ at $90^\circ$ and $0^\circ$ respectively, while rotating the $2\theta$ angle over some prescribed range (from $35^\circ$ to $85^\circ$ in this case). The resulting peaks of intensity correspond to $2\theta$ angles where pole figures may be measured. To determine which peak corresponds to $2\theta$ angles where pole figures may be measured. To determine which peak corresponds with which pole figure, the results of a pure aluminum powder specimen [29], shown in Table 2.3, were utilized. These angles agree well with the 2\(\theta\)-scan for each specimen, as shown in Figure 2.3. For the specimens near the center of the plate (t/3, t/2, and 2t/3) a non-aluminum peak was observed at about $42.1^\circ$. This peak likely corresponds to an orientation of a precipitate phase that may be highly concentrated at these plate locations. Due to the proximity of the peaks, the exact chemistry is unconfirmed, but likely candidates are either $\theta'$: $\text{Al}_2\text{Cu}$ ([220] peak @ $42.107^\circ$) [30] or $\text{T}_1$: $\text{Al}_2\text{CuLi}$ ([200] peak @ $42.127^\circ$) [31]. Both precipitate phases are expected in this material and directly influence strain hardening [13], which is also evident in the mechanical properties near the center of the plate. Since the $\theta'$ precipitate phase was observed to be preferentially oriented along the [100] direction [24] rather than [110], $\theta'$ is less likely to be the particulate chemistry responsible for the observed peak. It is probable that the peak is due to the needlelike $\text{T}_1$ phase, which was found in higher concentrations for peak-aged
and over-aged heat treatments [4] (as is the case near the plate center). Additionally, the
T$_1$ precipitates are often preferentially orientated in the [100] direction [4].

Table 2.3: Pole figure orientation vs. measured 2θ angles for pure aluminum [29]

<table>
<thead>
<tr>
<th>Polefigure Orientation</th>
<th>2θ Angle</th>
</tr>
</thead>
<tbody>
<tr>
<td>[111]</td>
<td>38.505</td>
</tr>
<tr>
<td>[200]</td>
<td>44.778</td>
</tr>
<tr>
<td>[220]</td>
<td>65.194</td>
</tr>
<tr>
<td>[311]</td>
<td>78.305</td>
</tr>
</tbody>
</table>

Figure 2.3: 2θ scans of the undeformed Al-Li plate at various thicknesses with an
N-normal polished surface.

The 2θ peak angles corresponding to the [111], [200], [220], and [311] peaks
were used to obtain the relevant pole figures for each specimen. By setting the 2θ angle
constant and incrementing the remaining two angles over 5° increments from 0-85° and
0-360° respectively, the four pole figure measurements were obtained along with
corresponding background measurements. The experimental pole figures were corrected
using both background measurements and a defocusing correction, which was scaled based on the Full-Width-Half-Max (FWHM) of the corresponding 2θ peak [32].

![Figure 2.4: [111], [100], and [110] pole figures for the 3 texture regimes of the Al-Li plate relative to an L-T-N reference frame.](image)

The N-face [111], [100], and [110] pole figures were obtained at nine plate thicknesses. The results showed approximate symmetry between the top and bottom of the plate, as expected from the 2θ-scans (Figure 2.3). Also there appears to be a smooth transition between three distinct textures through the plate. Beginning at the plate center (2t/5 - t/2), a strong N-oriented [110] component is evident (Figure 2.4). In the transition region of the plate (t/5 - 2t/5), a more typical rolling texture was observed [33]. Finally, near the outer surface of the plate (0 - t/5), a N-rotated cube texture was observed. This texture is highly anisotropic and is named for its large cube component in the N-direction. As the [100] pole figure illustrates, the N-cube component is dominant, but other components of a rolling texture are also evident. It should be noted that the density of the pole figures are scaled such that a uniform texture (random or untextured) material has an intensity of one everywhere. Pole figures and subsequent Rodrigues spaces were
plotted using equal-area projection with a Matlab [34] code, which borrowed heavily from Boyce’s DPLAB [35].

2.1.1.2 Orientation Mapping

Before delving into the various options for orientation mapping, first consider the aforementioned pole figures, which are directly measured during XRD experiments (after the aforementioned corrections). A pole figure displays the projections of a family of poles (such as \{111\}, \{100\} and \{110\}) with respect to the lab reference frame. For example, the center of a [111] pole figure corresponds to the density of orientations, whose \(\langle 111 \rangle\) axis is aligned with the normal direction chosen (experimentally it is often the measured surface). Since the measurement is a projection of a pole’s orientation, multiple crystallographic orientations occupy the same space, including any variant that is rotated about the projected pole’s axis. This ambiguity is commonly overcome though the used of multiple pole figures and assumptions on both material and crystal symmetry. A schematic illustration of the pole figure (Figure 2.5) is included for convenience; the reader is referred to the literature [33, 36-37] for further details and discussion.

Figure 2.5: Schematic illustrating a) the poles of a crystal extended to a unit sphere and b) the projection scheme for a stereographic pole figure [36].

There are situations when a single pole figure is sufficient to describe the crystallographic texture of interest; namely uniaxial deformation of single crystals or
uniform fiber textures, where only the relative orientation with respect to a loading axis is necessary. However, in the vast majority of scenarios a more complete orientation description is required to avoid ambiguity. The earliest method developed to define orientation was proposed by Euler [38] through the use of three ‘Euler’ angles. These three angles have several established conventions, but only the Bunge [39] convention is considered in this investigation. Bunge angles were reported by the XRD software [32] that was used to interpret the experimental pole figures. As it is necessary to implement these angles in subsequent analysis and modeling, defining the Bunge convention is appropriate. Specifically, the Bunge angle convention is a unique set of Euler angles that describes the orientation in terms of three sequential rotations corresponding to angles $\phi_1$ (rotation about $z_0$ or $z_1$ axis), $\Phi$ (rotation about $x_1$ or $x_2$ axis), and $\phi_2$ (rotation about the $z_2$ or $z_f$ axis) as illustrated in Figure 2.6. These rotations are combined to produce the orientation matrix, $g$ [39]:

$$g = R^\phi_2 R^\Phi R^\phi_1$$ \hspace{1cm} (2.1)

This orientation matrix is presented below in terms of Bunge angles.

$$g = \begin{bmatrix} 
\cos(\phi_1) \cos(\phi_2) - \cos(\Phi) \sin(\phi_1) \sin(\phi_2) & \cos(\phi_1) \sin(\phi_2) + \cos(\Phi) \cos(\phi_1) \sin(\phi_2) & \sin(\phi_2) \\
-\cos(\Phi) \cos(\phi_2) \sin(\phi_1) - \cos(\phi_1) \sin(\phi_2) & \cos(\Phi) \cos(\phi_1) \cos(\phi_2) - \sin(\phi_2) \sin(\phi_1) & \cos(\phi_1) \\
\sin(\phi_1) \sin(\phi_2) & \cos(\phi_1) \sin(\phi_2) & \cos(\phi_1) 
\end{bmatrix}$$ \hspace{1cm} (2.2)

Figure 2.6: Bunge angle illustration ($\phi_1$=30°, $\Phi$=45°, and $\phi_2$=60°)

Despite the widespread use and familiarity with Euler angles (Bunge), there are two particularly limiting features that inhibit their use as an effective orientation mapping
technique. The first is that the angle’s ordered coupling causes the effect of each angle to be a consequence of the angles previously prescribed. This ordering dependence makes angular interpretation rather awkward and asymmetric between each parameter. The second difficulty is the non-unique angular descriptions near zero rotation of the second Bunge angle, which makes any combination of first and third angles equivalent. To overcome these issues, one may consider the axis-angle orientation description, which utilizes a rotation about the axis, $\mathbf{n}$, by an angle, $\omega$. This axis-angle description may be presented in the form of a rotation matrix:

$$
\mathbf{g} = 
\begin{bmatrix}
(1 - n_i^2) \cos \omega + n_i^2 & n_i n_j (1 - \cos \omega) + n_j \sin \omega & n_i n_k (1 - \cos \omega) - n_k \sin \omega \\
n_i n_j (1 - \cos \omega) - n_j \sin \omega & (1 - n_j^2) \cos \omega + n_j^2 & n_j n_k (1 - \cos \omega) + n_k \sin \omega \\
n_i n_k (1 - \cos \omega) + n_k \sin \omega & n_j n_k (1 - \cos \omega) - n_i \sin \omega & (1 - n_k^2) \cos \omega + n_k^2
\end{bmatrix}
$$

or conversely, extracted from a rotation matrix by:

$$
\begin{bmatrix}
n_1 \\
n_2 \\
n_3
\end{bmatrix} = \frac{1}{\sqrt{(g_{23} - g_{32})^2 + (g_{31} - g_{13})^2 + (g_{12} - g_{21})^2}} \begin{bmatrix}
g_{23} - g_{32} \\
g_{31} - g_{13} \\
g_{12} - g_{21}
\end{bmatrix}
$$

$$
\omega = \cos^{-1} \left( \frac{1}{2} \left( g_{11} + g_{22} + g_{33} - 1 \right) \right)
$$

To avoid the ambiguity at a zero rotation angle, a vectoral description, which scales the axis (unit vector) by some function of the angle, is advantageous.

There are two specific mappings using a vector description that were employed in this investigation. The first is the Rodrigues vector, $\mathbf{R}^F$:

$$
\mathbf{R}^F = \mathbf{n} \tan \left( \frac{1}{2} \omega \right)
$$

which was introduced in 1840 by Rodrigues [40], but was ignored in most of the materials literature until it was popularized by Frank in 1988 [41]. It should be noted that Rodrigues’s work has been discussed in the literature by Gray [42]. This mapping is particularly useful because of its unique rectilinearity properties that make it the optimal choice for graphical representation, as will be illustrated subsequently. Any two sequential rotations described by Rodrigues vectors ($\mathbf{R}^{F(A)}$ and $\mathbf{R}^{F(B)}$) may be combined into a third Rodrigues vector ($\mathbf{R}^{F(C)}$) by:
The rotation matrix, \( g \), may be obtained in terms of any Rodrigues vector, \( \mathbf{R}^F \), with the following expression:

\[
g = \begin{bmatrix}
1 - \frac{1 - \cos(\|\mathbf{R}'\|)(R_{z}^2 + R_{y}^2)}{\|\mathbf{R}'\|^2} & \frac{1 - \cos(\|\mathbf{R}'\|)R_{y} R_{z}}{\|\mathbf{R}'\|^2} & \frac{1 - \cos(\|\mathbf{R}'\|)R_{x} R_{z}}{\|\mathbf{R}'\|^2} & \frac{1 - \cos(\|\mathbf{R}'\|)R_{x} R_{y}}{\|\mathbf{R}'\|^2} \\
\frac{1 - \cos(\|\mathbf{R}'\|)R_{y} R_{z}}{\|\mathbf{R}'\|^2} & 1 - \frac{1 - \cos(\|\mathbf{R}'\|)(R_{z}^2 + R_{y}^2)}{\|\mathbf{R}'\|^2} & \frac{1 - \cos(\|\mathbf{R}'\|)R_{x} R_{y}}{\|\mathbf{R}'\|^2} & \frac{1 - \cos(\|\mathbf{R}'\|)R_{x} R_{z}}{\|\mathbf{R}'\|^2} \\
\frac{1 - \cos(\|\mathbf{R}'\|)R_{x} R_{z}}{\|\mathbf{R}'\|^2} & \frac{1 - \cos(\|\mathbf{R}'\|)R_{x} R_{y}}{\|\mathbf{R}'\|^2} & 1 - \frac{1 - \cos(\|\mathbf{R}'\|)(R_{x}^2 + R_{y}^2)}{\|\mathbf{R}'\|^2} & \frac{1 - \cos(\|\mathbf{R}'\|)R_{y} R_{z}}{\|\mathbf{R}'\|^2} \\
\frac{1 - \cos(\|\mathbf{R}'\|)R_{x} R_{y}}{\|\mathbf{R}'\|^2} & \frac{1 - \cos(\|\mathbf{R}'\|)R_{x} R_{z}}{\|\mathbf{R}'\|^2} & \frac{1 - \cos(\|\mathbf{R}'\|)R_{y} R_{z}}{\|\mathbf{R}'\|^2} & 1 - \frac{1 - \cos(\|\mathbf{R}'\|)(R_{x}^2 + R_{y}^2)}{\|\mathbf{R}'\|^2}
\end{bmatrix}
\]

(2.7)

One disadvantage of a Rodrigues vector map is that in its most general format, it extends to infinity. This difficulty is often avoided with symmetry considerations, but for triclinic and purely mathematical applications there is another option, the Quaternion parameter, \( \mathbf{Q} \) [33]:

\[
\mathbf{Q} = \begin{cases} 
q_0 = \cos(\omega/2) \\
q_1 = n_1 \sin(\omega/2) \\
q_2 = n_2 \sin(\omega/2) \\
q_3 = n_3 \sin(\omega/2)
\end{cases}
\] and \( \|\mathbf{Q}\| = \sqrt{q_0^2 + q_1^2 + q_2^2 + q_3^2} = 1 \)

(2.8)

Like Rodrigues space, the combination of two Quaternions may be written as:

\[
\mathbf{Q}^{(C)} = \begin{bmatrix}
(q_0^{(C)}) \\
(q_1^{(C)}) \\
(q_2^{(C)}) \\
(q_3^{(C)})
\end{bmatrix} = \begin{bmatrix}
q_0^{(A)} q_0^{(B)} - q_1^{(A)} q_1^{(B)} - q_2^{(A)} q_2^{(B)} - q_3^{(A)} q_3^{(B)} \\
q_1^{(A)} q_1^{(B)} + q_1^{(A)} q_1^{(B)} + q_2^{(A)} q_2^{(B)} + q_3^{(A)} q_3^{(B)} \\
q_2^{(A)} q_2^{(B)} + q_1^{(A)} q_2^{(B)} + q_3^{(A)} q_3^{(B)} - q_2^{(A)} q_2^{(B)} \\
q_3^{(A)} q_3^{(B)} + q_1^{(A)} q_3^{(B)} + q_2^{(A)} q_3^{(B)} - q_2^{(A)} q_2^{(B)}
\end{bmatrix}
\]

(2.9)

where the corresponding rotation matrix is:

\[
g = \begin{bmatrix}
q_0^2 + q_1^2 - q_2^2 - q_3^2 & 2(q_1 q_2 - q_0 q_3) & 2(q_0 q_3 + q_0 q_2) \\
2(q_1 q_2 + q_0 q_3) & q_0^2 + q_1^2 + q_2^2 + q_3^2 & 2(q_2 q_3 - q_0 q_1) \\
2(q_1 q_3 - q_0 q_2) & 2(q_0 q_3 + q_0 q_1) & q_0^2 + q_1^2 - q_2^2 - q_3^2
\end{bmatrix}
\]

(2.10)

The Quaternion is mapped in four-dimensional Euclidean space as a unit sphere, which may be reduced with increasing symmetry. The orientation matrix, \( g \), can be employed to move between Quaternion, Rodrigues, and Bunge orientation descriptions. In this investigation, the Quaternion parameter was utilized for mathematical convenience to
describe the orientation distribution function (ODF). Rodrigues space is finite and provides a superior graphical representation for crystals with cubic symmetry.

**Figure 2.7: Rodrigues space illustrating axes of rotation and magnitude of angles.**

Since Rodrigues space will be utilized to graphically present orientation data, a brief description of the space specifically for cubic symmetry is appropriate. The Rodrigues vector may be plotted in 3D space without additional transformations or projections. Figure 2.7 illustrates the axes and angle description graphically in Rodrigues space. The axis of rotation (\( \mathbf{n} \) in Eq. 2.5) corresponds to the direction of the vector (Figure 2.7a). The magnitude of the vector is related to the tangent of half the angle of rotation (\( \omega \) in Eq. 2.5). This graphical representation corresponds to a nearly uniform spacing in angles by concentric spheres centered at the origin (Figure 2.7b-c).

Figure 2.8 displays several common texture components in Rodrigues space that correspond to the descriptions in Table 2.4 [33, 43-44]. Also of interest is the maximum angle of misorientation that corresponds to points on the surface of the Rodrigues region. The intersection of the \( <100> \), \( <110> \), and \( <111> \) axes of rotation with the outer surface correspond to rotation angels of \( 45^\circ \), \( 60.72^\circ \) and \( 60^\circ \) respectively. Hence, as you move out on an axis, the rotation about that axis increases. Other critical points of symmetry are along the \( <11(\sqrt{2}-1)> \) and \( <\sqrt{2} 11> \) axes, which correspond to the maximum angle of \( 62.8^\circ \) (corner of removed triangle) and \( 56.9^\circ \) (point at the center of the edge of the removed triangle) respectively [45]. This graphical representation will be used to illustrate both ODFs and stress values in orientation space.
Orientation Distribution Functions (ODF) were calculated assuming cubic crystal symmetry and orthorhombic specimen symmetry with the Phillip’s X’Pert Analytical
software [32], which reported results utilizing the Bunge angle convention. The resulting ODFs were representative of the experimental data. In many modeling methods, it is advantageous to discretely handle orientations for texture evolution and crystal stress estimates. The Bunge ODF was converted to discrete angles by a series of 8-node $5^\circ \times 5^\circ \times 5^\circ$ angular probability density elements. Nodal densities were prescribed by the calculated ODF and scaled with the sine of the 2nd Bunge angle, $\sin(\Phi)$ [33]. This scaling was applied due to the volume of unique orientations described as $\Phi$ changes: at $\Phi = 0^\circ$ (the volume of the element is very small) and at $\Phi = 90^\circ$ (the volume is comparatively large). The nodal probability densities serve to scale the number of random discrete angles subsequently sampled from each element.

To approximately sample each angular segment, a superposition of uniform and linear distributions was adopted for each of the 3 angles independently. The uniform distribution utilized a random number generator as summarized below:

$$P_i^U = \text{rand} \left( \overline{Q} - \frac{1}{2} \Delta Q_i \right)$$

(2.11)

where $\overline{Q}$ is the average probability density from the 8-nodes, $\Delta Q_i$ is the difference in average probability at opposing element faces, and $i$ is the angle number ($\phi_1$, $\Phi$, or $\phi_2$). The $\text{rand}(X)$ function generates an array of $X$ uniformly distributed random numbers ranging between 0 and 1.

Next, the linear distribution was constructed by distorting a set of uniformly distributed random numbers with their square root as the following expression illustrates:

$$P_i^L = 1 + \text{sign}(\Delta Q_i) \sqrt{\text{rand} \left( \frac{1}{2} \Delta Q_i \right)} - \frac{1 + \text{sign}(\Delta Q_i)}{2}$$

(2.12)

In this scenario, the favoritism to either 0 or 1 is determined by the sign of $\Delta Q_i$, which compensates for the different probability densities at each node. The linear character of this distribution was confirmed with several numerical trials that consisted of 100 to 10000 random numbers.

Combining the uniformly and linearly distributed random numbers computed for each angle, $i$, allows the construction of a list of angles representative of an ODF element. The $i^{\text{th}}$ set of random numbers were concatenated and scaled as follows:
\[ \theta_i = \theta_i^{(1)} + \Delta \theta_i \begin{bmatrix} P_i^I & P_i^L \end{bmatrix} \]  

(2.13)

where \( \theta_i^{(1)} \) is the constant angle on the reference face and \( \Delta \theta_i \) is difference in the angle on the opposing face (in this case \( \Delta \theta_i = 5^\circ \)). Once these orientations were generated for all elements of the ODF, they were subsequently randomly sampled to reduce the total number of discrete angles analyzed to a manageable size for simulation or calculation (often 1000 angles were utilized).

Alternatively, a similar procedure may be applied for an ODF defined in Rodrigues or Quaternion space. For these specimens, a Gaussian normal distribution may be assumed in the vicinity of each discrete ODF value, since they are not significantly distorted. Using a properly scaled random number generator with an appropriate standard deviation for each coordinate, a set of orientations statistically similar to the set resulting from the Bunge ODF could be obtained. Retrospectively, one of these alternative spaces may have provided a more straightforward approach.

The assumed orthorhombic sample symmetry of the Bunge ODF required the discrete sampling to be repeated three more times (4 total), one for each symmetry transformation. To confirm this procedure and unambiguously relate the ODF reference frame to the lab-frame, the samples aligned with respect to the L, T, or N surfaces were rotated to a common L-T-N reference frame. As Figure 2.9 illustrates, the rotated-frame textures near the center of the plate (t/2) agree very well. In contrast, the edge texture shows some differences, which are attributed to difference in plate location. The N-sample was obtained at t/6 and the L and T-samples were obtained very near the edge at t/10. However, the two t/10 samples show good agreement. It should be noted that a similar comparison in the transition regime showed fair agreement, but it exhibited increased sensitivity due the strong texture gradient and X-ray penetration direction.
2.1.1.3 Initial Texture Results

The measured initial textures are presented in Rodrigues space in Figure 2.10. The three distinct plate regions are demarked, and data suggests a smooth transition through the thickness of the plate. The center and edge regions may be characterized by distinct textures; however, the transition region seems to vary significantly with textures bridging the gap between the two extremes. Utilizing Rodrigues space, several features are evident that were obscure in the pole figure presentation. Specifically, the center of the plate exhibits a strong texture dominated by a brass component (L-face peaks) and an extrusion component (T-face peaks). Despite the fact that the center of the plate underwent the longest heat treatment, which would result in increased aging and slightly different chemistry from other plate regimes, the center texture does not seem to indicate recrystallization. The transition region at t/3 exhibits a texture with some similarity to the center of the plate but with a more pronounced recrystallized cube component. At t/4, the texture has a strong classic rolling character. Overall the transition from the center to the
edge appears smooth with a weakening of the brass and extrusion texture components and a strengthening of the cube (center peak) and shear texture components (N-face peaks). Somewhat surprisingly, the edge texture (t/6 and t/8) displays a strong N-rotated cube fiber texture. Such a texture is typically associated with recrystallization (N-fiber near cube) and shear deformation (center of N-face). More subtle trends are not discussed, but may be inferred from the figure.

Figure 2.10: Initial plate texture measurement illustrated in Rodrigues space for the three plate regions.
Electron Back-Scatter Diffraction (EBSD)

EBSD provides a means to obtain discrete orientation information of individual grains within the plate. Such information is ideal for models that require specific crystallographic orientation, such as crystal plasticity FEM, especially when considering adjacent grains and relative misorientation. Although this simplistic description provides an avenue for the most basic application of EBSD, further insight may be gleaned from these experiments (particularly on deformed samples discussed later) with a better understanding of the measurement process.

The initial plate was cut and polished into samples on the L, T, and N planes at plate thicknesses at the edge (t/6), transition region (t/3). No specimens near the center of the plate have been examined. Typical results are presented in Figure 2.11, corresponding to measurements normal to the L, T, and N orientations. Each figure shows an SEM image (right) next to the orientation measurements (left). In the orientation maps, the colors represent families of orientations relative to the plane normal to the specimen measured. White in the orientation maps indicates regimes whose orientation could not be resolved and should not be confused as an orientation falling in the center of the stereographic triangle. In these images, the unresolved points are attributed to the vast size of the region measured (magnification effect), rather than excessive deformation. This assertion was confirmed by considering smaller regions under higher magnification of the same sample, which resulted in improved measurements. It should be emphasized that the colors on each image should not be compared to each other, since each image corresponds to a 90° specimen rotation, and colors are relative to the surface normal.

In addition to local texture measurements, EBSD results also confirm the previous grain size measurements from optical microscopy. Although the window of resolution is too small to see the total grain length (in L or T), it is clear the microscopy results are reasonable. Due to the grain size of this material, EBSD results did not provide adequate data for bulk texture assessment. To obtain superior statistics for bulk orientations, X-ray diffraction was undertaken and is described in section 2.1.1. However, this technique did allow identification of specific grain orientation information around regions of localized deformation in deformed or delaminated specimens.
Orientations are somewhat ambiguous from the inverse pole figure coloring-scheme that was utilized in Figure 2.11. The raw data obtained from EBSD is more detailed and may also be presented with three figures utilizing Rodrigues vectors. Figure 2.12 illustrates the three Rodrigues vectors for each of the Edge texture EBSD maps discussed previously in Figure 2.11. In this case, all three measurements are presented such that the first component is the L-direction, the second is the T-direction, and the third is the N-direction. It should also be noted that the macroscopic Rodrigues representation of these EBSD maps is similar for all three cases and they match reasonably well with the X-ray measurements, considering the limited length-scale.

Figure 2.11: EBSD texture maps and SEM images for L, T, and N planes near the edge of the plate (t/10)
2.1.3 Auger Electron Spectroscopy (AES)

Auger Electron Spectroscopy (AES) [46] was employed to inspect a mode I fracture surface at the center (t/2), transition region (t/3), and edge (t/6) of the 2099-T861 plate. A Physical Electronics™ PHI 660 Scanning Auger Microprobe was utilized to conduct the Auger Electron Spectroscopy in this investigation. The Auger microprobe includes a Lanthanum Hexaboride (LaB₆) filament electron gun for excitation, a single pass cylindrical mirror analyzing detector, a differentially pumped 1-5 KeV argon Ion gun for sputtering, and a specialized stage for fracture. The specimen geometry relative to the plate orientation is illustrated in Figure 2.13. Each specimen was fractured under ultra high vacuum (pressure < 10⁻⁹ torr), and was observed to fail along elongated grain boundaries, as expected based on prior observation of other failures [1-23]. It should be noted that other investigations have explored the chemistry of fracture surfaces for a
variety of alloys and failure modes, including failure along grain boundaries [47]. Scanning Electron Microscopy (SEM) images presented in Figure 2.14 show the fracture occurred along grain boundaries. The boxed regions shown are areas where subsequent analyses utilizing the capabilities of the AES were preformed. While initial surface measurements of the fracture region were typically associated with the grain boundary, a sputtering process was used to remove material so information associated with possible gradients in chemical composition could be identified.

**Figure 2.13: Auger specimen geometry implemented with the notch centered at t/2, t/3, and t/6.**

![Auger specimen geometry](image)

*a all dimensions in mm*

In general, Auger Electron Spectroscopy relates peaks at certain electron energies with chemical composition. For a predominately aluminum alloy, which has relatively low atomic weight, the Auger analysis provides chemical information on the outermost 3-5 atomic layers [48]. For instance, the peak associated with aluminum occurs around 64 eV [49] and can be analyzed with other peak intensities to infer chemical composition. The basic Auger measurement varies the detected electron energy level and stores a number of counts over a time interval. Typical data over the range of electron energies examined in this investigation is presented in Figure 2.15a. Since the specific number of counts is very sensitive to surface geometry, beam time, and material composition, the
derivative of counts with respect to electron energy is the standard format used to present Auger data. Typically, a 9-point derivative Savitzky-Golay [50] algorithm is utilized with 1eV data spacing to estimate the derivative from raw data (Figure 2.15b). The derivative reduces sensitivity to specimen variables, and is used with standard sensitivity tables to determine chemical composition [51].

![Figure 2.15](image)

**Figure 2.15**: (a) Counts versus kinetic energy and (b) derivative versus kinetic energy for a survey at the grain boundary in the transition (t/3) region

Although the AES is unable to detect variations in lithium concentration, information on the copper content is feasible. Copper is more easily detected due to its higher sensitivity and its peak location relative to the dominant element, aluminum (Li peak is very close to Al). During the investigation, it was observed that copper content varied from location to location on the fractured surface. In order to visualize these variations, a point-by-point map was measured around the copper peak over a small region of the sample. Other AES research has employed chemical composition mapping particularly for detecting reinforcement size and distribution in particulate composites [52]. Figure 2.16 illustrates the SEM image and its corresponding copper concentration map for a small region at the edge (t/6) on the plate on the as-fractured surface. This mapped region contains two grains demarked by the rough and smooth characteristics of the fracture surface. The rough region of the map shows short elongated copper concentrated regions, corresponding to roughly 15 at% Cu as opposed to the bulk concentration of 1.5 at%, whereas the smooth fracture region shows 5 at% copper concentrations. Both regions are associated with failure along a grain boundary, but the rougher surface may accentuate grain boundary characteristics. The Cu concentrations
have been speculated to be dominated by $T_1$ precipitates based on TEM and EBSD observations of Tayon et al. [53].

![Figure 2.16: (a) SEM image of mapped region at t/6 indicated in Figure 2.14a (b) the corresponding copper concentration (black is positive) map](image)

To examine the chemical composition away from the grain boundary, ion sputtering was employed at 0.1 minutes per cycle (where the sputtering rate is $\sim$0.05 $\mu$m/min). During each cycle, the composition was measured at each of the numbered points shown in Figure 2.16. The points chosen for analysis correspond to a region of high copper content (1), and two ‘average’ regions (2, 3). An illustration of the copper content, as depth profiling proceeds, is presented in Figure 2.17a. As shown, the copper content at the grain boundary is 3-10 times greater than the bulk region. In many cases, the region just beneath the grain boundary shows a slight depletion of copper, which may be attributed to diffusion toward the grain boundary. It should be noted that the atomic percent was estimated based on simultaneous measurements of oxygen and aluminum (the contribution of lithium was neglected, but would not influence the trends observed). In a few analyses, the sputtering process was continued for $\sim$30 minutes (1.5 $\mu$m) to see if composition continued to change. However, for the edge of the plate, nothing notable was observed after the first few minutes. To emphasize this observation, copper content maps were taken after 3 minutes and 30 minutes of sputtering. Both cases displayed a uniform copper content of approximately 1.5 at%., as illustrated in Figure 2.17b. A similar analysis was completed on the transition (t/3) region of the plate, but minimal differences were noted relative to the edge of the plate and are omitted here for brevity.
Unlike the edge or transition region, the center (t/2) of the plate was significantly different than other thickness locations. Most notably, the center of the plate included aluminum (Al), oxygen (O), and copper (Cu) peaks but was also often accompanied by a manganese (Mn) peak. Another key difference was observed by comparing the copper concentration maps. At the edge of the plate, the copper concentrated regions were typically thin and elongated, but had a more spherical geometry at the center of the plate. Figure 2.18 illustrates an SEM image and its corresponding copper and manganese map. As shown, the fracture surface (or grain boundary region) contains many regions of high copper concentration, while manganese is much less common. Also it should be noted that the grain around point 2 appears similar to those observed at the edge (t/6) of the plate, but the region around points 1 and 3 is unique to the center of the plate.

Sputtering, utilizing the same protocol, was again employed at the center of the plate. In this case, Al, O, Cu and Mn peaks were included in the atomic concentration estimate for each point during the sputtering cycles (again lithium was neglected because it could not be detected). Figure 2.19a illustrates the copper and manganese composition during the sputtering process. Similar to the edge of the plate, a region ~0.015 µm thick, which corresponds to the approximate grain boundary thickness, is apparent on the figure. However, unlike the edge of the plate, regions analyzed at the center continue changing well after this grain boundary zone has been removed by sputtering. The copper and manganese mapped region is presented in Figure 2.19b after ~2 min of
sputtering. As the depth profile suggests, the map illustrates regions of elevated copper concentration, in comparison to the bulk, well within the grain. An increased manganese concentration was also observed within the grain. It should be emphasized that the region uniquely associated with the center of the plate (points 1 and 3) contained greater concentrations of copper (and additional Mn concentrations) to a greater depth than were observed in either the transition region or at the edge of the plate.

![SEM image of mapped region at t/2](image1)

**Figure 2.18:** (a) SEM image of mapped region at t/2 indicated in Figure 2.14b (b) the corresponding chemical composition (Cu\textsuperscript{green}, Mn\textsuperscript{red}) map

![Depth profile near the center (t/2)](image2)

**Figure 2.19:** (a) Depth profile near the center (t/2) of the plate illustrating the Cu and Mn atomic compositions at the points indicated (b) Map of the chemical composition (Cu\textsuperscript{green}, Mn\textsuperscript{red}) after sputtering of the same region in Figure 2.18

The Auger Electron Spectroscopy (AES) provides several unique insights on the aluminum 2099-T861 alloy under investigation. First, for all plate locations, the grain boundaries were decorated with copper concentrations as high as 15 at%. The grain boundary thickness was estimated at 0.015 \( \mu \text{m} \) based on the applied ion sputtering
process. Beyond the grain boundary, the edge and transition regions of the plate showed uniform copper content on the order of the bulk concentration (1.5 at%). Finally, the center of the plate showed several unique characteristics including regions of elevated manganese and copper concentrations at the grain boundary and well within a grain.

2.2 Small Strain Deformation

Because some phenomena, believed to be associated with delamination, are speculated to occur at small plastic nominal strains (< 0.5%), an investigation focusing on small strain deformation was executed. Various mechanical tests were conducted in the small strain range (less than 1% total strain). The experiments considered were named: Incremental step tests, Lock-in Thermography (LiT), Cyclic torsion, and Small strain compression. Unless otherwise specified, these tests were conducted on closed loop servo-hydraulic 100kN two-post Instron load frames. System control and data acquisition were handled with a 32-bit closed-loop computer controlled system with LabVIEW programming interfaces.

Because of the range of temperatures explored, two distinct experimental setups were employed in this investigation. For testing conditions between -100°C and 100°C, an environmental chamber surrounded the specimen and grips to provide a uniform temperature. A J-type thermocouple was attached to the gage section midpoint of the specimen with fiberglass sleeving (Figure 2.20a). Separate multi-thermocouple testing verified that the gage section was within ±2.5°C with this type of control. Using the thermocouple as feedback, a closed loop MicroStar temperature controller provided the necessary control for either heating or cooling. Liquid nitrogen was utilized for cooling, and resistance elements were used for heating. A fan provided circulation for the interior of the chamber to maintain uniform temperature for either heating or cooling. To measure deformation within the gage section, a knife edged 12.7 mm gage length extensometer with a 5% strain full scale was installed using springs to hold it in place. Due to the hydraulic gripping mechanism and limits on the extensometer in the chamber, the minimum achievable temperature was -100°C. The same factors limited heating to 100°C in the same chamber. Because of these limits, high temperature tests (above 100°C) were conducted with slightly modified setup. For these tests, a K-type
thermocouple was tied to the center of the gage section (Figure 2.20b) with similar closed-loop control of a 2.5kW radiant heat ceramic element furnace. The gage section deformation was measured using a 12.7 mm gage length quartz rod 10% full-scale extensometer with small dimples punched onto the specimen surface.

![Figure 2.20: Cyclic test setup of a) the environmental chamber and b) the high temperature frame, with an extensometer and thermocouple attached](image)

For the vast majority of uniaxial experiments, an 8 mm diameter with a 12.7 mm long extensometer gage length was chosen to provide adequate size and load capacity for the equipment available for this investigation. As discussed in the initial plate properties section, the initial grain size is approximately 1200 x 900 x 90 µm in L x T x N directions respectively. This gage section volume corresponds to measuring approximately 6500 grains simultaneously, which is more than sufficient for adequate bulk statistics, as indicated by the X-ray analysis. It should be noted that all stress-strain results have been converted to ‘true’ stress – ‘true’ strain by the elastic included conversion presented in Appendix A, unless otherwise specified.

### 2.2.1 Incremental Step Test

In this investigation the incremental step test is utilized to examine the small strain deformation at various strain rates and temperatures. The shape of the incremental step test’s controlled strain history with time is shown in Figure 2.21a. The range of strain is set to increase with each subsequent reversal until achieving some predetermined maximum value, then the range decreases using a similar algorithm. Each set of increasing and decreasing strain reversals is called a block. The advantage of this loading
path is that the material returns to approximately zero stress and strain after each block, even with plastic deformation at the larger cycles. This return to zero stress and strain allows blocks of different maximum strain amplitudes, strain rates and/or temperatures to be conducted on the same specimen without complexities associated with residual plastic deformation. Additionally, a stabilized cyclic microstructure was established for all data reported, unless otherwise specified. This procedure maximizes the data obtained for a material while eliminating the need to constantly change specimens, especially at non-ambient temperatures.

Figure 2.21: (a) Incremental step test control at 0.01%/s (b) Typical stress vs. strain for 1 block of the incremental test.

In this investigation, -100°C to 100°C specimens were tested in the L and T directions, at plate locations including t/8, t/6, 3t/8, and t/2. The temperature was controlled in 40°C increments including: -100, -60, -20, 20, 60, and 100°C. The specimen geometry chosen for these tests is illustrated in Figure 2.22a. Higher temperature tests were conducted in 50°C increments including: 200, 250, 300, 350, and 400°C. Higher temperature tests were restricted to the L-direction and at plate locations t/6 and t/2, because of the required button head geometry. An illustration depicting the button-head specimen geometry is available in Figure 2.22b. For both high and low temperature tests, the specimens were tested at a single temperature but experienced blocks of all strain rates (1.0, 0.1, 0.01, and 0.001%/s) after cyclic stabilization had occurred. For each test, approximately 10,000 data points were stored per block, which corresponds to about 0.002% strain between data points.
The incremental step test is limited to providing information under small strain conditions only. If the fully reversed strain range chosen is too large, then the specimen could buckle, never cyclically stabilize before specimen failure, or fail before a sufficient number of blocks can be conducted. It is with this in mind that a maximum axial strain of 0.75% was implemented for most tests conducted in this investigation. This maximum strain corresponds to a constant amplitude fatigue life of about 2000 cycles and a plastic strain amplitude of approximately 0.2%. To ensure the development of a cyclically stabilized microstructure, several test protocols were adopted. First, after taking a specimen to the desired testing temperature, 16 blocks at 0.1%/s were conducted to develop a cyclically stable microstructure. The cyclic stability is inferred if the difference in stress range between the 8th and 16th blocks is less than 2%. After initial stabilization, 2-4 block tests were conducted at strain-rates of 1%/s, 0.01%/s, and 0.001%/s. Finally, two blocks were repeated at 0.1%/s to compare with the original “stabilized” 16th block, and ensure that no cyclic damage that could alter deformation had occurred. With this procedure, most tests between -100°C and 100°C achieved “stable” cyclic deformation.

Besides the equipment and specimen differences previously mentioned, high temperature tests were conducted a little differently from those in the -100°C to 100°C window. First of all, a different maximum strain was chosen for each testing temperature, to eliminate excessive plastic strain development and buckling issues. This reflects the decrease in the elastic stiffness and yield strength at these elevated temperatures.
temperatures for this material. Secondly, these high temperature tests failed to show cyclically stabilized behavior, at least within the same tolerance achieved at lower temperatures. This instability in cyclic behavior is expected for a precipitation-hardened alloy when testing above the aging temperature (150°C). The difference between the bounding blocks (0.1%/s before and after other testing) infers the influence of the aging process and bounds the reliability of tests conducted. Even with rather large differences, trends are observable between adjacent blocks in the specimens testing history. However, at temperatures above 150°C, the assumption of a stable microstructure (from a precipitate size and distribution perspective) is probability inappropriate.

2.2.1.1 Non-Linear Elasticity

Due to the interest in very small plastic strains (< 0.2%), the definition of elastic behavior becomes more important than typical applications. The incremental step test consists of a series of increasing and then decreasing reversals, resulting in regions of elastic unloading over a broad range of stresses. A typical test highlighting these ‘elastic’ regions is displayed in Figure 2.23. These reversals provide an avenue to characterize elastic deformation over a relatively large range of stresses.

![Figure 2.23: Elastic regions of an incremental step test conducted at T=100°C, de=0.1%/s.](image-url)

The elastic regions were used to estimate elastic parameters for each incremental step test. Both linear and stress dependent elastic models were considered. For uniaxial loading, the non-linear relation chosen takes the following form:
\[
\frac{d\sigma}{de^e} = E + E_\sigma \sigma
\]  

(2.14)

where traditional linear elasticity is preserved as \(E_\sigma\) approaches zero. It should be noted that this choice of non-linearity is slightly simpler than the format suggested by Sommer et. al. [54], but both models would give similar results in this application. Integrating this expression results in the following expressions:

\[
e^e = \begin{cases} 
\frac{\sigma}{E} : & E_\sigma = 0 \\
\frac{1}{E_\sigma} \ln \left( \frac{E + E_\sigma \sigma}{E} \right) : & E_\sigma \neq 0
\end{cases} 
\]  

(2.15)

where it is assumed that zero stress implies zero elastic strain.

Stress dependence was considered due to the linear dependence evident when numerically computing the derivative of the stress with respect to the strain in the purely elastic regions. Figure 2.24a displays this numerical derivative and a linear and stress dependent curve fit. As intended, utilizing a stress dependent elastic model reduces the spurious behavior evident when examining the plastic strain from an incremental step test (Figure 2.24b). This representation shows unrealistic asymmetric behavior when linear elasticity is assumed. There are several experimental deficiencies that could result in similar stress dependent artifacts, such as machine alignment, extensometer placement, and specimen anisotropy. Machine alignment and extensometer placement were experimentally eliminated as the cause of the phenomenon. Specimen anisotropy is only significant under bulk plastic deformation, since bulk elastic anisotropy is very small for aluminum [55]. Additionally, X-ray texture measurements suggest the bulk plastic anisotropy should vary significantly through the plate thickness, but the stress dependence does not change appreciably with plate location, temperature, or strain-rate. Other possible phenomena associated with plastic deformation, such as anelasticity [56] are not considered in this research. Furthermore, other experimental investigations have observed similar behavior when comparing elastic deformation during unloading and reloading for a similar alloy [57].

37
Figure 2.24: (a) modulus vs. stress for the elastic regions (b) the Stress vs. plastic strain with removed linear and stress dependent elastic behavior; both plots are for an incremental step block (T=100°C, \( \dot{\varepsilon} = 0.1\%/s \))

In general, the elastic modulus has been shown to be temperature dependent for most materials. In this investigation, a modified Varshni \[58\] temperature dependence was adopted to model the elastic modulus over the entire experimental temperature range (-100°C to 400°C) and reasonably extrapolate to temperatures outside this range (if necessary). The Varshni model is presented below in its general form:

\[
E = E_1 - E_2 \left( e^{\left( \frac{C_1}{T} \right)} - 1 \right)^{-1}
\]  

(2.16)

where \( E_1, E_2, \) and \( C_1 \) are fit parameters, \( T \) is the temperature in degrees Kelvin and \( E \) is consistent with the nomenclature previously employed. A slight deviation from this model is apparent between 200 and 400 K (temperatures where delamination was observed). In this regime, the modulus is reduced and can be more accurately represented by an additional term shown below:

\[
E = E_1 - E_2 \left( e^{\left( \frac{C_1}{T} \right)} - 1 \right)^{-1} - E_3 e^{\left( \frac{T-C_2}{C_3} \right)^2}
\]  

(2.17)

where \( E_3, C_2, \) and \( C_3 \) are additional fit parameters. The format of this additional term is similar to a normal distribution function. The inclusion of this additional term is attributed to strain localizations, residual stresses, and negative strain rate sensitivity. It should be noted that the experimental data did not show any rate sensitivity for the elastic deformation. The result of applying this model to the experimentally measured data over the full temperature range is presented in Figure 2.25.
Figure 2.25: Linear elastic modulus vs. temperature for L-direction loading of the Edge texture illustrating modified Varshni temperature dependence

Since anisotropic elasticity is of interest in this investigation, the elastic modulus measurements of various textures and loading directions are useful. Figure 2.26a displays the elastic modulus over the temperature range where delaminations have been observed (-100°C to 100°C). The texture dependence appears to have a small effect on the measured elastic modulus, resulting in a 2-3% lower stiffness for the Edge texture than either the Center or Transition textures. The loading direction does not appear to be as significant, but differences are still observable. The stress dependent elastic modulus (Figure 2.26b) suggests the texture is more significant than the loading direction, as more stress dependence is apparent for the Edge texture than either the Transition or Center. It is also evident that the stress dependence shows a much weaker dependence on temperature than the elastic modulus.

Figure 2.26: (a) Elastic and (b) the stress dependent modulus vs. temperature for loading in the L and T-directions of the Edge, Transition, and Center textures.
One specimen had Tee Rosette strain gages attached to opposite sides of the specimen. Micrometres\textsuperscript{TM} gage designation CEA-P2-062UT-120, which has a gage resistance of 120 Ohms and a strain range of ±3%, was used on a t/8 specimen tested at room temperature. An extensometer was still used for control feedback, as was the case for all Incremental Step Tests. The strain-gauged specimen provides an avenue to estimate Poisson’s ratio during the elastic deformation. The elastic analysis is straightforward and is presented in Figure 2.27, illustrating the transverse and axial strain ratio. As the figure suggests, the bulk Poisson’s ratio is 0.30, which was used along with the other measurements to characterize anisotropic elasticity.

![Figure 2.27: Transverse strain vs. axial strain for the strain gage specimen illustrating Poisson’s ratio = 0.30.](image)

### 2.2.1.2 Cyclic Plasticity

The primary purpose of the incremental step test is to obtain information about the cyclic plastic deformation of a material. A series of assumptions was made to resolve the data into a useful format. The first of these assumptions is the additive nature of strains, which is valid for small strain deformation. To obtain the plastic strain, the following manipulation removes elasticity from the total strain, $\varepsilon^{\text{tot}}$:

$$
\varepsilon^p = \varepsilon^{\text{tot}} - \varepsilon^e 
$$

where the elastic strain, $\varepsilon^e$, was modeled including stress dependence (Eq. 2.15).

With recoverable deformation removed, plastic hysteresis loops, shown in Figure 2.28a, are now the baseline data. It is desirable to convert this hysteresis data to a format comparable to monotonic curves. The incremental step test forces the tested material to
exhibit Masing behavior, where the largest hysteresis loop establishes the cyclic microstructure, which dictates the plastic deformation for all amplitudes. Figure 2.28b illustrates the definition of Masing behavior [59]: after shifting the respective reversal points to a common origin the hysteresis loops follow a single ‘curve’. In this figure a congruence of the going tensile deformation (stresses become more positive with loading) is shown. A similar but mirror image shift is obtained for going compressive deformation. With the strain partitioning suggested in Eq. 2.18, the going tensile and compressive curves are approximately the same if the absolute values of stress and strain from outer hysteresis loops are compared. This is indicative of material symmetry.

![Plastic Hysteresis Loops and Masing Hysteresis Loops](image)

**Figure 2.28:** (a) Plastic hysteresis loops and (b) the corresponding Masing loops displaying the ‘going tension’ curve

With the Masing assumption confirmed, the conversion to a baseline tensile type curve is obtained with the following expressions:

$$\sigma_{\text{ten}} = \frac{\kappa_{\text{cyc}}}{2} (\sigma - \sigma_o + \sigma_{\text{max}} + \sigma_{\text{min}})$$  \hspace{1cm} (2.19)

$$\varepsilon_{\text{ten}}^p = \frac{\kappa}{2} (\varepsilon^p - \varepsilon_o^p)$$  \hspace{1cm} (2.20)

the coefficient $\kappa_{\text{cyc}} = \begin{cases} -1 : \text{going compressive} \\ 1 : \text{going tensile} \end{cases}$ and $\sigma_o$ and $\varepsilon_o^p$ correspond to the reversal point for each curve. Since the material under investigation showed material symmetry, $\sigma_{\text{max}} + \sigma_{\text{min}} = 0$ throughout this analysis. Figure 2.29a and Figure 2.29b display typical data for both the initial cycle and cyclically stable baseline tensile curves for -20°C and 100°C respectively. As is evident from the figures, the lower temperature (-100°C to
60°C) tests typically exhibit cyclic hardening with slightly negative strain-rate sensitivity at plastic strains greater than 0.05%. This observation is apparent by the higher stresses in the cyclically stable deformation and slightly higher stresses for the slower strain-rates. Conversely, the high temperature tests ($T \geq 100^\circ$C) exhibit cyclic softening with positive strain-rate sensitivity; opposite of the trends observed at lower temperatures. One should recognize that delamination is much more prevalent in the lower temperature regime, and was only rarely observed at the higher temperatures ($T \geq 100^\circ$C).

![Figure 2.29: Effective tensile stress versus plastic strain at a) -20°C and b) 100°C for L-direction incremental step tests illustrating the first cycle and subsequent stabilized cycles are each strain rate.](image)

One common analysis technique utilized to interpret experimental results is the use of various derivatives. For instance, the hardening slope and plastic strain rate are of primary interest in the current investigation. To obtain these derivatives, a variety of techniques exist including: general piecewise numerical differentiation and specific global curve-fitting algorithms. For the most part, both methods give similar results as long as sufficient care is taken in the numerical differentiation algorithm and appropriate curve-fit functions are available. Throughout this investigation, the general numerical differentiation method was employed for its generality and the broad scope of potential derivatives investigated in this analysis. Specifically, the numerical differentiation technique involves a repetitive polynomial curve-fitting process about the given data point of interest, similar to the Savitzky-Golay [50] algorithm implemented for AES or the 11-point polynomial suggested for crack growth estimates [60]. A set of adjacent data points are also included, where the number of points is specific to the application, but typically involved more than 5 points on each side and at least enough points to
minimize experimental noise effects. Successful implementation of this methodology requires a data window of about 3 times the transducer (ex: extensometer or LVDT) resolution. For the incremental step test’s stress-strain data, this corresponds to the hardening slope being estimated by repetitively fitting a second order polynomial to a data window of ±0.025% from the data point of interest. Experimental data intervals were such that sufficient data points were available within this window. The window range is increased for large strain tests due to decreased resolution of the experimental transducer (LVDT). The data window is specified in units of time for strain-rate estimates. Subsequent numerical integration supports the conclusion that these derivative estimates are representative of the original data.

The resulting stress-strain curve, normalized by the shear modulus, was utilized to determine the temperature and plastic strain rate dependence for various hardening slopes. A modified Fisher [61] parameter was chosen to model this behavior:

\[ x = \frac{T}{\mu} \left( \frac{\dot{\varepsilon}^p}{10^{-4}} \right)^{0.015} \]  

(2.21)

where

\[ \mu = \frac{E}{2(1 + v)} \]  

(2.22)

The modification of the Fisher parameter was necessary because the experimental evidence suggests the plastic strain rate dependence is significantly lower than the original parameter suggests. This observation is pertinent for lower temperature (T < 100°C) as well as higher temperature experiments. For the range of cyclic strain-rates tested (0.001 - 1.0 %/s) the data tends to segregate by temperature. This indicates that the coupling in Eq. 2.21 is more sensitive to temperature than plastic strain rate. The normalized stress is presented (Figures 2.30a-2.32a) versus this temperature / strain-rate parameter for multiple hardening levels from the incremental step experiments. A hardening slope of $9E$ corresponds to a small offset plastic strain between 0.003% and 0.005% for most experiments, while bulk plastic flow (3% plastic strain) develops when the hardening slope is approximately $0.01E$.

By inspecting Figures 2.30a-2.32a, some nuances of plate location are evident. In particular, the edge and transition regions of the plate (Figures 2.30a-2.31a) illustrate
negative strain-rate sensitivity at the largest hardening slope ($\frac{d\sigma}{d\varepsilon} = 9E$). This region of negative strain-rate sensitivity is most apparent in the range of -100°C to 60°C. Localization processes associated with this region are subsequently related to eventual cyclic delaminations. In contrast, the center of the plate (Figure 2.32a) only displays minimal strain-rate sensitivity for all hardening slopes. It is similar to the behavior observed for the other plate locations at a hardening slope of $\frac{d\sigma}{d\varepsilon} = 3E$. As the hardening slope decreases, the strain-rate insensitive regime trends toward a positive ‘stable’ relationship for all plate locations. In other words, once bulk plastic flow is achieved, a positive or traditional plastic response is expected, at least on the macroscopic scale. This observation could have several ramifications, including accentuated localizations during cyclic deformation at small plastic strains, due to the negative strain-rate regime at high hardening slopes. Unlike the complexity of the low temperature window, where delaminations are prevalent, the response above 100°C shows positive strain-rate sensitivity for all hardening slopes investigated. It should be noted that the lowest hardening slope (0.3E) was not always achieved in the incremental step test for lower temperature experiments (T < 100°C).

Figure 2.30: L-direction (Edge) incremental step test (a) normalized flow stress vs. temperature/strain-rate parameter for various hardening levels (b) fracture surfaces illustrating delamination trends with temperature.
Figure 2.31: L-direction (Transition) incremental step test (a) normalized flow stress vs. temperature/strain-rate parameter for various hardening levels (b) fracture surfaces illustrating delamination trends with temperature.

Figure 2.32: L-direction (Center) incremental step test (a) normalized flow stress vs. temperature/strain-rate parameter for various hardening levels (b) fracture surfaces illustrating delamination trends with temperature.

Figures 2.30b-2.32b also illustrate various cyclic failure surfaces from uniaxial specimens that underwent incremental step testing. As suggested when discussing the strain-rate sensitivity, the delamination process is temperature dependent and seems most prevalent around room temperature, where the negative strain-rate sensitivity is most pronounced. For experiments at temperatures above 100°C, delaminations were difficult to find, at least on the length-scale of those noted at lower temperatures. Higher
temperature tests are above the aging temperature, which may change the lithium precipitate or solute state in the material for these tests. For positive strain-rate sensitivity, there is a diminished propensity for localization. If localization is presumed to initiate the delamination process, then fewer delaminations are expected. Another aspect at higher temperatures that may influence the response is the heightened relaxation and recovery mechanisms due to obstacle and dislocation diffusion. Since the focus of this research is the delamination process, which occurs at lower temperatures, higher temperature mechanisms will not be investigated. To identify some of the possible parameters that influence cyclic delamination, EBSD and LiT (Lock-in Thermography) were pursued in subsequent sections.

2.2.1.3 EBSD Delamination Observations

The Electron Back Scatter Diffraction (EBSD) equipment was used to explore the crystallographic orientations around a few delaminations apparent on the fracture surface of incremental step test specimens. In particular a few room temperature test specimens tested in the L-direction were sectioned and polished such that the delaminations could be investigated with the EBSD. A small and large delamination from a 3t/8 specimen is presented in Figures 2.33-2.34. For both cases, the Scatter Electron Microscope (SEM) image is presented in (a) and the resolved EBSD crystallographic orientation texture map is available in (b). As previously discussed much better resolution was obtained for higher magnifications. However, for the length-scale of a delamination, the larger regions (lower magnification) would be more representative of macroscopic trends. The two delaminations presented (Figures 2.33-2.34) are high and low magnification regimes respectively. Both images show the delamination occurring between two grains with different crystallographic orientations. In particular both cases illustrate that one orientation is deforming more uniformly (green in Figure 2.33 and red in Figure 2.34) and the other orientation suggests the presence of localized slip (pink in Figure 2.33 and blue in Figure 2.34). This localized deformation is inferred by the bands of unresolved points (the white regions) within a grain. Unresolved points result from a crack or excessive lattice distortion, which is typical of larger deformations. These bands are at approximately 45° angles with respect to the axis of delamination, which is the loading axis of the cyclic experiment (L-direction).
Figure 2.33: (a) SEM image and (b) EBSD texture map of a small delamination cyclically loaded in the L-direction for the Transition texture

Figure 2.34: (a) SEM image and (b) EBSD texture map of a large delamination cyclically loaded in the L-direction for the Transition texture

Data from this technique raises speculation that delamination is most prominent between two grains (one more easily deformed than the other), resulting in one grain with localized slip bands feeding toward the delamination. It is undetermined whether these bands contribute to the development of a delamination or are the result of a delamination crack introduced between the grain boundaries. C. Calabrese and C. Laird [15] suggest that deformation bands can precede micro-cracking in a similar material. No delaminations were observed between similarly oriented grains. As with the other EBSD texture maps, it is useful to represent the orientation information by displaying the three components of Rodrigues space. Figure 2.35 shows the Rodrigues space of these delamination measurements for the Transition (3t/8) texture. With this representation, the crystallographic misorientation of the adjacent, delaminated, grain boundary interface may be calculated for subsequent analysis.
2.2.2 Lock-in Thermography (LiT)

Lock-in Thermography (LiT) measures the relative temperature field on a specimen during a cyclic loading process. Because of the accentuated delaminations observed during previous cyclic testing, LiT experiments were conducted to visualize deformation phenomenon both before and after delamination events. Ideally, measuring a relative temperature map during cyclic deformation should provide information about regions of localized heating, potentially due to localized plastic deformation, delamination initiation, or delamination propagation. Although there are some experimental limitations, LiT provides some clues on the delamination process.

Because of the cyclic loading, LiT analysis has similar aspects to thermo-elastic stress analysis (TSA). For details on TSA, refer to references by Harwood and Cummings among others [62, 63, 64]. Among the similarities, in-phase and out-of-phase temperature range signals were employed during LiT experiments. The in-phase signal refers to the peaks of the temporal cosine (the difference in intensity at maximum and minimum loads), while the out-of-phase signal refers to the temporal sine pattern (the difference in intensity at going-tensile and going-compressive mean loads) [65]. To help understand these signals, the following expressions are included:
In-phase: \[
\Delta T_{in} \propto \left( I^{\sigma_{\text{max}}} - I^{\sigma_{\text{min}}} \right) \tag{2.23}
\]

Out-of-phase: \[
\Delta T_{out} \propto I^{\frac{\sigma_{\text{max}} - \sigma_{\text{min}}}{2}} - I^{\frac{\sigma_{\text{max}} - \sigma_{\text{min}}}{2}} \tag{2.24}
\]

Where \( I^\sigma \) is the intensity measured when the stress is at the corresponding level, which are described by the minimum cyclic stress, \( \sigma_{\text{min}} \), the maximum cyclic stress, \( \sigma_{\text{max}} \), and the direction of loading, which include ‘going tensile’, ↑, and ‘going compressive’, ↓.

In this investigation, a 2-position zoom lens was coupled with a StressPhotonics DeltaTherm 1550 (320 x 256 pixel resolution, closed cycle cooled, InSb detector) to capture the thermal images. DeltaVision software was employed to lock-in data acquisition at the appropriate cycling rate (2 or 5 Hz) and average thermal difference images over 30 seconds once per minute. The thermal camera focused on a region of the test specimen approximately 32 x 26 mm in size. Strictly cyclic uniaxial tension tests (\( R = 0 \)) were conducted both to provide adequate reference temperature measurements (zero load) and to prevent buckling of the long test specimens, which were required to provide ample room for the thermal camera.

Specimens were polished to 600 grit sand paper and were painted flat black to provide uniform emissivity at constant temperature. The cycling rate was typically either 2 Hz or 5 Hz depending on the magnitude of the load investigated. This rate is slightly lower than is optimal for aluminum (\(~30\) Hz), whose high thermal conductivity may artificially decrease the readings at lower frequencies [66]. Two specimen geometries were tested in the L-direction including a straight specimen, plate location \( t/3 \) and \( t/2 \), (Figure 2.36a) and a smooth notched specimen, plate location \( t/4 \) (Figure 2.36b). Flat specimens were required to view a representative area and maintain thermal camera focus. The unnotched specimens were considered to detected localization for an otherwise uniform nominal stress state. The notched specimens were considered to ensure delamination or specimen failure initiated in the thermal camera’s field of view. It should be noted that the notched specimen has a minimal stress concentration of \( K_t = 1.26 \) [67].
The cycle rate of our tests was limited to 5 Hz maximum due to servo valve and pump capacity for the specimen size and deformation levels expected during testing. The specimen thickness was chosen to be 6.35 mm for comparison to other experiments, but may be larger than optimal for LiT experiments, where a smaller thickness could make detecting localizations in the specimen easier. Due to constraints of the thermal imaging equipment and software, the minimum averaging time for each image was 30 seconds. This timeframe is much longer than the localized plasticity events expected during the cyclic process. Another constraint is the experimental resolution, where 1 pixel was approximately 0.1 mm, or roughly the grain dimension (in the \( N \)-direction). This is limiting since initial localization may occur in regions much smaller than the grain size. It should be noted that for all subsequent LiT images, each image was auto-scaled such that the blue-red color range encompasses the range in intensity of readings on the specimen, rather than indicating any specific temperature.

All specimens were centered at either \( t/3 \) or \( t/2 \), but the LiT measurements were similar for all plate locations. For the majority of fatigue life of the straight bar specimens, very little changed in the in-phase or out-of-phase measurements. With careful observation, small regions of what is speculated to be localized plastic deformation were detected at random locations in the specimen. Figure 2.37 illustrates an example of these localized regions that became evident in an otherwise uniform temperature field after several thousand cycles. The pairs of blue and red regions in this figure correspond to specimen locations of ‘hot’ plastic deformation and are approximately 0.45 mm apart. Specimen motion was estimated to be 0.7 mm over the
whole specimen from LVDT data and 0.45 mm in the region of the specimen where data was acquired. The in-phase data is computed from the difference in temperature at the peak tensile load and at the minimum load (zero). Therefore a localized ‘hot spot’ would show a cold region when the hot spot is at zero load and a hot region when the hot spot is at the maximum tensile load. These ‘hot spots’ are interpreted to be the result of localized plastic deformation. The number of pixels in these ‘hot spots’ is consistent with the scale anticipated from EBSD observations, meaning very few pixels or on the order of the grain dimension (100 µm). Even though localized deformation was observed, delamination and subsequent specimen failure initiated outside the camera’s field of view, due to grip effects. Only delaminations propagating into the field of view were measured during these experiments, and they propagated too quickly to collect meaningful data. Due to these difficulties, the notched specimen geometry was tested.

In-Phase Data ($\Delta \sigma = 300$ MPa, 5 Hz)

**Figure 2.37: Straight specimen in-phase data illustrating localized plasticity**

The notched and unnotched specimens were tested under similar conditions. One key difference is that the notched specimens have a non-uniform stress state due to the stress concentration of the notches. For these experiments, the gradient of the stress field proved to overwhelm the small plastic localizations observed in the unnotched measurements (red and blue spots). However, the initiation of delamination was observed within the camera’s view. Figure 2.38 illustrates a sequence of in-phase and out-of-phase data for moderate nominal stress range ($\Delta \sigma = 340$ MPa, $R = 0$) cycled at 5 Hz. As shown, the initial temperature field is slightly asymmetric, which may be due to a gradient in properties through the plate’s thickness. As the cycles accumulate, the temperature range on the left-hand side of Figure 2.38 increases gradually, which is
especially evident in the out-of-phase data where the concentration of red intensifies in
the upper left corner of the second image. Shortly after this change, a delamination
occurs on the upper left side of the third image at approximately 54,000 cycles. As the
cycling continues more delaminations initiate and propagate toward the upper and lower
regions of the specimen until after 74,027 cycles the specimen fails entirely.

a) In-Phase Data:

b) Out-of-Phase Data:

![Image]

Figure 2.38: Thermal Stress cyclic test at t/4, T=20°C with $\Delta \sigma = 340$ MPa (R=0) @
5Hz for (a) In-Phase data and (b) Out-of-Phase data progressions.

Macro-scale delaminations occupy a very small life fraction of lower stress level
tests. Furthermore, the unnotched uniaxial specimen tested at 200 MPa did not result in
delamination after 140,000 cycles (when it failed at the grips). These observations
indicate that some minimum stress state, which results in some amount of plastic
deformation, is necessary for the delamination process. While approximately one third of
the total life has significant delaminations at higher stress levels, it is unclear whether
their presence necessarily improves fatigue durability. Improvement could be stipulated
in some specimen orientations because the delamination would arrest a Mode I crack.

2.2.3 Cyclic Torsion

Torsion experiments are often conducted on thin-walled tubes because the elastic-
plastic analysis is simplified. Because of machining costs and that the internal material
may contribute to the delamination process, solid bars were chosen over thin-walled
pipes. It is desirable to determine if delamination can be driven by nominal shear stresses
and strains alone. A 100kN, 5000 N-m two-post Instron biaxial load frame was used to
conduct a few small strain torsion tests on this alloy. Specimens oriented in the L-
direction and centered at \( t/6 \) and \( t/2 \) plate thickness locations were tested at room temperature with the geometry presented in Figure 2.39. A quartz-rod 25 mm gage length biaxial extensometer with a \( \pm 2.5\% \) axial strain range and a \( \pm 5\% \) shear strain range was used. Like the high temperature tests, small dimples were punched onto the specimen surface. The use of a high temperature extensometer facilitated the use of periodic video imaging to track the development of delaminations on the specimen surface. Three basic tests were conducted in torsion: a load control cyclic test, a strain control cyclic test, and the incremental step test.

![Figure 2.39: Solid bar torsion test specimen geometry oriented in the L-direction.](image)

The load control cyclic test was conducted at \( R=0 \) with a peak torque of 52 N-m at 1 Hz. Assuming only elastic deformation, this range corresponds to a peak shear stress of 144 MPa at the outer surface. From the perspective of previous uniaxial experiments and a von Mises criteria, this nominal stress level is well below even a small offset yield strength \( (\tau_{0.001\%} \sim 175 \text{ MPa}) \). Figure 2.40 shows the calculated elastic shear stress-strain response during this loading process. A least squares linear regression estimates the shear modulus, \( \mu \), as 30.5 GPa at room temperature. This shear modulus estimate is an essential component for the anisotropic elastic parameter assessment presented in a subsequent section. Additionally it should be noted that the shear modulus is close to what an isotropic elastic model would predict (30.0 GPa) using the previously discussed Poisson’s ratio (0.30) and an approximate linear elastic modulus (78 GPa) from axial experiments at room temperature. Although stress dependent elasticity was discussed previously for the incremental step test, it is only expected to affect the bulk modulus and would not be observed for torsion testing. Upon fatigue failure, at 1.7 million cycles, no delamination was observed. This lack of delamination may indicate that some minimum amount of plastic deformation is required to initiate the delamination process.
A strain control cyclic test to failure was also conducted to observe plastic deformation and delamination. Shear strain endpoints of ±1.5% were chosen to ensure some cyclic plastic deformation was present during the fatigue process. A shear strain rate of 2%/s was used for convenience. It should be noted that the strain control cyclic test was conducted after several incremental step test blocks of similar amplitude. With this in mind, initial delamination began on about the 64th cycle and slowly progressed until eventual specimen failure at 1059 cycles (initial incremental step test blocks could be approximately 100 effective cycles utilizing a linear damage approach). A compilation of cyclic torque - shear strain curves is presented in Figure 2.41a, illustrating the effect of delamination on the torsional mechanical response of the specimen. It should be noted that the degradation of mechanical properties is attributed to delaminations, not cyclic softening. Significant delaminations were observed before cycle 128. Figure 2.41b shows the delaminated state of the short-life fatigue specimen.

When cyclic deformation occurs at sufficiently small loads (≤ 200 MPa uniaxial and ≤ 144 MPa in torsion), the absence of delamination is consistently observed. It should be noted that the 144 MPa shear stress corresponds to a 250 MPa uniaxial stress using a von Mises conversion. The shorter life of the 200 MPa axial experiment is not significant due to the failure occurring at the grips. As previously mentioned, this supports the assertion that a minimum amount of plastic strain is required to result in delamination, and nominal shear stresses and strains alone are sufficient. Furthermore, a
large enough resolved shear stress along the delamination interface was achieved in the higher strain test.

**Figure 2.41: (a) Short life fatigue cycles illustrating decreasing compliance with growing delaminations. (b) Final delaminated state after 1059 cycles.**

Some basic analysis on a solid torsion specimen can provide an estimate of the shear stress-strain curve. The solution method adopted in this analysis was originally outlined by Nadai [68]. Nadai begins by assuming small strain deformation, which defines the shear strain, $\gamma$, as the product of radius, $r$, and unit twist, $\Theta$ (rotation/length).

$$\gamma = r\Theta \quad (2.25)$$

Then recall the definition of the twisting moment, or torque is represented by the integral:

$$T = 2\pi \int_0^a \tau r^2 dr \quad (2.26)$$

where $a$ is the outer radius, and $\tau$ is the shear stress. It is then assumed the shear stress is a function of shear strain for pure shear monotonic loading.

$$\tau = f(\gamma) \quad (2.27)$$

By combining Eqs. 2.25 - 2.27, and realizing the maximum shear strain, $\gamma_{\text{max}}$, also corresponds to the strain at the outer radius, the following expression can be formulated.

$$T = \frac{2\pi}{\Theta} \int_0^{\gamma_{\text{max}}} f(\gamma) \gamma^2 d\gamma \quad (2.28)$$

Nadai [68] suggests the following rearrangement of Eq. 2.28, where the shear strain is replaced with radius and unit twist terms presented in Eq. 2.25.

$$\Theta^3 T = 2\pi \int_0^{a\Theta} f(a\Theta)(a\Theta)^2 da\Theta \quad (2.29)$$
Then taking the derivative of both sides with respect to unit twist results in:

\[ 3\Theta^2 T + \Theta^3 \frac{dT}{d\Theta} = 2\pi a^3 \Theta^2 f(\alpha\Theta). \]  

(2.30)

Finally Eq. 2.30 can be rearranged to solve for the shear stress at the surface as a function of the torque and the unit twist.

\[ f(\alpha\Theta) = \tau_{\text{shear}} = \frac{1}{2\pi a^3} \left( 3T + \Theta \frac{dT}{d\Theta} \right) \]  

(2.31)

This expression can be used for both hardening and softening materials with complete generality [69]. The main complexity in solving Eq. 2.31 is determining the derivative of torque with respect to twist.

It should be emphasized that applying the above analysis requires the stress-strain to be in a monotonic format. Either cyclic or incremental step test data was modified as discussed for the uniaxial incremental step tests utilizing the Masing assumption (Section 2.2.1.2). For the ensuing discussion, the torque and twist have been appropriately converted from torsional incremental step tests. With the experimental data converted, the shear strain is easily calculated from Eq. 2.25. By utilizing the torque, \( T \), versus unit twist, \( \Theta \), data, the shear stress is estimated with Eq. 2.31, through the use of a numerical derivative approach. Figure 2.42 illustrates the shear stress vs. shear strain for each strain rate considered in this investigation for plate locations \( t/2 \) and \( t/6 \). Both locations display lower stresses at the endpoints for faster strain-rates, which is indicative of slight negative strain-rate sensitivity. This is similar to the results of the uniaxial testing.

**Figure 2.42:** Shear stress vs. shear strain at various strain rates at (a) \( t/2 \) and (b) \( t/6 \).
2.2.4 Small Strain Compression

The primary purpose of small strain compression tests is to complement large strain compression tests discussed in a subsequent section. By providing small strain hardening and yield information, large strain tests conducted without an extensometer become much more meaningful. Additionally, small strain compression tests provide an avenue at sampling strain-rate/temperature sensitivity in a more traditional way. Thus, a comparison between monotonic compression and cyclically stabilized incremental step test data may highlight differences from monotonic to cyclic behavior at the various plate locations. Any trends that may be unique to either case may be clarified and those trends that appear representative in both may be enhanced.

Using the same equipment as for incremental step tests, small strain compression tests were conducted from -100°C to 100°C in 40°C increments. Because of limited specimen quantity, only a 0.1%/s total strain rate was considered for the monotonic compressive loading. Specimens were tested at plate locations corresponding to t/10, 3t/10, and t/2 in the L-direction only. The specimen geometry is a simple cylinder 30 mm long and 8 mm in diameter (Figure 2.43a). During testing Dow Corning™ 321 dry film lubricant, and SAF-T-EZE™ nickel SBT-16N anti-seize were employed on the specimen ends and the compressive fixture to minimize barreling and end effects. A picture of the experimental setup is presented in Figure 2.43b. Notice the extensometer and thermocouple installation was identical to the incremental step test. None of the tests displayed barreling or buckling behavior at the deformation range considered.

Figure 2.43: Small strain compression (a) specimen geometry and (b) Experimental setup
The initial compressive elastic behavior and plastic hardening were analyzed in an analogous manner as the incremental step test results. The only difference being instead of shifting and inverting, the compressive data only required inversion (to obtain positive values for stress and strain). The inversion was necessary due to the numerical technique used to fit the data. The stress versus plastic strain for various temperature tests is presented for each plate location in the L-direction in Figure 2.44. As illustrated, the
temperature affects the stress response by as much as 15% at a given strain for the temperature window investigated. Often, a lower temperature resulted in a lower flow stress at the same plastic strain, which suggests negative strain-rate sensitivity, since temperature is inversely coupled to the strain-rate. As with the incremental step tests, a temperature/strain-rate parameter, \( x \) (Eq. 2.21), was utilized to explore the strain-rate sensitivity at various hardening slopes. The right-hand side of Figure 2.44 illustrates the normalized flow stress versus \( x \) for the stress-plastic strain curves displayed on the LHS.

By comparing the small strain compression (monotonic) temperature/strain-rate results to the cyclic results presented previously, compressive monotonic versus cyclic observations on flow stress magnitude and strain-rate sensitivity are possible at each plate location and hardening slope. In general, incremental step tests at low temperatures (<100°C) exhibited initial cyclic hardening to achieve stabilized cyclic deformation (Figures 2.30-2.32). By comparing the normalized flow stress at lower hardening levels \( (d\sigma/d\epsilon^p < 3E) \), the monotonic response shows a lower flow stress than the corresponding cyclic response. The same trend does not hold true for higher hardening slopes (especially \( d\sigma/d\epsilon^p = 9E \)), where initial microstructural instabilities and possibly retained residual stresses may dominate the response, particularly in the monotonic specimens. The high hardening slope results illustrate a difference in monotonic versus cyclic strain-rate sensitivity for different plate locations. In particular, the edge of the plate displayed the most severe negative rate sensitivity during cyclic deformation and showed a strain-rate insensitive regime during monotonic deformation. In contrast, the center of the plate displayed a strain-rate insensitive region during cyclic deformation and showed the most severe negative strain-rate sensitivity during monotonic deformation.

Once the maximum strain level was reached for each small strain compression test the total strain was held constant for approximately 4 hours. This abrupt change in deformation is essentially a fast-slow strain-rate ‘jump’ test. However, since the constant strain period drives deformation internally, ‘stable’ mechanisms dominate the response. Thus, the anticipated negative strain-rate sensitivity is overshadowed by relaxation mechanisms. Relaxation is the decrease in stress magnitude observed when total strain is held constant at non-zero stress levels. This behavior is typically associated with creep
deformation, or the gradual diffusion of dislocations and obstacles subjected to stress [70-71]. Creep is typically associated with deformation at elevated temperatures, where it is often the dominant deformation mechanism. Typical experimental results illustrating the relaxation of stress during the strain hold period are presented in Figure 2.45a for results near the edge of the plate in the L-direction. A few curves are truncated to illustrate only the regime of relaxation, eliminating data when reloading occurs due to experimental complication, temperature variation, or aging effects beyond the scope of this discussion. Not surprisingly, using this data in conjunction with traditional steady-state creep modeling results in very poor correlation. This observation is expected due to the low temperatures considered and the importance of primary creep on the deformation in this regime. For clarity, an estimated creep rate versus stress is presented in Figure 2.45b implementing a power-law curve fit to estimate stress-rate at times exceeding 20 seconds from the start of the relaxation data. As illustrated, the creep rate does not resemble typical high temperature trends (the stress-temperature dependence on creep rate seem exceedingly complex, especially at -60°C). If one were to pursue a fully rate-dependent analysis, then these mechanisms are important. However, when rate independence dominates the mechanical behavior, which is the case for the temperature regime where delaminations were observed, the relaxation and recovery behavior may be neglected.

![Figure 2.45: (a) Stress relaxation versus time for small strain compression tests in the L-direction at the edge of the plate and (b) estimated creep rate versus stress.](image)

### 2.3 Large Strain Deformation

Previously discussed experimental results have shown that only small macroscopic cyclic strains are required to cause eventual delamination in the aluminum-
lithium alloy under investigation. Evidence of strain localization suggests local strains are much larger than the homogeneous approximation. Since localizations are critical in determining the onset of delaminations, large deformation should be understood and modeled accurately to characterize localized strain events. A variety of tests were conducted with these goals in mind, including large strain compression, and interface strength experiments.

### 2.3.1 Large Strain Compression

To determine an approximate saturation stress, hardening under large strains, plastic anisotropy, texture evolution, and other bulk plastic deformation characteristics, large strain compression tests were conducted in this investigation. The specimen geometry chosen for these experiments is presented in Figure 2.46a. The small ‘cup’ region [72] was included to store sufficient lubrication during testing to minimize barreling and end effects. The same lubricants utilized for the small strain compression tests were again used here. In general the small end effect did not change the bulk response, but helped prolong the specimen integrity through larger deformations than specimens without a cupped region. Due to the small specimen length, experiments were conducted in displacement control since none of the available extensometers would fit on the specimen or provide adequate strain measurement. The L, T, and N-directions were tested at temperatures ranging from -100°C to 100°C in 40°C increments. The strain rates investigated mirror the incremental step test, including rates at 0.001, 0.01, 0.1 and 1.0%/s. Example images of an undeformed and deformed specimen are shown in Figure 2.46b, which illustrates the plastic anisotropy observed during large strain compression.

![Figure 2.46: Large strain compression (a) specimen geometry and (b) images of undeformed and deformed specimens.](image)

Although the tests were conducted in displacement control, it was desirable to mirror prior strain-rate controlled experiments. Furthermore, the large deformation mandated that these tests be performed under approximate constant true strain-rate
conditions to better estimate mechanical properties. By decomposing the crosshead displacement into specimen and machine components, the displacement rate corresponding to the desired constant true strain-rate deformation is presented below:

\[
\dot{\Delta} = \left( L_o + \Delta - \Delta^{\text{thres}} - \frac{P - P^{\text{thres}}}{K_{\text{mach}}} \right) \dot{\varepsilon}_{\text{true}} + \frac{\dot{P}}{K_{\text{mach}}}
\]  

(2.32)

where \( L_o \) is the initial specimen length neglecting cup depth (~10 mm), \( \Delta^{\text{thres}} \) and \( P^{\text{thres}} \) are reference displacement and load (these will be the topic subsequent discussion) and \( \dot{\varepsilon}_{\text{true}} \) is the true strain rate. The machine stiffness, \( K_{\text{mach}} \), was approximately constant (Appendix B). Although the expression presented in Eq. 2.32 is accurate for the idealized machine stiffness, the loading rate, \( \dot{P} \), is difficult to compute during testing by the control software available. To compensate for this difficulty, the loading rate term was neglected when approximating true total strain rate control.

Since the specimen end-cup and machine stiffness are not well behaved during initial loading, obtaining small strain results from these specimens is difficult. In order to approximate the stress-strain curve for the initial portion of the loading, small strain compression test data, conducted at the same plate location and temperature, were used. The small strain compression tests were all conducted at a strain rate of 0.1%/s, but were used in the analysis of large strain tests with strain rates ranging from 0.001 to 1.0 %/s. This does not limit the analysis since this material exhibits strain-rate insensitivity at small plastic strains. Additionally, the small strain compression tests were restricted to specimens compressed in the rolling (L) direction. The large strain compression tests were conducted in the 3 plate orientations (L, T, and N). In order to convert small strain data to other directions, the Taylor factor (calculated from X-ray diffraction measurements) was applied. The Taylor factor is defined by the following expression:

\[
M_x = \frac{1}{N} \frac{1}{\sqrt{2}} \frac{\mathbf{D}^p : \mathbf{D}^p}{\sum_{i=1}^{N} \mathbf{g}^{r(i)} \cdot \mathbf{g}^{(i)}}
\]  

(2.33)

where, \( N \) is the number of crystal orientations, \( \mathbf{D}^p \) is the symmetric part of the velocity gradient (in the reference frame), \( \mathbf{g}^{(i)} \) is the orientation matrix for each crystal, and \( \mathbf{g}^{r(i)} \) is the normalized crystal stress for each orientation with the applied velocity gradient. In
general the Taylor factor varies with the direction of applied loading (L, T, or N), and plate texture (t/10, 3t/10, and t/2 textures). Unlike the rate insensitivity assumption, which was experimentally verified at small strains, the Taylor factor has limitations.

The small strain compression test data, corresponding to strain-rate and temperature conditions closest to the large strain compression test under investigation, was used to determine a elastic and plastic strain offset between data sets \( \varepsilon_{\text{offset}}^\text{tot} = \varepsilon_{\text{offset}}^p + \varepsilon_{\text{offset}}^e \). To further explain this offset concept, consider the typical small strain compression test presented in Figure 2.47a. The strain offset was chosen to be the maximum strain achieved during the small strain experiment. The load corresponding to this strain offset defines the load threshold \( P_{\text{thres}} \) of the large strain test. This load threshold is assumed to be the beginning of the useful portion of the large strain data. Additionally, the elastic and plastic strains at the end of the small strain experiment are assumed to be those at the threshold load of the large strain experiments. When the small and large strain tests were conducted in different directions (L vs. T for example), the Taylor factor was applied to the small strain data. Finally, load and displacement thresholds for the large strain data are computed using the expressions (Figure 2.47b):

\[
P_{\text{thres}} = A_{\text{LSC}} \frac{M_{\text{LSC}}}{M_{\text{SSC}}} \sigma_{\text{thres}}^*
\]

\[
\Delta_{\text{thres}} = \Delta @ \left( P = P_{\text{thres}} \right)
\]

where, \( M_{\text{SSC}} \) and \( M_{\text{LSC}} \) are the small strain compression and large strain compression Taylor factors. The cross sectional area of the large strain compression sample is \( A_{\text{LSC}} \) and \( \sigma_{\text{thres}}^* \) is the engineering stress at the end of the small strain compression test. The subsequent engineering strain in the large strain compression specimen can be computed from the following equation:

\[
\varepsilon_{\text{eng}} = \frac{1}{L_{\text{thres}}} \left( \Delta - \Delta_{\text{thres}} - \frac{P - P_{\text{thres}}}{K_{\text{mach}}} \right) + \varepsilon_{\text{offset}}^p + \varepsilon_{\text{offset}}^e
\]

where, \( K_{\text{mach}} \) is the machine stiffness determined experimentally using a strain-gauged specimen (Appendix B), and the offset strains from the small strain experiments are:

\[
\varepsilon_{\text{offset}}^p = \frac{M_{\text{SSC}}}{M_{\text{LSC}}} \varepsilon_{\text{offset}}^*\]

63
\[
\varepsilon_{\text{offset}}^* = \begin{cases} 
\frac{1}{E} \frac{M_{\text{LSC}}}{M_{\text{SSC}}} \sigma_{\text{thres}}^* & (E_\alpha = 0) \\
\frac{1}{E_\alpha} \ln \left( 1 + \frac{E_\alpha}{E} \frac{M_{\text{LSC}}}{M_{\text{SSC}}} \sigma_{\text{thres}}^* \right) & (E_\alpha \neq 0)
\end{cases}
\] (2.38)

where \(E\) and \(E_\alpha\) are elastic moduli defined in Eq. 2.14, and \(\varepsilon_{\text{offset}}^*\) is the plastic strain from the small strain compression test that corresponds to \(\sigma_{\text{thres}}^*\).

\[d\sigma \over d\varepsilon^* = \frac{\theta_o}{\tanh(k)} \left( \tanh(k) - \tanh \left( k \frac{\sigma}{\sigma_{\text{sat}}} \right) \right) \] (2.39)

A representative selection of stress-strain curves compressed at 0.1%/s in the L, T, and N loading directions are presented in Figures 2.48-2.50 for the edge (t/10), transition (3t/10), and center (t/2) textures. The curves illustrate relative temperature / strain-rate insensitivity between -60°C and 60°C for most cases. Notable exceptions are N-direction loading of the edge texture and L and T-direction loading of the center texture. For each of these exceptions, the compression curves appear regularly spaced and properly ordered for typical positive strain-rate sensitivity. Several curves,
particularly at the center of the plate, do not achieve the full 60% strain magnitude. For these specimens, bulk softening was often observed at a smaller strain due to regions of localized slip, which will be discussed in greater detail subsequently.

By following the analysis procedure previously discussed, the stress, strain-rate, and hardening slope could be estimated at any point of interest during each experiment. The normalized flow stress is presented versus the same temperature/strain-rate parameter, \( x \) (Eq. 2.21), that was implemented in the previous sections (i.e. Figure 2.30) in Figures 2.48-2.50. In this case, the hardening slopes vary from where the others left off (0.3\( E \)) to a minimal slope that is flat for any practical application (0.0009\( E \)). Often the experimental data did not achieve the 0.0009\( E \) slope because either the deformation was not sufficient, or bulk localization overwhelmed the response. In general, high hardening slopes show a rate insensitive regime, while as hardening slope decreases, positive rate sensitivity dominates the behavior. It should be emphasized that when bulk localization was observed, the data after localization was neglected. This indicates that despite the trend toward stable plastic flow, bulk localizations are still observed and are even common for compressive loading at the center of the plate.

One observation from the data in Figures 2.48-2.50 is the variation in location of the temperature/strain-rate plateau depending on texture and loading direction. From the temperature/strain-rate representation, a plateau regime is evident for all cases, even the textures and loading directions (N-Edge, T-Center, N-Center) that show only positive strain-rate sensitivity from the representative 0.1%/s curves. This emphasizes the usefulness of this representation over lone stress-strain curves. Another observation from these figures is the amount of hardening present for each texture and loading direction. This trend may be easily quantified by comparing the 0.3\( E \) and 0.003\( E \) (generally \( \epsilon_p < 20\% \)) normalized stress levels for a given temperature/strain-rate combination. Specifically, the trend illustrates that lower temperatures and higher strain-rates (lower \( x \)) typically result in more plastic hardening (larger change in stress between 0.3\( E \) and 0.003\( E \)). Furthermore, the texture appears to contribute significantly to this trend, where significant hardening is observed for the edge (\( t/10 \)) and transition (3\( t/10 \)) textures, while relatively little hardening is observed for the center (\( t/2 \)) texture. Differences grain
structure and plate chemistry, which probably activates different hardening mechanisms, may also contribute to these observations.

Figure 2.48: Large strain compression of the Edge texture in the L, T, and N-directions illustrating the stress-strain at various temperatures and the flow stress vs. temperature/strain-rate at various hardening slopes.
Figure 2.49: Large strain compression of the Transition texture in the L, T, and N-directions illustrating the stress-strain at various temperatures and the flow stress vs. temperature/strain-rate at various hardening slopes.
Figure 2.50: Large strain compression of the Center texture in the L, T, and N-directions illustrating the stress-strain at various temperatures and the flow stress vs. temperature/strain-rate at various hardening slopes.
2.3.1.1 Texture Evolution

To measure the evolved texture after large strain compression, specimens were cross-sectioned and polished only at t/10, 3t/10, and t/2 for an additional X-ray diffraction study. These regions were representative of the three microstructures and textures previously identified. Using the same procedure previously discussed, the textures after compression are presented in Figures 2.51-2.53, which illustrate the Rodrigues space for compression in the N, T and L-directions for each plate location.

First consider N-direction compression (Figure 2.51), which shows a nearly equivalent evolved texture for all three plate locations. Furthermore, the resulting texture is essentially the initial texture at the center of the plate. This is not particularly surprising because a compressive stress state is expected near the plate center during rolling.

One sees a similar trend from the evolved texture in the T-direction (Figure 2.52). In this case, the texture appears to be evolving toward a rotated variant of the final N-compression texture, or the original t/2 texture. One primary difference from the N-compression is that the texture evolution seems to be much more gradual. Also, the T-face displays a subtle shear component that may result from the elongated (pancake-like) grains shearing with respect to one and other. It should be noted that localizations and delaminations were both relatively unlikely in T-direction compression as compared to N or L compression.

Lastly, consider the evolved texture due to L-direction compression (Figure 2.53). Unlike the other directions, the initial texture appears to play a significant role in the resulting texture for this loading direction. The initial center texture (t/2) appears to evolve toward a texture variant similar to that in the N-direction or T-direction. The rate of evolution appears much like the observations in the T-direction. The other plate locations (3t/10 and t/10) both illustrate a strong shear texture component, similar to the subtle component observed in T-direction compression. Like before, this shear component is deemed to result from the shearing of adjacent elongated grains. Furthermore, L-direction compression typically results in the most pronounced compressive delaminations, which may be coupled to the increased localized shear texture component observed.
Figure 2.51: N-direction compression for center (t/2), transition (3t/10) and edge (t/10) plate regimes

Figure 2.52: T-direction compression for center (t/2), transition (3t/10) and edge (t/10) plate regimes
Figure 2.53: L-direction compression for center (t/2), transition (3t/10) and edge (t/10) plate regimes

2.3.1.2 Localization Observations

Macroscopic localizations were most commonly observed at the center of the plate. Even when no macroscopic localization was observed, the large strain compression samples were sectioned parallel to the loading direction, polished, and etched with an identical procedure that was previously discussed for grain size characterization (Section 2.1). Upon careful observation, nearly every large strain compression specimen displayed evidence of localized deformation when $\varepsilon_p > 10\%$. Using optical microscopy, it was evident that localized deformation and delaminations were occurring even when no macroscopic quantities, such as stress-strain response or visual inspection, showed evidence of localization. Figure 2.54 illustrates an edge crack or delaminated region of an t/10 L-Direction large strain compression test conducted at 0.1%/s at room temperature. Delaminations would not be expected in large strain compression, if initial speculation that the necessity of a substantial transverse stress inherent in a mode I crack field was the driving force for delamination. Texture evolution and potential grain orientation mismatch may lead to shear deformation at grain boundary interfaces. This deformation could lead toward delamination, particularly in
orientations (such as L or T-compression) when the stress in the N-direction is potentially positive. Nevertheless, a region of severe deformation is apparent between delaminations in the figure presented. Overall only a small region of a few samples exhibited this form of localization under large strain compression. Due to the limited number of specimens that were sectioned, it may have occurred at other locations.

Figure 2.54: An optical micrograph of a large strain compression specimen in the L-direction at the edge of the plate illustrating heavy deformation between edge cracks or grain delaminations

Figure 2.55: Large strain compression in the L-Direction in the plate transition region illustrating localized slip bands in (a) SEM image and (b) EBSD Texture map

The most common form of localization, pronounced localized slip band formation, occurred in all plate locations and compression directions. One example is presented in Figure 2.55 for compression in the L-direction in the transition (3t/10) plate regime. As illustrated, slip band deformations are apparent in both the SEM image (Figure 2.55a) and the texture map found from an EBSD investigation (Figure 2.55b). The localized slip regions are represented by thin white bands in both images due to the heavy deformation associated with this type of slip. The presence of these regions does not assure that macroscopic localization will occur. However, the existence of such
regions may be precursors to the development of other forms of localization including delamination.

Figure 2.56: Large strain compression in the N-direction at the center of the plate illustrating macroscopic slip localization for (a) image sequence of strain levels, (b) stress-strain, and (c) an optical micrograph showing localized deformation

Often, near the center of the plate, localized deformation develops on the macroscopic scale. One example is presented in Figure 2.56 for large strain compression at room temperature in the N-Direction located at the center (t/2) of the plate. Figure 2.56a shows a sequence of images at corresponding macroscopic strain levels, including the development of a macroscopic slip region particularly apparent above -20% strain. The stress versus strain curve illustrated in Figure 2.56b corresponds to theses images showing that just above -20% strain the stress magnitude decreases rapidly. It should be noted that when this phenomenon was observed, the subsequent deformation was neglected when the stress-strain properties were being determined. An optical micrograph is presented in Figure 2.56c showing a region of severe localized slip (near the top of the image). Regions of macroscopic localization are associated with the plate location (t/2), but minimal delaminations were observed during cyclic deformation at this plate location. It should be emphasized that this type of localization is not delamination, but is another mechanism that occurs at large strains for compressive stress states.
2.3.2 Split Hopkinson Bar

Throughout this investigation, strain-rates have been limited to approximately 1%/s due to equipment constraints and the relevance of slow mechanical tests to most engineering applications. High strain-rate applications are beyond the scope of this investigation, but with a temperature/strain-rate coupling, mechanical deformation at cryogenic temperatures can be estimated from high strain-rate room temperature testing. To better complete the temperature/strain-rate hardening relationship, split Hopkinson bar testing was utilized to provide high strain-rate (> 500 s\(^{-1}\)) deformation measurements.

Small cylindrical specimens (Figure 2.57a) were compressed at room temperature in the L-direction only for plate locations corresponding to t/10, 3t/10, and t/2. A 12 inch steel strike bar was accelerated into the input bar by a chamber of compressed air set at 20-40 psi. The input and output bars are 1520 and 760 mm long respectively. Both bars were carefully aligned along the center of the loading axis utilizing vacuum grease at the specimen interface to minimize barreling and end effects. Each C350 maraging steel bar has a 12.7 mm diameter, and is assumed to behave linearly elastic during loading. A 200 GPa elastic modulus and 8100 kg/m\(^3\) volumetric density is anticipated for each steel bar, which corresponds to an estimated wave speed of 5000 m/s \(c_{\text{bar}} = \sqrt{\frac{E_{\text{bar}}}{\rho_{\text{bar}}}}\) [78]. A CEA-06-250UW-10C Micrometricals\textsuperscript{TM} strain gage was installed near the center of each bar to measure the incident, transmitted and reflected deformation waves after impact (a schematic is available in Figure 2.57b).

Upon impact, an oscilloscope was employed to record voltage versus time data at both strain-gage locations for a period of 1 microsecond, including a 0.1 ms buffer before the trigger voltage was exceeded. Typical incident and transmitted wave data are presented in Figure 2.58a, illustrating the incident, transmitted and reflected components. Converting the voltage signal of each wave to the corresponding strain seen by the input or output bars involves applying the following conversion:

![Figure 2.57: (a) Specimen geometry (b) Schematic of the experimental setup](image-url)
\[ \varepsilon_{\text{wave}} = \frac{4}{G_f G_a X_v} V_{\text{wave}} \]  

(2.40)

where \( V_{\text{wave}} \) is the measured wave voltage, \( G_f \) is the strain gage gain factor (2.105), \( G_a \) is the amplifier gain, and \( X_v \) is the excitation voltage. The most common approach to analyze this data involves assuming homogenous deformation after dynamic equilibrium is achieved, which estimates the stress with the transmitted wave and the total strain-rate with the reflected wave [78] as the following equations indicate:

**stress:**
\[ \sigma = E_{\text{bar}} \frac{A_{\text{bar}}}{A_o} \varepsilon_{\text{trans}} \]  

(2.41)

**strain-rate:**
\[ \dot{\varepsilon} = -\frac{2c_{\text{bar}}}{L_o} \varepsilon_{\text{ref}} \]  

(2.42)

where \( \varepsilon_{\text{trans}} \) and \( \varepsilon_{\text{ref}} \) are the resolved transmitted and reflected strains measured in the steel output and input bars. The other constants include: the initial specimen area, \( A_o \), length, \( L_o \), the input or output bar area, \( A_{\text{bars}} \), elastic modulus, \( E_{\text{bars}} \), and wave speed, \( c_{\text{bar}} \). The estimated stress and strain-rate using the homogenous 1-wave analysis is presented in Figure 2.58b. Alternative approaches include a 2-wave analysis, which employs all three measured wave sections to estimate stress and strain-rate by balancing the forces on the front and back faces of the sample [79].

![Figure 2.58](image)

**Figure 2.58:** (a) Typical split Hopkinson bar raw data for t/10 illustrating the incident, transmitted and reflected wave components. (b) Resulting stress and strain-rate magnitudes versus time for the homogeneous deformation assumption.

By numerical integration of the strain-rate versus time, the total engineering strain was estimated. However, due to the sensitivity of the start of the reflected wave, the integration was initiated such that the initial elastic slope was reasonable. An initial strain-rate magnitude of 250 s\(^{-1}\) provided some level of consistency. Figure 2.59a shows
the stress versus strain for specimens at $t/10$, $3t/10$, and $t/2$. The plastic strain was computed by subtracting the stress-dependent elastic strain, whose parameters were assumed to match the results from the incremental step test discussed previously. With the prescribed initial strain-rate, the plastic strain was approximately zero for all tests until a minimum of 450 MPa. The normalized stress versus the temperature/strain-rate parameter, $x$, is presented in Figure 2.59b. Clearly the level of noise and fluctuating strain-rate make subsequent analysis more difficult than the other mechanical tests previously discussed. To account for this deficiency, only bound estimates in stress, plastic strain-rate, and plastic hardening slope were considered for each plate location. It’s important to note that only data with greater than 2% plastic strain was considered in the hardening estimates (Table 2.5). There is too much variation in the strain-rate and deformation data at smaller plastic strains. This strain threshold also allowed ample time for dynamic equilibrium (>0.004 ms) to be achieved. The range of hardening slopes was estimated by a bilinear curve fit where the first line estimates the initial or highest slope and the second estimates the final or lowest slope. To compute these lines the data were separated into two halves for each linear fit. As a reference to previous data, the hardening slope range corresponds to 0.003-0.01$E$. Due to a majority of flow stresses being defined at lower hardening levels and large plastic strains for these tests, the rate insensitivity previously observed should not be displayed by these tests. The variation in strain-rate during the tests and the limited amount of data did not allow the determination of strain-rate sensitivity for the higher strain-rate regime.

Figure 2.59: Split Hopkinson bar compression in the L-direction illustrating (a) stress vs. strain and (b) normalized flow stress versus $x$ for each texture
Table 2.5: Split Hopkinson bar summary

<table>
<thead>
<tr>
<th></th>
<th>Stress (MPa)</th>
<th>Strain Rate (s(^{-1}))</th>
<th>Hardening Slope (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Min</td>
<td>Max</td>
<td>Min</td>
</tr>
<tr>
<td>Edge (t/10):</td>
<td>490</td>
<td>560</td>
<td>600</td>
</tr>
<tr>
<td>Transition (3t/10):</td>
<td>547</td>
<td>603</td>
<td>530</td>
</tr>
<tr>
<td>Center (t/2):</td>
<td>540</td>
<td>610</td>
<td>900</td>
</tr>
</tbody>
</table>

2.3.3 Tension Testing

Extensive cyclic (incremental step) testing and compressive (large strain compression) testing were preformed to characterize the mechanical response of the 2099-T861 aluminum alloy under investigation. To complement these results limited tensile data were examined from a previous investigation where an additional in-plane direction was tested [74]. Also, some smaller specimens were tested in this study to ascertain size effects and thru-thickness (N-direction) strength. Additionally, strain-rate jump tests were conducted to confirm the strain-rate sensitivity apparent from other experiments.

Alcoa conducted tension tests of the 2099-T861 alloy under investigation at both room (20°C) and cryogenic (-182°C) temperatures. The plate location was restricted to the edge (t/6) regime and the loading rate was not specified, but was on the quasi-static time-scale. Figure 2.60 illustrates typical results from their experiments for monotonic tensile loading in the L, T, and 45° between L and T. As illustrated, the orientation dependence of yield and ultimate strength is moderately significant (on the order of 5% difference was observed) and is consistent at both testing temperatures. The testing temperature appears to be more significant than orientation as a 20% increase in strength was observed at cryogenic temperature. However, only one plate location (t/6) and a single strain-rate were considered. These results are consistent with the current observations during large strain compression tests, where the -100°C experiments were consistently stronger than their room temperature counterparts (Figure 2.48).
Despite the apparent positive temperature/rate sensitivity for this temperature difference, incremental step test and large strain compression results suggest a slightly negative or insensitive strain-rate regime for a smaller temperature range around room temperature. This trend was explored along with the effect of plate location and tensile loading in the N-direction with sub-size tensile specimens. The specimen geometry for these experiments is presented in Figure 2.61 and has approximately one quarter of the cross-sectional area of the other specimens used in this investigation. For the L-direction, the number of grains in the gage cross-section is about 100, while only 10 grains are expected in the N-direction. These mechanical tests were conducted with a 100 kN rated Zwick-Roell 1476 two-post screw machine, with a 10 kN load cell and 10 kN wedge clamp grips, and were displacement-rate controlled with a 32-bit computer system using a TestXpert™ interface at room temperature. Strain measurements were taken optically with a Rudolph™ CCD line scan sensor. The details of this experimental setup are available in the literature [75]. A variety of displacement rates (between 0.003 – 0.3 mm/s) were considered for loading in the L and N-directions. The L-direction plate locations considered were the t/6 (Edge texture) and t/3 (Transition texture). Testing in the N-direction was possible with these specimens, but the gage section encompassed plate locations between t/4 and 3t/4. It should be noted that tensile testing in the N-direction consistently displayed failures at the center (t/2) of the plate (Figure 2.61c).
The strength results for the L and T directions are displayed in Figure 2.62a-b. Only engineering stress is displayed because strain measurements were not taken during the entire deformation. Nevertheless, several useful observations are possible from these experiments. First, the difference between loading in the L versus the N-direction indicates that the N-direction is harder ($\sigma_u = 500$ vs. 480 MPa) and less ductile ($\Delta_f = 6$ vs. 7 mm displacement). The strength observation is somewhat surprising since N-direction loading is perpendicular to the ‘weak’ grain boundary interface where delamination is often observed. The N-direction data may be combined with other interface strength tests to estimate the grain boundary strength and possible shear-normal stress interactions.

Another useful observation from these experiments is the confirmation of negative or insensitive strain-rate dependence that was also observed previously. This trend is more pronounced for loading in the L-direction, but is also displayed in the N-direction. Since machine compliance dominates the initial deformation for this data, comparison of stress at a given displacement is difficult. Close observation of the deformation response during the plastic deformation of these experiments (particularly in the L-direction) exhibits significant stress serrations (on the order of 3-5 MPa), as
displayed in Figure 2.63a-b. The serrations were observed for all loading rates for the L-direction, but were restricted to the slowest (0.003 mm/s) rate for the N-direction. These serrations are similar to those reported as the PLC effect [8] for a similar aluminum alloy. Additionally, these serrations may be related to the negative strain-rate sensitivity that has been consistently observed around room temperature throughout this investigation. Both negative strain-rate sensitivity and serrated plastic flow have been associated with unstable localized deformation [8, 55]. It should be noted that testing of larger specimens did not display these load drops, even when using very similar testing equipment (i.e. screw load frame and wedge clamp grips). For this reason, these serrations may be attributed to a mechanism that persists on a relatively small length scale, but dampens at larger scales.

![Figure 2.63: ‘Zoomed’ stress-displacement curves for (a) L-direction and (b) N-direction illustrating stress serrations](image)

Additional tensile jump test experiments were conducted with the same specimen geometry, as the incremental step tests (Figure 2.20a). These experiments were conducted after cyclic stabilization (8-16 incremental step blocks) and were subsequently pulled in tension using the same equipment previously described (Section 2.2.1). Two quasi-static strain-rates were considered during these experiments: Slow (0.001%/s) and Fast (1.0%/s). The unique component of these tests was a jump in strain-rate was applied at either the proportional limit (0.5%), after some plasticity (0.75%), or after substantial plastic deformation (3.0%). Both slow-fast (0.001-1.0%/s) and fast-slow (1.0-0.001%/s) jump tests were conducted. The results from these experiments are presented in Figure 2.64a-d, where additional plots are included to highlight the region where the transition occurred. 

80
First consider the jump near the proportional limit (0.5% strain). This jump occurs when most grains are not deforming plastically and elasticity is still dominating the mechanical response. As illustrated, the slow-fast jump displays negligible effect and the fast-slow jump shows a slight shift in strain that may be an experimental control artifact. Next consider the jump after some plastic deformation (0.75% strain), where a relatively high plastic hardening slope dominates the mechanical response. At this jump a stress peak for slow-fast and a stress drop for fast-slow was observed. Other than the jump response, the stress-strain curves display subtle strain-rate dependence. Convergence of the curves at higher strains after the jump indicates a higher hardening slope for a slower strain-rate, which is associated with negative strain-rate sensitivity. At this strain magnitude, the effects of the strain-rate jump are still subtle. Lastly consider the jump after significant plasticity (3.0% strain), when plastic flow in all grains dominates the behavior. In this case, the slow-fast jump again begins with an initial
stress peak, but quickly trends toward a softer response than extrapolation of the initial response would suggest. Conversely, the fast-slow jump begins with an initial stress drop, but quickly hardens toward a harder stress-strain response than the initial fast deformation. Unlike the other jump tests, the jump at 3.0% strain clearly displays negative strain-rate sensitivity after the initial transient behavior at the jump. With these observations, it is clear that the slight negative (insensitive) temperature/strain-rate behavior is evident during plastic deformation and is most mechanically significant when hardening is minimal and plastic strains are sufficiently large.

### 2.3.4 Shear Interface Strength

A novel experiment was devised to obtain an estimate for the shear grain boundary interface strength. Compressive loading (in the L-direction) was employed on the specimen geometry presented in Figure 2.65a. The primary feature of this specimen is 3 pairs of grooves. Each groove pair, on opposite sides of the specimen, flanks a ligament of primarily shear deformation. This shear deformation is aligned with the elongated grain boundary interface. When the interface is sufficiently weaker than the bulk material (and when the bulk material is sufficiently stiff), this specimen geometry should result in shear failure along the grain boundaries.

![Figure 2.65: (a) Shear test specimen geometry (b) ASTM D695 [76] support fixture](image)

Three ligaments were incorporated into the specimen design to provide adequate statistics and explore sequential failures. Due to the specimen height and nominal compressive loading, specimen buckling is a serious concern. A fixture (Figure 2.65b), used in the past for plastics testing ASTM D695 [76], was installed around the specimen...
to minimize buckling effects. Graphite based lubricant was included to minimize frictional effects on the specimen-fixture interface.

All experiments were conducted on the 100kN two-post load frames described previously. Each shear test was run in position control until the onset of failure at final ligament, when the test was stopped and the final fracture interface was examined under a microscope to confirm that failure occurred along the grain boundaries. Tests were conducted with the failure interface aligned with plate locations: t/10, 3t/10, and t/2. Typical results from this test are displayed in Figure 2.66a, along with a summary presented in Figure 2.66b, which shows the average shear strength for t/10, 3t/10, and t/2 to be 245, 228, and 225 MPa respectively. It should be emphasized that the approximate grain boundary interface shear strength is on the order of half the axial yield stress and 1/3 of the saturation stress. Even converting the shear stress to an effective axial stress, results in an interface strength that is on the order of the monotonic yield strength and much lower than the ultimate tensile strength of the material.

The state of stress at the test specimen’s failure location was investigated by Kalyanam and Dodds [77] by utilizing finite element analysis with the displacement boundary conditions employed in the experiment. The resolved shear stress in the failure region is uniform for more than 95% of the ligament between grooves, as shown in Figure 2.67 [77]. No notable stress concentration that would add constraint was found. Furthermore, the value of shear stress was very close to that calculated via the nominal load and ligament area. The shear failure strengths observed lend credence to the notion

---

**Figure 2.66:** (a) Shear Test illustrating three ligament failures (b) Summary of the grain boundary shear strength at t/10, 3t/10, and t/2.
that a material weakness exists along the elongated grain boundaries, which may contribute to delamination. A possible interaction with normal stresses was not possible with this specimen geometry.

![Shear Stress Simulation](image)

**Figure 2.67**: FEM simulation presenting the shear stress field in the interface strength specimen [77].

### 2.4 Experimental Summary

The results of this experimental investigation reveal several features associated with delamination, which was observed to occur at elongated grain boundaries. Based on the results in the initial plate properties, small strain deformation, and large deformation subchapters, the following observations are salient. These observations may be categorized into aspects relating to delamination process: properties of the grain-boundary, mechanisms of plastic flow, and material anisotropy.

**Properties of the grain-boundary:**

- Large elongated pancake-shaped grains with a significant aspect ratio relative to the N-direction were observed (Optical Microscopy, EBSD). The most elongated grains occur near the edge of the plate, where the average grain dimensions are $1.2 \times 0.9 \times 0.09$ mm in the L x T x N directions respectively.

- Grain boundaries are decorated with thin copper precipitates (Auger Spectroscopy) that are not characteristic of the bulk grain, particularly near the edge of the plate where delamination is most prevalent.
• The elongated grain boundary interface is relatively weak in shear, approximately 225 MPa, as compared to the tensile strength in the N-direction, which was approximately 500 MPa. The cyclic torsion experiments indicate a range of 150 to 600 MPa for lives of $10^6$ (no delamination) and $10^2$ (many delaminations).

**Mechanisms of plastic deformation:**

• Delamination failure requires a significant amount of bulk plastic deformation ($\Delta \varepsilon^p > 0.005\%$) to initiate, even in cyclic applications (Torsion / LiT).

• Insensitive to negative strain-rate/temperature sensitivity of the plastic deformation, was observed in the regime where the delamination was most prevalent (around room temperature). This type of macroscopic behavior has been associated with localized deformation. Conversely, positive strain-rate sensitivity dominated the behavior at higher temperatures ($T > 150^\circ C$), where delaminations were not observed.

• Slip banding (Micros / EBSD) and localized plastic deformation (LiT) were observed in the vicinity of delaminations, suggesting that localized deformation is associated with the initiation or growth of delaminations at the grain boundary.

**Material anisotropy:**

• The macroscopic stress-strain behavior suggests that the properties in the L, T, and N directions are not significantly different.

• Electron backscatter diffraction (EBSD) results indicate that significant grain misorientation is typical at the delaminated grain boundary interface.

• Texture measurements (X-ray) were included to statistically characterize the potential crystallographic misorientation at grain boundaries.

The delamination process has been hypothesized to be driven by the stress state at the relatively weak elongated grain boundary interface. These stresses are assumed to result from both the mechanisms of plasticity and the local grain orientation mismatch. To estimate the stress state that leads to delamination, a model that reflects these mechanisms on the grain length scale is most appropriate (i.e. crystal plasticity).
3 Modeling Material Behavior

In this chapter, the modeling framework employed to examine grain boundary effects on cyclic deformation is presented. This chapter begins with a background of related modeling efforts and continues with details of the model that was implemented. Specifically, a rate independent, anisotropic elastic-plastic finite strain crystalline model with additive kinematic hardening on independent slip systems was utilized in a uniform deformation polycrystalline model. This modeling framework was incorporated into a bicrystal model whose goal is to statistically estimate the stress state on grain boundaries.

3.1 Modeling Background

Material modeling has been an important aspect in many engineering applications for generations. The earliest efforts in material modeling involved bulk material response, which include linear elasticity as postulated by Hooke and plastic yielding behavior as forwarded by Tresca [55]. In both cases, the modeling efforts were based on experimental observation and clever intuition of the mechanical behavior. Henceforth, theoretical and modeling improvements have evolved as the understanding of such phenomena has improved. One such significant insight was the proposal of a fundamental component of matter, called an atom, by Dalton in 1808 [80]. When a material exhibits some particular arrangement of atoms, it is often referred to as a crystalline structure. Solid crystalline materials include almost all engineering metals and were first confirmed to exhibit specific crystalline structures by W. L. Bragg in 1912 by utilizing X-ray diffraction [28]. Currently, engineering materials are known to exhibit particular crystalline structures depending on temperature and composition. The most common metallic structures include Face-Centered-Cubic (FCC), Body-Centered-Cubic (BCC), and Hexagonal-Close-Packed (HCP) structures [55].

The relationship between crystalline structure and plastic deformation was first observed by Taylor and Elam in 1923 [81]. They observed the slip of an FCC aluminum single crystal pulled in tension through the use of engraved markings on the specimen’s surface. The experiments showed that slip bands occurred on \{111\} planes along the family of \(<110>\) crystallographic directions. Despite the experimental evidence and geometric understanding, a physical explanation for such slip behavior was a mystery.
until 1934, when Orowan [82], Polanyi [83], and Taylor [84] independently postulated the interaction of line defects (dislocations) and crystallographic slip to explain the discrepancy between experimentally observed strengths and estimates from atomistic theories. With this physical interpretation, modeling efforts based on the material’s crystalline structure have been pursued.

The first crystal plasticity model was introduced in 1924 by Erich Schmid [85]. The model assumes plastic slip occurs on the slip system with the highest resolved shear stress, once it reaches some critical value. The relationship between this resolved shear stress and an applied uniaxial stress is appropriately named the Schmid factor [55]. Most early work on crystal plasticity involved the onset of slip deformation (initial yield). This restricted the successful modeling to orientations where single slip conditions dominate the plastic deformation. The first yield criterion for multiple independent slip system activity was introduced by Koiter [86] in 1953. In 1966, Hill [87] formulated a general rate independent crystal plasticity hardening law. However, the model required stipulating the number of non-redundant active slip systems to maintain uniqueness of the solution. By exploring a similar problem, Rice [88] recognized that including rate dependence of plastic flow makes the previously ambiguous state at corners, such as those inherent in the Tresca yield criteria, unique. This was shown more rigorously by Pan and Rice in 1983 [89]. Coincidentally, rate independent crystal plasticity models typically exhibit corners on the yield surface for a single crystal. Nevertheless, in 1976 Hutchinson [90] was inspired by the rate dependent creep behavior common at elevated temperatures in most engineering metals to overcome this ambiguity. He applied a creep-like power law on each independent slip system, which effectively eliminates the uniqueness issue involved in rate independent formulations, while more accurately replicating the physical response of many materials. It should come as no surprise that the vast majority of more recent crystal plasticity modeling efforts have this rate dependence embedded in their formulations.

Most early theoretical work utilized the small strain assumption to make analysis more tractable. This limited deformation to a small scale, relative to the overall geometry. Under many circumstances such as texture evolution or deformation localization, small strain models do not accurately reproduce behavior under finite strain
conditions. A fundamental concept used in most finite strain formulations involves the multiplicative decomposition of elastic and plastic deformation, which was first introduced by Lee and Liu in 1967 [91]. Lee [92] showed that the multiplicative formulation is consistent with the additive decomposition for small strains. Adopting this multiplicative decomposition and incorporating concepts from the work of Hill, Rice, and others, Asaro [93-94] presented an initial framework of finite strain crystal plasticity for both rate dependent and rate independent plastic slip behavior. Subsequently, Pierce et. al. [95] considered a rate dependent formulation, which included latent hardening and considered the effect of plastic strain-rate on localization. Latent hardening encompasses the interaction of hardening on the active slip systems with those that are currently inactive. It should be noted that since crystal plasticity is significantly coupled with material anisotropy, resolving the orientation is essential. Including other features of the finite strain approach does not result in much added complexity.

The vast majority of crystal plasticity models were developed for monotonic loading scenarios to predict yield, anisotropy, or texture evolution. However, there are many relevant applications that may be enhanced by the ability to model cyclic deformation of single or polycrystals. The most common phenomenon included in continuum cyclic plasticity is kinematic hardening, where strain hardening is often envisioned as the translation of the yield surface rather than the isotropic expansion. As early as 1962, Budiansky and Wu [96] incorporated kinematic hardening concepts into a crystal plasticity framework, but failed to explain a physical mechanism to support the implementation. In 1979, Weng [97] implemented kinematic hardening concepts into crystal plasticity and included a mechanistic interpretation relevant to the single crystal length scale. As was the case for many early kinematic hardening models implemented on slip systems, Weng’s model requires the separation of each slip system for positive and negative slip directions. For example, this separation requires the use of 24 slip systems in FCC metals, which usual have only 12 primary slip systems. This reflects the difficulty in incorporating most monotonic hardening models into a cyclic format. In 1980, Weng [98] added isotropic hardening to the kinematic hardening capabilities of his previous work. In many applications a combination of both isotropic and kinematic type hardening may be important to adequately reproduce physical mechanical behavior.
Frequently, kinematic hardening implementations in cyclic crystal plasticity fall into two basic categories: crystal backstress or slip system backstress. The crystal backstress method was employed in the work of Budiansky and Wu [96], where a backstress term almost identical to the classical continuum plasticity models was used. In other words, the backstress was subtracted from the stress state before resolving the shear stress on each slip system. This application requires some specialized slip system coupling for interpretation and does not fully reflect the contributions of individual slip systems. Other researchers that have nuanced this basic interpretation include: Khan and Cheng [99], who utilized Armstrong-Fredrick [100, 101] concepts for backstress evolution, and Voyiadjis and Huang [102], who constructed a crystal backstress based on the combined contributions from each slip system.

Alternatively, the slip system backstress method developed by Weng [97] considers each slip system to have an independent backstress term that affects the onset of slip differently in the positive and negative directions. In 1992, Qin and Bassani [103] employed the slip system backstress with non-Schmid hardening contributions. More recently, Xu and Jiang [104] decomposed each pseudo-Armstrong-Fredrick slip system into additive components, where the numerically required number of slip systems is back down to 12 (in FCC). In nearly all the investigations that included kinematic hardening concepts, a significant latent hardening contribution was stipulated, but a rigorous understanding of this coupling phenomenon is still limited at best.

Improvements considering dislocation mechanisms for specific obstacles and deformation capabilities may provide additional insight. According to Weng [97], kinematic behavior on single slip systems is potentially generated by a combination of Seeger’s dislocation pile-up theory and Orowan’s dispersion hardening. An overview of dislocation mechanisms in crystal plasticity is presented in the work by Kuhlmann-Wilsdorf [105]. Concepts of particular interest include: a more complete understanding of temperature/rate dependence or latent hardening and corresponding choices of dislocation mechanisms. Further enhancements have been forwarded for complex mechanisms such as dynamic strain aging or the Portevin-Le Châtelier effect that have been observed [8, 106]. However, the consideration of these phenomena is not included in the current investigation.
With a choice of material model and mechanical framework, some estimation of polycrystalline behavior based on single crystal theory is required. The first model to connect single and polycrystalline behavior was introduced by Sachs in 1928 [107]. In this work, the average macroscopic stress was applied to each crystallographic orientation, and the resulting plastic strains were averaged over all orientations. In 1938, Taylor [108] proposed a method to estimate polycrystalline behavior by applying uniform plastic strain equal to the average macroscopic strain onto each crystallographic regime. The Taylor and Sachs models are analogous to Voight and Reuss models in elasticity. In general it was shown in 1951 by Drucker [109] and Hill [110] that a uniform strain model (Voight or Taylor) acts as an upper bound and a uniform stress model (Reuss or Sachs) acts as a lower bound for the yield stress behavior. In 1958, Kröner [111-112] introduced what is often called the self-consistent model, which considers each orientation as a circular inclusion surrounded by an isotropic matrix representing the bulk material response. The model utilizes the Eshelby method [113] and averages the results over all representative orientations. An excellent discussion of Sachs, Taylor, and self-consistent polycrystalline models is available in the literature [114]. In Kocks’s discussion, the Taylor model is noted to become increasingly representative of the nominal response as the magnitude of deformation increases, since corrections to enforce equilibrium become relatively small (assuming no localization). It was also illustrated that the Taylor assumption reproduces experimental trends observed for many polycrystals.

Hutchinson [90] identified similarities between the self-consistent and uniform strain-rate models for rate dependent creep behavior of polycrystals. Similar approaches have been utilized to predict experimental textures at finite plastic strains. For instance, Asaro and Needleman [115] utilized an elastic-viscoplastic Taylor model to predict texture evolution during uniaxial tensile loading. Molinari [116] utilized an “interactive strain-rate” term in a self-consistent framework to improve in texture predictions in comparison to a traditional Taylor model. In 1998, Marin and Dawson [117] employed the Taylor model in an elastic-viscoplastic framework to predict textures and concluded that elasticity has negligible effect on the resulting texture for plane strain compression. Overall, both the self-consistent and Taylor approaches have been shown to be useful
techniques to estimate polycrystalline mechanical response without consideration of specific neighboring grains.

With increasing computational capabilities, the implementation of crystal plasticity into the finite element method (FEM) has become possible in recent years. The primary advantage of such a method is the simultaneous weak enforcement of equilibrium and compatibility on individual crystals or elements. Improvement of such a technique over Sachs, Taylor or self-consistent models is expected in most cases, but the enhanced complexity and computational overhead makes the method tractable only for specific length scales. One of the earliest works involving the FEM and crystal plasticity was reported by Harren et. al. in 1988 [118]. In this work, experimental and computational evidence of shear band formation was examined for both single and polycrystals deformed in plane strain compression. This early work illustrates one of the problems that FEM is best suited to examine: localization due to geometric softening. In 1991, Becker [119] employed the finite element method to an aggregate of crystal orientations to simulate a layer of grains subjected to plane strain compression. Grain interactions were examined, and it was recognized that grains whose deformation is dominated by shear have the largest effect on neighboring grains. To increase the length scale using the FEM, in 1992 Kalidindi et. al. [120] simulated 100 crystallographic orientations at each element gauss point, utilizing a homogenization by the Taylor assumption (uniform strain). This model was shown to reasonably reproduce experimental textures of a non-homogeneous, non-steady-state, plane strain forging. Beaudoin et. al. [121] has discussed the advantages and feasibility of FEM polycrystal plasticity modeling on large strain operations, such as rolling and forging. In 1998, Marin and Dawson [122] showed overall agreement between the plane strain compression of a 3D elastic-plastic crystalline formulation and the results of a traditional Taylor model [117]. More recently, the FEM has been utilized to successfully explore various material effects, such as temperature and strain-rate sensitivity in the work of Kok et. al. [123]. Although the finite element method remains the most general framework for crystal plasticity modeling, difficulties such as grain geometry, macroscopic constraint, mesh refinement, and computational overhead make other methods more attractive in many situations. Such applications are typically statistical in

91
nature, such as estimating properties on the bulk scale (texture) or the probability of some value on the mesoscale (stress).

One example of modified polycrystalline formulations is the ‘relaxed constraints’ model, introduced in the work of Honneff and Mecking [124] in 1978. In the context of crystal plasticity, ‘relaxed constraint’ refers to relaxing the applied uniformity of certain velocity gradient components in a Taylor based model. In rolling applications, these relaxed directions are usually the normal-longitudinal shear and/or the normal-transverse shear components. These relaxed constraints permit incompatibility in the specific velocity gradient components and reflect the observed behavior of certain grain geometries such as elongated or pancake-like. In 1982, the works of Kocks and Chandra [125] and Van Houtte [126] both showed the implications of partial constraint on slip system activation. In general, these relaxed constraint models showed no improvement in texture predictions over the fully constrained Taylor model [127] and further investigation was sparse for a time. Besides rolling, a similar relaxed Taylor model concept was utilized for low symmetry crystals that exhibit less than 5 independent active slip systems in the work of Schoenfeld et. al. [128]. In 2002, Delannay et. al. [129] showed that the relaxed constraint concepts could be coupled with grain interaction effects in relaxed directions to predict intergranular stress-strain behavior during uniaxial tension experiments. This was one of the few investigations utilizing a relaxed constraint polycrystalline plasticity model to explore an application other than texture development.

In order to include the effect of elongated/pancake-like grain interactions, a two grain Lamel model (named for its assumed lamellar grain structure) was developed by Van Houtte et. al. [130] in 1999. The primary objective of the model was to improve texture predictions over both the Taylor model and the ‘relaxed constraint’ model without the computational overhead of FEM. The Lamel model chooses grain pairs statistically based on the orientation density function (ODF). For each pair of grains subjected to plane strain compression, the longitudinal and transverse directions are left undistorted, but the normal velocity gradient components are free to distort such that equilibrium may be enforced between the pair of crystals. It should be noted that such an arrangement also preserves compatibility on the grain interface and overall on set of grain pairs. In 2002, Van Houtte et. al. [131] compared texture evolution results of the plane strain
compression utilizing the Lamel model with FEM results with a practical mesh size. The Lamel model showed better agreement with experimental measurements than the FEM, which was partially attributed to the simplicity of the mesh. This finding illustrates the potential advantage of Lamel like models compared to robust, yet complex, implementations such as the FEM, which may not improve predictions without sufficient geometric resolution. In 2005, Van Houtte et. al. [127] improved the Lamel model to accommodate more general nominal loadings. His work also provides a review and comparison of results employing a variety of methods including: Taylor, Lamel, visco-plastic self-consistent, and crystal plasticity FEM for plane strain compression (rolling simulations).

Many modeling efforts have utilized the underlying crystalline structure to enhance elastic and plastic mechanical response for various applications. The modeling length scales are typically on the order of the grain size (or sub-grain size), but several techniques have been developed to apply appropriate boundary conditions that allow estimation of nominal material behavior at larger length scales. Much of the previous work has focused on the development of anisotropy or texture at relatively large deformations. However, in this investigation, similar concepts involving the crystalline material response will be utilized to statistically examine stresses on elongated grain boundary interfaces. Since small nominal strains during cyclic fatigue are of interest for the delamination phenomenon, anisotropic elasticity and rate independent kinematic hardening crystal plasticity with an additive slip system backstress were implemented to reflect many of the experimental observations. A finite strain framework was deemed appropriate to accommodate potential localizations, but is not a significant feature for many of the cyclic loadings considered. Due to the cyclic nature of fatigue, highly stressed localized regions of relatively small length scales can significantly influence the delamination process. Furthermore, a statistical approach was deemed appropriate to identify potential localized regions within a generalized polycrystalline microstructure without excessive computational overhead. To obtain many statistical quantities that may be relevant to the delamination phenomenon, a uniform deformation (Taylor-like) model was employed for its computational efficiency for any potential crystallographic textures. Additionally, a bi-crystal (Lamel-like) model was used to estimate the grain boundary
interface stresses for specific pairs of crystallographic orientations, to estimate critical misorientations associated with the onset of delamination.

### 3.2 Finite Deformation

The deformation gradient, \( \mathbf{F} \), is defined as the derivative of deformation in the current (Cauchy) frame \( \mathbf{x} \) with respect to the Lab reference frame \( \mathbf{X} \):

\[
\mathbf{F} = \frac{d\mathbf{x}}{d\mathbf{X}}
\]

(3.1)

It should be noted that 2\textsuperscript{nd} order tensors are displayed in bold without any underline(s) and vectors are in bold with a single underline. The deformation gradient is separated into elastic \( (\mathbf{F}^e) \) and plastic \( (\mathbf{F}^p) \) components that are related by the following multiplicative decomposition [91]:

\[
\mathbf{F} = \mathbf{F}^e \mathbf{F}^p.
\]

(3.2)

The velocity gradient, \( \mathbf{L} \), is related to the deformation gradient and the rate of the deformation gradient, \( \dot{\mathbf{F}} \), by the usual definition [92]:

\[
\mathbf{L} = \frac{d\dot{\mathbf{x}}}{d\mathbf{X}} = \frac{d\dot{\mathbf{x}}}{d\mathbf{X}} \frac{d\mathbf{X}}{d\mathbf{x}} = \dot{\mathbf{F}} \mathbf{F}^{-1}
\]

(3.3)

where the upper dot represents a time derivative. To accommodate the incremental nature of plastic deformation, it is desirable to describe the deformation with respect to a time increment. The deformation gradient increment, \( \Delta \mathbf{F} \), which relates the current deformation gradient, \( \mathbf{F}^{(i+1)} \) at \( t = t_0 + \Delta t \), to the previous deformation gradient, \( \mathbf{F}^{(i)} \) at \( t = t_0 \), is defined by the following expression [132]:

\[
\mathbf{F}^{(i+1)} = \Delta \mathbf{F} \mathbf{F}^{(i)}
\]

(3.4)

where \( \Delta \mathbf{F} \) is determined by integrating Eq. 3.3. If the velocity gradient is assumed to be constant over a time increment, \( \Delta t \), the deformation gradient increment can be integrated utilizing the exponential map function, \( \exp(\mathbf{A}) \) [133]:

\[
\Delta \mathbf{F} = \exp(\mathbf{L} \Delta t).
\]

(3.5)

The plastic velocity gradient, \( \mathbf{L}^p \), is related to the plastic part of the deformation by the following expression, which is analogous to Eq. 3.3 [92]:

\[
\mathbf{L}^p = \dot{\mathbf{F}}^p \mathbf{F}^{p^{-1}}.
\]

(3.6)
As before, the incremental form may be expressed utilizing the current \( F_p^{(i+1)} \) and previous \( F_p^{(i)} \) plastic deformation gradients:

\[
F_p^{(i+1)} = \Delta F_p F_p^{(i)} \tag{3.7}
\]

where the plastic deformation gradient increment, \( \Delta F_p \), is found by integrating Eq. 3.6. When \( L^p \) is assumed constant over \( \Delta t \), \( \Delta F_p \) can be solved utilizing the exponential map:

\[
\Delta F_p = \exp(L^p \Delta t). \tag{3.8}
\]

Figure 3.1 illustrates the incremental form of the multiplicative decomposition, distinguishing four reference frames: Lab-Frame, Crystal-Frame, Previous-Frame, and Current-Frame.

![Figure 3.1: Multiplicative decomposition of the deformation gradient for an arbitrary time increment.](image)

To distinguish many of the stress definitions appearing subsequently, the elastic deformation gradient, \( F^e \), is manipulated using the right polar decomposition [134]:

\[
F^e = R^e U^e \tag{3.9}
\]

where the rigid rotation, \( R^e \), relates the crystal lattice to the current frame, and the elastic stretch, \( U^e \), is commonly related to the stress in the crystal frame.

The highlighted path (red) depicted in Figure 3.1 relates the current time to the previous time state. Utilizing that path to describe the deformation change (\( \Delta F \)) at time \( t = t_o + \Delta t \) is presented below:

\[
\Delta F = F^{e(i+1)} \Delta F_p F^{e(i)-1} \tag{3.10}
\]
where the elastic deformation at $t = 0$ ($F^{e(0)}$) is the initial rotation from the crystal lattice to the lab frame in the absence of any initial residual stresses in the body. A description of the rotations relating the various frames is presented in Appendix C.

### 3.3 Elasticity

The elastic deformation gradient, $F^e$, is defined to have a unique relationship to stress in the crystal reference frame. If the elastic deformation is assumed to be hyper-elastic [92]:

$$S^e = \rho \frac{\partial W^e}{\partial E^{Ge}}$$  \hspace{1cm} (3.11)

and,

$$E^{Ge} = \frac{1}{2} (F^{e*} F^e - I) = \frac{1}{2} (U^e U^e - I)$$  \hspace{1cm} (3.12)

where $E^{Ge}$ is the elastic Green strain (analogous to the engineering elastic strain) and $S^e$ is the corresponding engineering stress (or second Piola-Kirchoff stress). For clarity, the engineering stress is described below in terms of the current Cauchy stress, $\sigma$ and the rotated Cauchy stress, $\hat{\sigma}$.

$$S^e = J^e F^{e-1} \sigma F^{e-T} = J^e U^{e-1} R^{sT} \sigma R^s U^{e-T} = J^e U^{e-1} \hat{\sigma} U^{e-1}$$  \hspace{1cm} (3.13)

where $J^e = \det(F^e) = \det(U^e)$. The current Cauchy stress is the true stress in the current reference frame and likely has the most physical relevance. The Mandel stress [135], $\Sigma^e$, is the work conjugate stress for plastic deformation and will be subsequently related to the resolved shear stress by Eq. 3.33. Utilizing the definition of this stress in terms of the elastic Green strain, results in the following expression:

$$\Sigma^e = J^e F^{e-1} \sigma F^e = J^e U^{e-1} \hat{\sigma} U^e = S^e U^e U^e = S^e \left(2E^{Ge} + I\right)$$  \hspace{1cm} (3.14)

Note that this stress is not necessarily symmetric and is the transpose of the Mandel stress defined by Lubliner [136]. For completeness, the rotated Cauchy stress and current Cauchy stress can be related to the other stress definitions by:

$$\hat{\sigma} = R^s \sigma R^s = \frac{1}{J^e} U^e S^e U^e = \frac{1}{J^e} U^e \Sigma^e U^{e-1}$$  \hspace{1cm} (3.15)

$$\sigma = R^s \hat{\sigma} R^s = \frac{1}{J^e} F^e S^e F^{e-T} = \frac{1}{J^e} F^e \Sigma^e F^{e-1}$$  \hspace{1cm} (3.16)

Experimental evidence suggests that the delamination process may occur at small nominal deformations and requires plastic flow in adjacent grains. Due to the small
nominal strains being considered, the elastic anisotropy potentially has relevance to the stress state when plastic flow is initiated. No systematic investigation that illustrates the effect of anisotropic elasticity in a crystal plasticity formulation was found in the literature for FCC crystal structures. However, elastic anisotropy was examined with dislocation dynamics models [138] and HCP crystal plasticity [139], which found that it is significant on the grain size length scale because it increases local stresses and suppresses stress redistribution effects.

For materials whose crystallographic structure exhibits cubic symmetry (FCC or BCC), a three-parameter model is appropriate to describe the elastic anisotropy (instead of two for isotropy). The elastic stiffness, $C^e$, is presented below with respect to the physical parameters chosen:

$$ C^e = \rho \frac{\partial V^e}{\partial E^g \partial E^g} = 2\mu \mathbf{K} + 3\kappa \mathbf{J} + \zeta \mathbf{X} $$

(3.17)

where $\mu$ is the shear modulus, $\kappa$ is the bulk modulus, $\zeta$ characterizes the anisotropy, and the 4th order tensors $\mathbf{K}$, $\mathbf{J}$, and $\mathbf{X}$ are defined in component form utilizing the kronecker delta, $\delta_{ij}$:

deviatoric

$$ K_{ijkl} = \frac{1}{2}\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right) - \frac{1}{3}\delta_{ij}\delta_{kl} $$

(3.18)

spherical

$$ J_{ijkl} = \frac{1}{3}\delta_{ij}\delta_{kl} $$

(3.19)

anisotropic

$$ X_{ijkl} = \begin{cases} 1 & : i = j = k = l \\ 0 & : \text{otherwise} \end{cases} $$

(3.20)

It should be noted that these components have some useful attributes as listed below:

$$ \mathbf{J} : \mathbf{J} = 1 \quad \mathbf{J} : \mathbf{I} = 0 \quad \mathbf{J} : \mathbf{K} = \mathbf{K} : \mathbf{J} = 0 $$

$$ \mathbf{K} : \mathbf{K} = \mathbf{K} \quad \mathbf{K} : \mathbf{I} = 0 \quad \mathbf{K} : \mathbf{K} = \mathbf{K} : \mathbf{K} = \mathbf{K} - \mathbf{J} $$

(3.21)

where $\mathbf{0}$ and $\mathbf{0}$ refer to the 2nd order and 4th order zero tensors respectively, and $\cdot$ is the dot product on the inner two components, as described below:

$$ (\mathbf{A} : \mathbf{B})_{ijkl} = A_{ijmn}B_{mnkl}. $$

(3.22)

When $\zeta = 0$, the model reverts to classic isotropic elasticity (Hooke’s Law) [55]. Utilizing the definitions forwarded in Eq. 3.21, it can be shown that the elastic compliance may be written:
\[
\mathbb{E}^{-1} = \frac{1}{2\mu} \mathbb{K} + \left( \frac{1}{3\kappa + \zeta} + \frac{\zeta}{2\mu(\kappa + 2\mu)} \right) \mathbf{J} + \frac{-\zeta}{2\mu(\kappa + 2\mu)} \mathbf{K}
\]  

The literature [55] commonly reports anisotropic parameters \( S_{11}, S_{12}, \text{ and } S_{44} \), which are related to those utilized above by:

\[
S_{11} = \frac{1}{3} \left( \frac{1}{3\kappa + \zeta} - \frac{\zeta}{\mu(\kappa + 2\mu)} + \frac{1}{\mu} \right); \quad S_{12} = \frac{1}{3} \left( \frac{1}{3\kappa + \zeta} + \frac{\zeta}{2\mu(\kappa + 2\mu)} - \frac{1}{2\mu} \right); \quad S_{44} = \frac{1}{\mu}
\]

or conversely,

\[
\mu = \frac{1}{S_{44}}; \quad \kappa = \frac{1}{3S_{44}} \left( \frac{-S_{11} - 2S_{12} + S_{44}}{2S_{12} + S_{11}} + \frac{2S_{11} - 2S_{12} - S_{44}}{S_{11} - S_{12}} \right); \quad \zeta = \frac{S_{44} - 2S_{11} + 2S_{12}}{S_{44}(S_{11} - S_{12})}
\]

Stress dependence of the bulk modulus is considered in Appendix D.2 and a description of the elastic strain energy density is available in Appendix D.1.

In most formulations, assuming small strain elastic behavior is paramount in producing a tractable elastic-plastic solution. Within the proposed framework, which utilizes anisotropic elasticity, only small simplifications for the small elastic strain hypothesis are possible. Subsequent simulations will highlight the ramifications of assuming small strain elasticity, where both a rigorous definition (large strain elasticity) and a simplification associated with small strain elasticity are compared.

There are a few notable variations associated with the choice of elastic formulation. First, consider the different relationships of the stretch, \( \mathbf{U} \), with respect to the elastic Green strain, \( \mathbf{E}^{Ge} \):

**Definition:**

\[
\mathbf{E}^{Ge} = \frac{1}{2} \left( \mathbf{F}^{eT} \mathbf{F}^{e} - \mathbf{I} \right) = \frac{1}{2} \left( \mathbf{U}^{e} \mathbf{U}^{e} - \mathbf{I} \right)
\]  

**Small strain** (\( \|\mathbf{U}^{e} - \mathbf{I}\| \ll 1 \)):

\[
\mathbf{\varepsilon} = \mathbf{U}^{e} - \mathbf{I}
\]

These nuisances influence the calculation of the Mandel stress, which can be obtained from either of the ensuing equations:

**Definition:**

\[
\mathbf{\Sigma}^{e} = \mathbf{S}^{e} \left( 2\mathbf{E}^{Ge} + \mathbf{I} \right) = \frac{1}{2} \left( \mathbb{E}^{e} : \left( \mathbf{F}^{eT} \mathbf{F}^{e} - \mathbf{I} \right) \right) \left( \mathbf{F}^{eT} \mathbf{F}^{e} \right)
\]  

**Small strain:**

\[
\mathbf{\Sigma}^{e} = \mathbf{S}^{e} = \mathbb{E}^{e} : \mathbf{\varepsilon}.
\]

Notice, the definition of the Mandel stress does not require the use of a polar decomposition to distinguish the stretch, \( \mathbf{U}^{e} \), and the rotation, \( \mathbf{R}^{e} \). By requiring this decomposition, the small strain elasticity simplification loses much of its purposed
benefit in the proposed framework. Differences are also apparent in the formulations of the current Cauchy stress, $\sigma$, which are shown below:

**Definition:**

$$\sigma = \frac{1}{J^e} F^e \Sigma^e F^{e-1} = \frac{1}{J^e} F^e \left( \varepsilon^e : \left( F^e F^e - I \right) \right) F^{eT}$$  \hspace{1cm} (3.29)

**Small strain:**

$$\sigma = RS^e R^T = R \left( \varepsilon^e : \varepsilon \right) R^T$$  \hspace{1cm} (3.30)

In the subsequent discussion and modeling, only the large strain elastic definition was employed unless otherwise specified.

### 3.4 Plasticity

In this investigation, a crystal plasticity framework was adopted to describe the deformation due to slip. Specifically the plastic velocity gradient is related to the plastic strain-rate on each slip system, $\dot{\gamma}_p$, by the following expression [94]:

$$L^p = \sum_s \dot{\gamma}_p \left( b_{(s)} \otimes n_{(s)} \right)$$  \hspace{1cm} (3.31)

where, $n_{(s)}$ represents the normal vector of the slip plane and $b_{(s)}$ is the corresponding slip direction. For a Face-Centered-Cubic (FCC) crystal structure, the normal and slip direction vectors are presented in Table 3.1 for the 12 primary slip systems. The shear stress resolved onto each slip system is defined below with respect to the Cauchy stress, $\sigma$, and the Mandel stress, $\Sigma^e$ [95]:

$$\tau_{(s)} = \left( F^e b_{(s)} \right) : \left( J^e \sigma \right) \left( n_{(s)} F^{e-1} \right)$$  \hspace{1cm} (3.32)

or

$$\tau_{(s)} = \Sigma^{eT} : \left( b_{(s)} \otimes n_{(s)} \right).$$  \hspace{1cm} (3.33)

The corresponding rate of plastic work, $\dot{\Psi}^p$, may be expressed in macro and micro variables as [137]:

$$\dot{\Psi}^p = \Sigma^{eT} : L^p = \sum_s \tau_{(s)} \dot{\gamma}_p$$  \hspace{1cm} (3.34)

The resolved shear stress, $\tau_{(s)}$, should equal the plastic flow stress, $\tau^{* p}_{(s)}$, on the each slip system that is plastically deforming (i.e. $\dot{\gamma}_p \neq 0$):

$$\tau_{(s)} \left( \Sigma^e \left( F^e \right) \right) = \tau^{* p}_{(s)} \left( \dot{\gamma}_p, q_{(p)} \right)$$  \hspace{1cm} (3.35)

$$\dot{q}_{(s)} = f \left( \dot{\gamma}_p, q_{(p)} \right)$$  \hspace{1cm} (3.36)

where $q_{(p)}$ are internal state variables associated with the slip system, $\beta$. 

99
It should be noted that determining the evolution of plastic deformation in a crystal plasticity framework is exceedingly difficult due to the non-uniqueness relating the shear stress and plastic strain-rate on each slip system [88]. The vast majority of crystal plasticity models employ a visco-plastic type constitutive equation on the slip-system level [90]. Alternatively, one can in some measure incorporate the traditional concept of a yield stress in this framework by assuming a plastic hardening slope much greater than the elastic stiffness prior to plastic flow. This assumption maintains uniqueness of the solution even when slip systems are redundant. Since the material under consideration displays regimes of relative strain-rate insensitivity, the adoption of this modified plastic hardening approach is advantageous.

Table 3.1: Primary slip systems for an FCC crystal structure [55]

<table>
<thead>
<tr>
<th>Slip System</th>
<th>( \mathbf{n}_{(s)} )</th>
<th>( \mathbf{b}_{(s)} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1)</td>
<td>( \frac{1}{\sqrt{3}}(1\ 1\ 1) )</td>
<td>( (\sqrt{2})[0\ 1\ -1] )</td>
</tr>
<tr>
<td>(2)</td>
<td>( \frac{1}{\sqrt{3}}(1\ 1\ 1) )</td>
<td>( (\sqrt{2})[1\ 0\ -1] )</td>
</tr>
<tr>
<td>(3)</td>
<td>( \frac{1}{\sqrt{3}}(1\ 1\ 1) )</td>
<td>( (\sqrt{2})[1\ -1\ 0] )</td>
</tr>
<tr>
<td>(4)</td>
<td>( \frac{1}{\sqrt{3}}(-1\ 1\ 1) )</td>
<td>( (\sqrt{2})[0\ -1\ 1] )</td>
</tr>
<tr>
<td>(5)</td>
<td>( \frac{1}{\sqrt{3}}(-1\ 1\ 1) )</td>
<td>( (\sqrt{2})[1\ 0\ 1] )</td>
</tr>
<tr>
<td>(6)</td>
<td>( \frac{1}{\sqrt{3}}(-1\ 1\ 1) )</td>
<td>( (\sqrt{2})[1\ 1\ 0] )</td>
</tr>
<tr>
<td>(7)</td>
<td>( \frac{1}{\sqrt{3}}(1\ -1\ 1) )</td>
<td>( (\sqrt{2})[0\ 1\ 1] )</td>
</tr>
<tr>
<td>(8)</td>
<td>( \frac{1}{\sqrt{3}}(1\ -1\ 1) )</td>
<td>( (\sqrt{2})[-1\ 0\ 1] )</td>
</tr>
<tr>
<td>(9)</td>
<td>( \frac{1}{\sqrt{3}}(1\ -1\ 1) )</td>
<td>( (\sqrt{2})[-1\ -1\ 0] )</td>
</tr>
<tr>
<td>(10)</td>
<td>( \frac{1}{\sqrt{3}}(1\ 1\ -1) )</td>
<td>( (\sqrt{2})[0\ -1\ -1] )</td>
</tr>
<tr>
<td>(11)</td>
<td>( \frac{1}{\sqrt{3}}(1\ 1\ -1) )</td>
<td>( (\sqrt{2})[-1\ 0\ -1] )</td>
</tr>
<tr>
<td>(12)</td>
<td>( \frac{1}{\sqrt{3}}(1\ 1\ -1) )</td>
<td>( (\sqrt{2})[-1\ 1\ 0] )</td>
</tr>
</tbody>
</table>

The independent slip-system (Schmid type) model [86] chosen for this investigation relates each slip-system’s shear stress, \( \tau_{(s)}^* \), to the state variables, \( q_{(s)(a)} \):

\[
\tau_{(s)}^* = \sum_{a=1}^{M} q_{(s)(a)} \quad (3.37)
\]

\[
\text{sign}\left(\dot{\gamma}_{(s)}^p q_{(s)(a)} < r_{(a)} \right) \dot{q}_{(s)(a)} = \theta_{(a)} \dot{\gamma}_{(s)}^p \\
\text{sign}\left(\dot{\gamma}_{(s)}^p q_{(s)(a)} = r_{(a)} \right) \dot{q}_{(s)(a)} = 0 \quad (3.38)
\]

where the hardening slope(s), \( \theta_{(a)} \), may be related to the strain hardening for a given obstacle to slip which saturates at a hardening strength of \( r_{(a)} \). It should be noted that the first slope, \( \theta_{(1)} \), has been assumed to be on the order of 1000 times the shear modulus, and
the first hardening strength, \( r_{(1)} \), is related to an initial yield definition. This additive structure is similar to the format introduced by Xu and Jiang [104]. Mechanistically, saturation refers to some critical strength value when the obstacles causing the strain hardening, \( \theta_{(a)} \), exhibit a balance between trapping and releasing of dislocations, or the ability to bypass the saturated obstacles. Other mechanistic interpretations may be forwarded, but the model has the ability to reflect the physically observed change of strain hardening as hardening progresses. Despite recognition that latent hardening has a significant impact on plasticity modeling, slip system independence was stipulated because a physically based representation for slip system coupling was not readily available. Furthermore, if precipitate obstacles rather than dislocation obstacles dominate hardening, slip system independence may be appropriate.

For clarity, an illustration is presented in Figure 3.2 for unidirectional loading of a single slip system with the changes in slip resistance resolved into five distinct linear regions. The other demarcations chosen in this figure broadly assume that the range of obstacle resistance to slip can be adequately categorized with five hardening strengths. The shear stress at each slope change can be described by the following expression:

\[
\tau^*_{(x)} = \left( \sum_{a=1}^{x} r_{(a)} \right) + m_{(x+1)} \gamma^p_{(x)}
\]

where,

\[
\gamma^p_{(x)} = \frac{r_{(x)}}{\theta_{(x)}} , \quad \gamma^p_{(0)} = 0
\]
and
\[ m_{(x)} = \sum_{a=x}^{M} \theta_{(a)} , \quad m_{(M+1)} = 0. \]  

In the previous expression, \( m_{(x)} \) represents the slip system hardening slope and \( \gamma^p_{(x)} \) is the corresponding slip system plastic strain (for monotonic loading). When these expressions are employed, the appropriate shear stress-strain relationship may be distinguished by optimizing \( \theta_{(x)} \) and \( r_{(x)} \) as necessary. The primary advantage of this linearly segmented formulation is for numerical convenience and the robustness to handle kinematic hardening during cyclic deformation without introducing “negative” slip systems. Another distinct advantage of this model is that the integration during a step is very simple, which is particularly useful due to the chosen framework, where integration is implemented during an iterative procedure.

In a classical plasticity sense, each independent slip system model is analogous to the 1-D equivalent of an Armstrong-Fredrick [100] / Chaboche [142] type model. The 1-D simplification is appropriate because the direction of slip was assumed to be dictated by the independent crystal slip systems. Most kinematic hardening models are associated with a ‘backstress’. One does not appear explicitly in the current form of this model due to the incorporation of the modified plastic hardening approach, which maintains uniqueness of the solution. Hence, an additive slip system ‘backstress’ could be inferred:

\[ \alpha_{(x)} = \sum_{a=2}^{M} q_{(s)(a)} \]  

which is equivalent to the kinematic format proposed by Weng [97]. The mechanism of a ‘backstress’ in most kinematic hardening models assumes sufficient obstacles to slip on a scale much smaller than the volume of the modeled region. This mechanistic assumption has been attributed to polycrystalline behavior whose grain size is smaller than the representative volume. However, one may expect similar behavior on the grain level when sufficient obstacles (such as precipitates, or dislocation cell structure) exist that cause slip of a single slip system to behave differently in opposing directions. Weng [97] suggested that Seeger’s dislocation pileup theory or Orowan’s dispersion hardening hypothesis may exhibit similar directional slip behavior. In cyclically stable microstructures, it is forwarded that these obstacles may act together as a 1-D ‘backstress’ even in single crystals, as is supported by experimental evidence [143].
Currently, slip-system coupling is ignored, but may be essential to refine modeling of single crystal behavior under more complex multiaxial loadings. Nevertheless, for a cyclically stable microstructure the interaction between slip systems is expected to have been established.

Having chosen a framework that is well behaved and numerically stable for rate independence, it is worth noting modifications necessary for including rate dependence. For positive rate sensitivity, uniqueness is maintained and the implementation involves a choice between allowing the hardening slope, \( \theta_{(a)} \), and/or the hardening strength, \( n_{(a)} \), to depend on the plastic slip-rate, \( \dot{\gamma}_{(a)} \). Allowing only the hardening strength to vary with strain-rate could be physically motivated by the limiting nature of the term. Each of the hardening strengths/slopes need not have the same rate dependence. Experimental data (incremental step tests Section 2.2.1) for the material considered suggests rate insensitivity at higher slopes (after initial yield), while positive rate sensitivity is prevalent at lower hardening slopes (larger plastic strains). This data also indicates a slightly negative rate sensitivity at the highest slopes (near yield). However, difficulties in maintaining uniqueness and providing a mechanistic interpretation is avoided by requiring the rate dependence to be strictly greater-than or equal to zero in the ensuing discussion.

### 3.5 General Solution Implementation

A general non-linear solution algorithm was adopted to employ the model described previously. Either the velocity gradient \( (L) \) or the new and previous deformation gradients \( (F^{(i)}, F^{(i+1)}) \) are specified prior to the iterative procedure, depending on the application. First, the deformation gradient increment is determined from the appropriate form:

\[
\Delta F = \exp(L \Delta t) \quad (3.43)
\]

or

\[
\Delta F = F^{(i+1)} F^{(i-1)} \quad (3.44)
\]

The previous elastic deformation gradient, \( F^{(e)} \), is also known, and can be manipulated to extract both the stress and crystallographic orientation. The current elastic deformation gradient, \( F^{(e)(i+1)} \), may be expressed by rearranging Eq. 3.10:
\[ \mathbf{F}^{(i+1)} = \Delta \mathbf{F} \mathbf{F}^{(i)} \Delta \mathbf{F}^{-1}. \]  

(3.45)

If one recognizes that the inverse of the plastic deformation gradient increment, \( \Delta \mathbf{F}^{-1} \), is only a function of \( \mathbf{F}^{(i+1)} \), then a non-linear solution algorithm may be constructed that minimizes the following residual equation:

\[ \Xi^e = \frac{1}{2} \left( \mathbf{F}^{(\text{guess})} - \mathbf{F}^{(i+1)} \right) : \left( \mathbf{F}^{(\text{guess})} - \mathbf{F}^{(i+1)} \right), \]

(3.46)

where the elastic deformation gradient is guessed and updated until convergence is achieved \( (\mathbf{F}^{(\text{guess})} = \mathbf{F}^{(i+1)}) \). To clarify how the plastic deformation gradient may be expressed as a function of the elastic deformation increment, first consider the Mandel stress:

\[ \Sigma^e = \frac{1}{2} \mathbf{C}^e : \left( \mathbf{F}^T \mathbf{F} - \mathbf{I} \right) \left( \mathbf{F}^T \mathbf{F} \right) \]

(3.27)

which is a function of only \( \mathbf{F}^e \). Next, the shear stress resolved on each slip system can be determined as described previously:

\[ \tau^{(s)} = \Sigma^e : (\mathbf{b}^{(s)} \otimes \mathbf{n}^{(s)}). \]

(3.33)

Presuming a unique relationship exists between this resolved shear stress and the plastic strain-rate on each slip system, the plastic strain-rate may be determined from the resolved shear stress:

\[ \dot{\gamma}^{p\,(s)} = f(\tau^{(s)}), \]

(3.47)

where the function \( f \) corresponds to the inverse of Eq. 3.35, which is defined for strain hardening. These plastic strain-rates may be combined to determine the plastic velocity gradient, as previously discussed for plastic slip:

\[ \mathbf{L}^p = \sum_s \dot{\gamma}^{p\,(s)} (\mathbf{b}^{(s)} \otimes \mathbf{n}^{(s)}) \]

(3.31)

Similar to the total deformation increment, the inverse plastic increment is estimated by integrating \( \mathbf{L}^p \) with respect to time:

\[ \Delta \mathbf{F}^{-1} = \exp(-\mathbf{L}^p \Delta t), \]

(3.48)

where the negative sign indicates direct calculation of the inverse. This integration process was inspired by personal communication with Aravas [144] and is similar to the work of de Souza [133]. For both the total (Eq. 3.43) and plastic (Eq. 3.48) integrations, the exponential map was computed using the Padé approximation [145]. With this
procedure, the elastic deformation gradient may be solved iteratively using a number of methods including successive substitution and Newton’s method. For example, solving the following expression for the elastic deformation gradient guess increment, \( \Delta F_{e\text{(guess)}} \), is one potential solution method:

\[
\frac{dF_{e\text{(i+1)}}}{dF_{e}} - \Delta F_{e\text{(guess)}} = F_{e\text{(guess)}} - F_{e\text{(i+1)}}.
\]  

(3.49)

The derivative of the current elastic deformation gradient with respect to the guess is determined using the chain rule:

\[
\frac{dF_{e\text{(i+1)}}}{dF_{e}} = \frac{dF_{e\text{(i+1)}}}{d\dot{\gamma}^p_{(s)}} \frac{d\dot{\gamma}^p_{(s)}}{d\tau_{(s)}} \frac{d\tau_{(s)}}{d\Sigma^e} \frac{d\Sigma^e}{dF_{e}^{-1}}.
\]  

(3.50)

where the derivative of the slip-system plastic strain-rate with respect to the shear stress is defined from Eq. 3.47, and the other derivatives are described in Eqs. 3.54-3.56.

Although the aforementioned approach is instructive, some complexity arises when plastic deformation exhibits relatively little strain hardening on any slip system (a small change in \( \tau_{(s)} \) results in a large change in \( \dot{\gamma}^p_{(s)} \)). To overcome this sensitivity while utilizing a Newton based approach, the residual (Eq. 3.46) was recast onto each slip system by observing \( F_e \) may be written as a function of the plastic strain-rate, \( \dot{\gamma}^p_{(s)} \). The following slip-system residual, involving a difference of shear stresses, was employed in this investigation:

\[
\Xi^r = \frac{1}{2} \sum_{a=1}^{M} \left( \tau_{(s)} - \tau^*_{(s)} \right)^2 < 10^{-12}.
\]  

(3.51)

The first shear stress, \( \tau_{(s)} \), is a function of \( \dot{\gamma}^p_{(s)} \), which was obtained through the manipulation of Eqs. 3.33, 3.27, 3.45, 3.48, and 3.31. The other shear stress, \( \tau^*_{(s)} \), is a function of only \( \dot{\gamma}^p_{(s)} \), as was previously stipulated for the rate-independent kinematic hardening model:

\[
\tau^*_{(s)} = \sum_{a=1}^{M} q_{(s)(a)} \theta_{(a)} \dot{\gamma}^p_{(s)}
\]  

(3.37)

\[
\text{sign} \left( \dot{\gamma}^p_{(s)} \right) q_{(s)(a)} < r_{(a)} : \dot{q}_{(s)(a)} = \theta_{(a)} \dot{\gamma}^p_{(s)}
\]  

\[
\text{sign} \left( \dot{\gamma}^p_{(s)} \right) q_{(s)(a)} = r_{(a)} : \dot{q}_{(s)(a)} = 0
\]  

(3.38)
It should be noted that saturation was approximated with a finite slope of $10^8 \mu$ in this investigation to avoid non-uniqueness of the slip-system strain-rates. This algorithm only requires Eq. 3.47 to exist for uniqueness and does not explicitly utilize it during the solution procedure.

Newton’s method was adopted to obtain an updated guess if the residual condition was not satisfied for the current choice of $\dot{\gamma}^p_{(s)}$. This involves solving the linearized system of $M$ equations for the plastic strain-rate increment, $\Delta \dot{\gamma}^p_{(s)}$:

$$\begin{bmatrix} \frac{\partial \tau_{(s)}}{\partial \dot{\gamma}^p_{(t)}} - \frac{\partial \tau^*_s}{\partial \dot{\gamma}^p_{(t)}} \end{bmatrix} \{ \Delta \dot{\gamma}^p_{(t)} \} = \{ \tau^*_s - \tau_{(s)} \}. \tag{3.52}$$

The first partial derivative (the first term on the left-hand side of Eq. 3.52) is estimated using the chain-rule:

$$\frac{\partial \tau_{(s)}}{\partial \dot{\gamma}^p_{(t)}} = \frac{d \tau_{(s)}}{d \Sigma^e} \frac{d \Sigma^e}{d F^e} \frac{d F^e}{d \dot{\gamma}^p_{(t)}}. \tag{3.53}$$

The derivative of slip-system shear stress with respect to the Mandel stress is determined from Eq. 3.33, as shown below:

$$\frac{d \tau_{(s)}}{d \Sigma^e} = n_{(s)ij} b_{(s)j}. \tag{3.54}$$

The derivative of the Mandel stress with respect to the elastic deformation gradient is estimated by:

$$\frac{d \Sigma^e_{ij}}{d F^e_{kl}} = \frac{1}{2} \left( \mathcal{C}^e_{isnm} F^e_{om} F^e_{on} \delta_{ji} - \mathcal{C}^e_{ismn} \delta_{ji} + \mathcal{C}^e_{jmst} F^e_{om} F^e_{oj} \right) (F^e_{kl} \delta_{li} + F^e_{ki} \delta_{il}). \tag{3.55}$$

If the small strain elasticity approximation were utilized, then a more complex expression would involve the derivative of the right polar decomposition, which is detailed in the literature [134].

The derivative of the elastic deformation gradient is estimated using Eq. 3.45 and the derivative of the plastic strain increment with respect to the plastic strain-rate:

$$\frac{\partial F^e_{ij}^{(s+1)}}{\partial \dot{\gamma}^p_{(t)}} = -\Delta t \Delta F^p_{ik} F^e_{kl}^{(s+1)} \exp(-\mathbf{L}^p \Delta t) \mathbf{b}_{(s)mn} \Delta \mathbf{n}_{(s)lm}, \tag{3.56}$$

where the derivative of the exponential map, $\exp(\mathbf{A})$, is calculated in the manner presented by de Souza [133]:

106
The remaining term in the linearized equation (the second term on the left-hand side of Eq. 3.52) involves the derivative of the plastic shear stress, \( \tau^*_{(s)} \), with respect to the plastic strain-rate on each slip system. For the plasticity model incorporated in this investigation, this derivative takes the following form:

\[
\frac{\partial \tau^*_{(s)}}{\partial \dot{\gamma}_{(s)}^p} = \sum_{a=1}^{M} \theta_{(a)} \left[ \text{sign} \left( \dot{\gamma}_{(s)}^p \right) \right]_{q_{(a)} \leq \tau_{(a)}},
\]

This results in an \( M \times M \) diagonal matrix since the slip systems are assumed to be independent. With these derivatives, a plastic strain-rate increment may be calculated from Eq. 3.52. The plastic strain-rate guess is then updated with the following:

\[
\dot{\gamma}_{(s)}^p = \dot{\gamma}_{(s)}^p + \Delta \dot{\gamma}_{(s)}^p.
\]

This process is repeated until the convergence criterion is satisfied. It should be noted that the plastic strain-rate increment is scaled such that the plastic strain-rate does not change signs (i.e. cross zero) during a single iteration. This stipulation is included due to the heightened sensitivity (increased stiffness) of the plastic deformation at a reversal. Figure 3.3 illustrates the typical convergence rate of this internal iterative scheme. As shown, the convergence rate is very rapid when the residual is small, but slow when the residual is large. This trend is due to the sensitivity of the plastic strain-rate when its direction (sign of the plastic slip) changes. Convergence rates are slowed when these sign changes occur (unloading or initial plastic flow), and can require as many as 20-25 iterations to converge.

Figure 3.3: Typical residual convergence for plastic strain-rates
After convergence of the plastic strain-rates, the Cauchy stress may be determined by the following expression for large strain elasticity:

\[ \sigma = \frac{1}{2 \det(F^e)} F^e \left( \mathcal{E} : \left( F^{eT} F^e - I \right) \right) F^{eT}. \]  

(3.60)

The derivative of the Cauchy stress with respect to the increment of the deformation gradient is desirable for many applications (including Uniform Deformation, Bi-crystal or Abaqus implementation):

\[ \frac{d\sigma}{d\Delta F} = \frac{d\sigma}{dF^e} \left( \frac{\partial F^e}{\partial \Delta F} + \frac{\partial F^e}{\partial \gamma^p} \left( \frac{\partial \tau^e_{(s)}(s)}{\partial \gamma^p_{(s)}} - \frac{\partial \tau^e_{(s)}}{\partial \gamma^p_{(s)}} \right) \right) \left( \frac{d\tau_{(s)}}{d\Delta F} \frac{d\Sigma^e}{dF^e} \frac{\partial F^e}{\partial \Delta F} \right). \]  

(3.61)

The derivative of the Cauchy stress with respect to the elastic deformation gradient for large elastic strains is:

\[ \frac{d\sigma_{ij}}{dF^e_{kl}} = \frac{1}{2 \det(F^e)} \left( \delta_{ik} F^e_{jm} \mathring{\mathcal{E}}_{lnop} + F^e_{im} \delta_{jk} \mathring{\mathcal{E}}_{lnop} \right) \left( F^{eT}_{pq} \delta_{qp} - \delta_{ip} \right) - 2 \sigma_{ij} \frac{d \left( \det(F^e) \right)}{dF^e_{kl}} \]  

(3.62)

where the derivative of the determinant is readily defined for a 3x3 matrix. The partial derivative of the elastic deformation gradient with respect to the deformation gradient increment can be defined as:

\[ \frac{\partial F^e_{ij}}{\partial \Delta F_{kl}} = \delta_{ik} F^e_{lm} \delta_{mj} \Delta F_{ij}^{-1}. \]  

(3.63)

The other terms in Eq. 3.61 have been obtained as part of the slip-system plastic strain-rate solution technique (Eq. 3.52) with Eqs. 3.54-3.56.

Obtaining the derivative of the Cauchy stress with respect to the deformation gradient increment, allows the implementation of the chain rule to determine the appropriate derivative for the application under consideration. When utilizing a given \( F^{(i+1)} \) or \( L \), the appropriate derivative is described below with the necessary substitutions:

\[ \frac{d\sigma_{ij}}{dL_{kl}} = \frac{d\sigma_{ij}}{dF_{mn}} \frac{d\Delta F_{mn}}{dL_{kl}} = \frac{d\sigma_{ij}}{d\Delta F_{mn}} \frac{d\exp(L \Delta t)}{dL_{kl}} \]  

(3.64)

\[ \frac{d\sigma_{ij}}{dF_{kl}^{(i)}} = \frac{d\sigma_{ij}}{d\Delta F_{mn}} \frac{d\Delta F_{mn}}{dF_{kl}^{(i)}} = \frac{d\sigma_{ij}}{d\Delta F_{mn}} \delta_{mn} F_{ln}^{(i)} \]  

(3.65)
Typical convergence for this solution procedure with 1000 crystallographic orientations modeled with the uniform deformation model and five stress boundary conditions is presented in Figure 3.4. The residual in question for this example is defined as the difference in the prescribed traction boundary condition and the average simulated value:

$$
\Xi_{ij}^\gamma = \frac{1}{2} \left( \sum_{\alpha=1}^{N} \sigma^{(\alpha)} - \sigma^{(BC)} \right) \cdot \left( \sum_{\alpha=1}^{N} \sigma^{(\alpha)} - \sigma^{(BC)} \right) < 10^{-4}.
$$

where the summation of $N$ terms represents the grain averaging. As illustrated, the convergence rate is manageable, but is not as well behaved as the internal iterations. Nevertheless, 5-7 iterations is typical to achieve the rather loose convergence criteria adopted for the uniform deformation model. Furthermore, the aforementioned difficulty at reversal points did not occur for this part of the solution.

![Figure 3.4: Typical residual convergence for the uniform deformation model](image)

### 3.6 Uniform Deformation Model

Often times it is desirable to combine a set of crystalline orientations into an aggregate to approximate deformation on a length scale larger than the grain size. Under such circumstances, a wide variety of assumptions are often employed to obtain a reasonable estimate of the aggregate behavior. One such method is to ensure that compatibility is trivially enforced everywhere, by applying uniform deformation to each crystallographic orientation. This method is attributed to Taylor [108] for polycrystalline plastic deformation, and has been postulated to be a reasonable estimate of deformation, particularly at large strains [114]. Furthermore, uniform strain methods generally act as upper bounds on stress response [109, 110]. It should be noted that other aggregate methods such as the self-consistent method [111, 112] typically require relative isotropy.
on the macroscopic scale and do not necessarily result in an upper bound. In this investigation, a uniform deformation model was employed for its relatively simple boundary conditions within the framework of relatively complex anisotropic models.

As the name indicates, the distinct feature of this polycrystalline model is the uniform deformation applied to each crystal. In some applications, the macroscopic deformation may be stipulated in all components, such as plane strain compression. However, for other realistic loadings there are nominal stress boundary conditions that should be enforced. For instance, during uniaxial tension, the nominal deformation may be prescribed in one direction, but the other tensorial components of deformation are determined by the traction-free boundary condition on the remaining free surfaces. In such situations, the appropriate deformation should result in an average (or nominal) stress of zero for these traction free components.

To elaborate on the use of the uniform deformation model, consider an aggregate of $N$, crystallographic orientations that represent the Orientation Distribution Function (ODF) of the material under investigation. The velocity gradient, $L$, at any instant is assumed to be uniform, and the macroscopic stress, $\sigma^{\text{avg}}$, observed by the material may be written as the average of the crystal stresses overall all orientations:

$$\sigma^{\text{avg}} = \frac{1}{N} \sum_{i=1}^{N} (\sigma^{(i)})$$

where each crystal stress, $\sigma^{(i)}$, is determined from the appropriate definition (Eq. 3.60). Since the macroscopic stress is determined from an average, equilibrium is not strictly enforced on the crystal scale; it is only weakly enforced on the macro-scale in the boundary value problem sense. In other words, each crystallographic orientation independently influences the polycrystalline response, neglecting any influence of a specific neighboring grain. However, the aggregate of the ODF does play a substantive role. This implementation of the Taylor-like model mirrors the polycrystalline aggregate simulated by FEM at individual Gauss points by Kalidindi et. al. [120], where the nominal stress in the polycrystal was adjusted by varying the applied (uniform) velocity gradient until equilibrium is satisfied. In order to relate the velocity gradient to the average macroscopic stress, a Newton iterative scheme was adopted. In the most general
case (if all nominal stress components were given), the change in the velocity gradient can be estimated by solving following equation:

\[
\left[ \sum_{\alpha=1}^{N} \left( \frac{d\sigma^{(o)}}{dL} \right) \right] \{\Delta L\} = \left[ \sigma^{(BC)} - \left( \sum_{\alpha=1}^{N} \sigma^{(o)} \right) \right].
\] (3.68)

Slight modifications are needed when some components of \( L \) are specified as part of the boundary value problem.

To clarify this concept, consider the implementation of the uniform deformation model to symmetric uniaxial loading in the 1-direction. In this case, the following components of the velocity gradient and nominal stress are specified:

\[
\begin{align*}
L_{11} &= \Delta & \sigma_{22}^{\text{avg}} &= 0 \\
L_{12} &= L_{21} & \sigma_{33}^{\text{avg}} &= 0 \\
L_{13} &= L_{31} & \sigma_{12}^{\text{avg}} &= \sigma_{21}^{\text{avg}} = 0 \\
L_{23} &= L_{32} & \sigma_{13}^{\text{avg}} &= \sigma_{31}^{\text{avg}} = 0 \\
& & \sigma_{23}^{\text{avg}} &= \sigma_{32}^{\text{avg}} = 0
\end{align*}
\] (3.69)

where \( \Delta \) is the applied uniaxial strain-rate and \( \sigma_{11}^{\text{avg}} \) is the only non-zero macroscopic component of stress. Clearly, there are five components of \( L \) that need to be determined: \( L_{22}, L_{33}, L_{12}, L_{13}, \) and \( L_{23} \). In order to determine these components of the velocity gradient, the following Newton system of equations were implemented:

\[
\begin{pmatrix}
\frac{d\sigma_{22}^{(o)}}{dL_{22}} & \frac{d\sigma_{22}^{(o)}}{dL_{23}} & \frac{d\sigma_{22}^{(o)}}{dL_{32}} & \frac{d\sigma_{22}^{(o)}}{dL_{33}} & \frac{d\sigma_{22}^{(o)}}{dL_{12}} & \frac{d\sigma_{22}^{(o)}}{dL_{13}} \\
\frac{d\sigma_{33}^{(o)}}{dL_{22}} & \frac{d\sigma_{33}^{(o)}}{dL_{23}} & \frac{d\sigma_{33}^{(o)}}{dL_{32}} & \frac{d\sigma_{33}^{(o)}}{dL_{33}} & \frac{d\sigma_{33}^{(o)}}{dL_{12}} & \frac{d\sigma_{33}^{(o)}}{dL_{13}} \\
\frac{d\sigma_{12}^{(o)}}{dL_{22}} & \frac{d\sigma_{12}^{(o)}}{dL_{23}} & \frac{d\sigma_{12}^{(o)}}{dL_{32}} & \frac{d\sigma_{12}^{(o)}}{dL_{33}} & \frac{d\sigma_{12}^{(o)}}{dL_{12}} & \frac{d\sigma_{12}^{(o)}}{dL_{13}} \\
\frac{d\sigma_{13}^{(o)}}{dL_{22}} & \frac{d\sigma_{13}^{(o)}}{dL_{23}} & \frac{d\sigma_{13}^{(o)}}{dL_{32}} & \frac{d\sigma_{13}^{(o)}}{dL_{33}} & \frac{d\sigma_{13}^{(o)}}{dL_{12}} & \frac{d\sigma_{13}^{(o)}}{dL_{13}} \\
\frac{d\sigma_{23}^{(o)}}{dL_{22}} & \frac{d\sigma_{23}^{(o)}}{dL_{23}} & \frac{d\sigma_{23}^{(o)}}{dL_{32}} & \frac{d\sigma_{23}^{(o)}}{dL_{33}} & \frac{d\sigma_{23}^{(o)}}{dL_{12}} & \frac{d\sigma_{23}^{(o)}}{dL_{13}} \\
\end{pmatrix}
\begin{pmatrix}
\frac{d\sigma_{22}^{(o)}}{dL_{12}} \\
\frac{d\sigma_{33}^{(o)}}{dL_{12}} \\
\frac{d\sigma_{12}^{(o)}}{dL_{12}} \\
\frac{d\sigma_{13}^{(o)}}{dL_{12}} \\
\frac{d\sigma_{23}^{(o)}}{dL_{12}} \\
\end{pmatrix}
= \begin{pmatrix}
\Delta L_{22} \\
\Delta L_{33} \\
\Delta L_{12} \\
\Delta L_{13} \\
\Delta L_{23} \\
\end{pmatrix}
\]

(70)

where convergence is determined when the sum of squares of the average stresses nears zero. At convergence, the uniform velocity gradient is the estimated macroscopic deformation observed by a polycrystal. It should be noted that the stress for each crystallographic orientation under uniform deformation could easily be queried through Eq. 3.60 for statistical analysis.
3.7 **Bi-Crystal Model**

In the delamination of Al-Li alloys, grain boundaries are observed to play a crucial role; the interface between grains is where cracking or delamination is observed. Although a high precipitate volume fraction (Auger Section 2.1.3) and a relatively weak grain boundary interface (Interface Strength 2.3.2) have been experimentally observed, crystallographic mismatch may significantly contribute to the delamination phenomenon. To obtain an improved statistical estimate of grain boundary interface stresses, a bi-crystal model was developed.

Suppose there exists an adjacent pair of orientations, demarked as grain A and grain B, as illustrated in Figure 3.5. First consider the schematic in Figure 3.5a, which illustrates that both grains are required to deform identically, as was the case for the Taylor model. Although this assumption provides an upper bound for stress estimates (on average), it ignores equilibrium at the grain boundary interface. A uniform deformation model over constrains a pair of orientations with an infinitesimal interface. Compatibility may remain satisfied in both the polycrystalline and grain boundary interface length scales even when permitting deviation in 3 components of the velocity gradient: $L_{13}$, $L_{23}$, and $L_{33}$. Illustrations of each of these component inequalities are depicted in Figure 3.5b-d where the dashed lines illustrate the uniform deformation (Figure 3.5a). These three components are determined by enforcing equilibrium on the grain boundary interface.

![Figure 3.5: Potential deformation modes of the bi-crystal model](image)
This type of bi-crystal simulation is not unique to this investigation. For instance, Hadamard [146] enforced equilibrium along an interfacial plane in 1903. The Lamel and advanced Lamel models were formulated by Van Houtte [130, 127] to obtain texture predictions for elongated grain structures by utilizing a similar bi-crystal arrangement. In their work, the relaxed constraint in bi-crystals provided an avenue toward improved estimates of experimentally observed textures over the Taylor model and polycrystalline FEM results [131]. Unlike the Taylor model, these stipulations directly infer the influence of an adjacent crystallographic orientation on the deformation. At relatively small strains, texture evolution is minimal. However, these relaxed constraint conditions may result in a more realistic stress state at the material interface, the grain boundary. To clarify this concept, consider when a relatively soft grain is adjacent to a hard grain with uniformly applied deformation. The soft grain will be subjected to a relatively low stress and the hard grain will see a high stress. These stresses will trend toward an intermediate value due to the bi-crystal’s relative flexibility. If one considers the interplay of multiple tensoral stress components, then the stress state at the interface can change in a more complex way.

To fully characterize the bi-crystal model, an appropriate choice of boundary conditions is necessary. Several options analogous to the single grain orientation case are possible, including uniform deformation, uniform stress, self-consistent, and FEM. As before, the FEM provides the most complete tool to determine stresses on the bi-crystal interface, but the computational requirements for a sufficient number of neighboring grain pairings make it impractical for statistical evaluation. Alternatively, a uniform deformation boundary condition approach may be adopted on the bi-crystal length scale, which relaxes equilibrium requirements but provides a plausible avenue for statistical considerations. Much like the uniform deformation model previously discussed, imposing uniform deformation to pairs of bi-crystals satisfies compatibility on both the macroscopic and bi-crystal length scales. Furthermore, since compatibility is trivially satisfied, the prescribed deformation provides an upper bound for stress estimates between grain pairs. If the uniform deformation boundary conditions stipulated is a contribution of the material’s texture (ODF) via the uniform deformation model, then the macroscopic boundary conditions are mirrored. In short, a statistically feasible
estimation providing a conservative upper bound is maintained by ensuring that the average velocity gradient is equivalent to that stipulated by the uniform deformation model. On the bi-crystal length scale, the average velocity gradient, \( \mathbf{L} \), is comprised of contribution from grain A and grain B:

\[
\mathbf{L} = \frac{1}{2} \left( \mathbf{L}^A + \mathbf{L}^B \right)
\]

where the superscripts \( A \) and \( B \) refer to grain A and grain B respectively. A similar expression is derivable for the average stress, but is only useful for finite element implementations and would serve little purpose in lone bi-crystal analysis, since equilibrium is ignored between the bi-crystal and bulk polycrystalline length scales.

For a general bi-crystal, the planar orientation interface (grain boundary) may be described by the unit normal vector, \( \mathbf{m} \). If \( \mathbf{m} \) is only non-zero in the 3-direction, then no rotation is required. Otherwise, the following rotation matrix, \( \mathbf{R}^{3m} \), transforms the \( m \)-direction to the 3-direction:

\[
\mathbf{R}^{3m} = \begin{bmatrix}
1 + \frac{(1-m_3)m_1^2}{m_1^2 + m_2^2} & \frac{(m_3-1)m_1m_2}{m_1^2 + m_2^2} & -m_1 \\
\frac{(m_3-1)m_1m_2}{m_1^2 + m_2^2} & 1 + \frac{(1-m_3)m_2^2}{m_1^2 + m_2^2} & -m_2 \\
m_1 & m_2 & m_3
\end{bmatrix}
\]

Since the velocity gradient is a 2\(^{nd}\) order tensor, the velocity gradient and stress in grain A may be written such that the interface aligns with the 3-direction by:

\[
\text{velocity gradient:} \quad L_{ij}^A = R_{ik}^{3m} R_{jl}^{3m} L_{kl}^A
\]

\[
\text{stress:} \quad \sigma_{ij}^A = R_{ik}^{3m} R_{jl}^{3m} \sigma_{kl}^A.
\]

Similarly, the rotated derivative of the stress with respect to the velocity gradient is:

\[
\frac{d\sigma_{ij}^A}{dL_{kl}^A} = R_{im}^{3m} R_{jn}^{3m} R_{ko}^{3m} R_{lp}^{3m} \frac{d\sigma_{mn}^A}{dL_{op}^A}.
\]
\[ L_{11}^3 = L_{41}^3, \quad L_{21}^3 = L_{21}^3 \]
\[ L_{22}^3 = L_{22}^3, \quad L_{31}^3 = L_{31}^3 \]
\[ L_{12}^3 = L_{12}^3, \quad L_{32}^3 = L_{32}^3 \]
\[ \alpha_{33}^3 = \alpha_{33}^3 \]
\[ \text{Compatibility:} \]

\[ \sigma_{13}^3 = \sigma_{31}^3 = \sigma_{13}^B = \sigma_{31}^B, \]
\[ \sigma_{23}^3 = \sigma_{32}^3 = \sigma_{23}^B = \sigma_{32}^B \]
\[ \text{Equilibrium:} \]

It should be noted that since the bi-crystal velocity gradient, \( L \), is given, only 3 velocity gradients are unknown: \( L_{13}^3 \), \( L_{23}^3 \) and \( L_{33}^3 \), which have all been written in terms of grain A. Equation 3.71 may be used to determine the deformation in grain B. With this in mind, a Newton method was employed to update the velocity gradient in grain A, \( L^A \), by solving the following system of three equations:

\[ \begin{aligned}
\left[ \frac{d\sigma_{13}^3}{dL_{j3}^3} + \frac{d\sigma_{23}^3}{dL_{j3}^3} \right] \{\Delta L_{j3}^3\} & = \left\{ \sigma_{13}^B - \sigma_{13}^A \right\} \\
\end{aligned} \]  

(3.78)

which essentially enforces equilibrium on the interface. After determining the increment in the velocity gradient, the updated velocity gradients of each grain can be obtained by rotating back to the lab-frame:

\[ L_{ij}^A = R_{ki}^3 \hat{R}_{lj}^3 \left( L_{kl}^3 + \Delta L_{kl}^3 \right) \]

\[ L_{ij}^B = R_{ki}^3 \hat{R}_{lj}^3 \left( L_{kl}^3 - \Delta L_{kl}^3 \right) \]

(3.79)

At convergence, local equilibrium at the bi-crystal interface and compatibility on both the local and global scale are enforced.

This model provides an estimate of the stresses near a grain boundary interface. The stress components that may act on the interface itself include the normal stress, \( \sigma_{33}^3 \), and the resolved shear stress:

\[ \tau_{3A} = \sqrt{\sigma_{13}^{3A} + \sigma_{23}^{3A} \left( \sigma_{33}^B - \sigma_{33}^A \right)} \]

(3.80)

Both of these stresses may act on the interface to promote grain-boundary delamination or other interfacial mechanisms. Because of the observed low ultimate shear stress on the elongated grain boundary interface in Al-Li alloys, the resolved shear stress is expected to be of particular importance. However, considering mechanisms similar to Findley fatigue damage parameter [147] or micro-crack mechanisms, a positive normal stress may also significantly contribute to the initiation of delamination. Utilizing a statistical
approach, the bi-crystal model may estimate the probability of potential interface stresses, and relate these stresses to a potential driving force for delamination.

### 3.8 Modeling Summary

A material model has been developed to estimate the state of stress at the grain boundary interface that is stipulated to provide a driving force for delamination. A statistical approach was chosen to highlight the influence of crystallographic orientation. The principle features of this modeling effort are concisely described below in some detail:

- The interest in cyclic deformation also influenced the choice of plasticity modeling, which couples the geometric contributions of crystal plasticity with stable kinematic hardening on independent slip systems. Rate insensitivity was stipulated to complement experimental evidence. This would potentially enhance localization phenomena in a spatially discretized application.

- Two simplified deformation models were employed, uniform deformation and bi-crystal models. While neither model accommodates localization phenomena, they provide statistically representative, orientation dependent, stress estimates at the grain interior and boundary.

- An implicit finite deformation scheme was adopted to accommodate potentially large deformations due to localized plastic behavior. This feature was not fully utilized due to other modeling constraints, namely employing the uniform deformation model rather than a spatially discretized method (i.e. FEM).

- Cubic anisotropy, large strain elasticity, and stress dependence were considered to describe the elastic deformation, due to the interest at small strains under stable cyclic deformation. Subsequent results indicate that these features are insignificant for the alloy under investigation.

- The current material model is amenable to discrete implementation including commercial Finite Element software, which would allow an investigation of localization phenomena.
4 Results and Discussion

The goal of this modeling effort is to estimate the stress state at grain boundaries due to local orientation mismatch. This stress state is hypothesized to be linked with the origin of the delamination phenomenon. In this chapter, the procedure for parameter determination is outlined and the proposed slip system material parameters are presented. The primary discussion begins with uniaxial cyclic behavior of the uniform deformation model, which is utilized to examine both bulk and local stress estimates, particularly components on the elongated grain boundary interface. A Findley-based shear-normal coupling is proposed for monotonic and cyclic loading to quantify potential damaging stress states. Next, the bi-crystal model is employed to statistically examine the effect of local grain misorientation as a driving force for the initiation of delamination. The chapter continues by examining the effect of changing texture, loading direction, and alternative macroscopic states of stress. The states of stress range from relatively uniform to those with a significant stress gradient, including: shear, plane strain, and near a crack tip.

4.1 Modeling Parameters

When determining the parameters of material models, tensile or compressive mechanical experiments are commonly utilized. Such experiments at the macro-scale (poly-crystals) may be employed to “tune” parameters on the micro-scale (single-crystals) through the use of a material model. In this investigation, the uniform deformation model is combined with the experimentally determined polycrystalline texture to estimate the deformation on the micro-scale. With the appropriate grain-based material parameters, the nominal behavior of the polycrystalline experiments is reproduced.

4.1.1 Anisotropic Elasticity

Cubic, stress-dependent, anisotropic elasticity was chosen to model the elastic behavior of the 2099-T81 plate under investigation. At a given temperature, this model requires 4 distinct parameters including the shear modulus, \( \mu \), bulk modulus, \( \kappa \), anisotropic modulus, \( \zeta \), and stress-dependent bulk modulus, \( \kappa^\sigma \). The relationship of the engineering stress to the elastic Green strain is described below:
\[
\frac{dS^e}{dE^e_{\text{tot}}} = 2\mu J^e + \left(3\kappa + 3\kappa_\text{e} \psi_{\text{e}} \right) J + \zeta R
\]  

(4.1)

A more detailed discussion of this model is provided in Appendix D.2.

Cyclic experiments in the L and T-directions of the three distinct textures (Edge, Transition, and Center) made up the majority of data available to determine the elastic parameters at temperatures ranging from -100°C to 100°C. However, these uniaxial experiments alone did not sufficiently decouple the shear and bulk modulus behavior. To distinguish the shear and bulk deformation, Poisson’s ratio (0.30) was measured in the T-direction with L-direction loading for the edge texture at room temperature. Since other experimental temperature and orientation measurements of Poisson’s ratio were not available, the value of 0.30 was assumed to be constant over the -100°C to 100°C temperature range where delaminations were observed. Poisson’s ratio for other textures and orientations were not directly imposed and are a byproduct of the parameter fitting process. These experiments are described in a previous section (Section 2.2.1).

At each temperature, the macroscopic measurements were utilized in a least squares regression to optimize the crystallographic elasticity parameters. The estimates of the uniaxial experiments took the following form:

\[
E = \frac{\Delta \sigma_{11}}{\Delta e'_{11}}
\]  

(4.2)

where the orientations utilized are representative of the corresponding material texture and loading direction, which is demarked by subscript 1. The value of Poisson’s ratio was modeled with the following relationship:

\[
\nu = -\frac{\Delta e'_{22}}{\Delta e'_{11}}.
\]  

(4.3)

It should be noted that both uniform strain and uniform stress estimates provided nearly identical results for the four material parameters under investigation, although uniform stress was assumed for the calculations presented.

The temperature dependence of each parameter is illustrated in Figure 4.1. Over the temperature range under investigation, linear temperature dependence was considered adequate to quantify the experimental trends. The shear modulus and bulk modulus are adequately described with a linear dependence with slopes of -10.8 MPa/K and -23.4
MPa/K respectively. The anisotropic modulus and stress-dependent bulk modulus show no clear temperature dependence and were chosen to be constant with values of \(-3725\) MPa and \(-16.98\) respectively. The anisotropic elastic parameters for pure aluminum at room temperature have been reported by Boas and MacKenzie in Hosford’s text [55]. The values \(\mu = 28300\) MPa, \(\kappa = 79850\) MPa, and \(\zeta = -10200\) MPa agree reasonably well with the values resulting from the fitting procedure.

![Graphs showing temperature dependence of various moduli.](image)

**Figure 4.1:** Temperature dependence of the a) shear b) bulk c) anisotropic and d) stress-dependent moduli.

The anisotropic modulus, \(\zeta\), found in this investigation is relatively small compared to the other moduli and even the one reported in the literature [55]. Because of this magnitude, the level of anisotropy in the elasticity is expected to be very small and likely negligible under most circumstances. If a material were to have a larger anisotropic modulus, the texture and orientation dependence of the elastic stiffness would increase, and anisotropic elasticity would display increased significance. The stress dependent bulk modulus, \(\kappa''\), is a large enough to have 1% impact on the bulk modulus...
for every 50 MPa of stress applied. The effect of elastic anisotropy and other elastic assumptions are quantified in Appendix D.3.

4.1.2 Independent Slip-System Plasticity

The material parameters chosen to represent slip resistance for independent slip system plastic deformation were discussed in Section 3.5. Experimental observations of hardening versus temperature and strain-rate have been presented in Sections 2.2-3. The experimental results indicate that a region of temperature / strain-rate insensitivity is appropriate within the temperature regime (−100°C to 100°C) where delaminations are prevalent. With this in mind, the plasticity parameters were chosen assuming them to be independent of temperature and strain-rate for the current investigation.

To adequately describe the hardening parameters, five distinct hardening slopes, which encompass five orders of magnitude, were chosen as ratios of the elastic shear modulus. Additionally, pseudo-hardening slopes of 1000 $\mu$ and $10^{-8}$ $\mu$ were employed to represent behavior before yield and after saturation respectively. These non-infinite and non-zero slopes were chosen for mathematical uniqueness purposes, as discussed in Section 3.5. Each of these hardening slopes is associated with a shear stress increment related to distinct strengthening obstacles. Various strengthening obstacles include solutes, precipitate structures, and forest dislocation interactions. Each period of shear hardening starts with a limited ability for dislocations to bypass a given type of obstacle. As the slip system stress increases, more bypassing occurs; but supply of additional dislocations exceeds the bypass rate, which results in hardening. Finally an equilibrium state between additional dislocation supply and dislocation bypass is achieved, and no further hardening is achieved from these obstacles is expected. This interpretation reflects the mathematical stipulation of each backstress strength, $r^{(i)}$ (Section 3.5).

Slip system parameters were chosen on the basis that the uniform deformation model (Section 3.7) provides a reasonable representation of the bulk deformation. It is recognized that employing a sophisticated optimization technique would have likely improved the experimental agreement, but the additional complexity and computational overhead were a sufficient deterrent. The resulting plasticity parameters and the shear stress-strain response of a single slip system are presented in Figure 4.2.
To illustrate that these parameters are representative of the material under investigation, uniform deformation simulations corresponding to uniaxial deformation of the three plate textures (edge, transition, and center) loaded in the L-direction are presented in Figure 4.3. By comparing the simulations (Figure 4.3b) with the experimental small strain monotonic and cyclic results (Figure 4.3a), it is evident that the magnitude of the simulation is significantly higher than the monotonic behavior (10-20% higher at 2% axial strain). This is a result of determining the plastic slip parameters based on the hardened cyclic behavior, which was limited to 0.75% strain. It should be noted that a larger average stress magnitude during uniaxial deformation was subsequently shown to result in lower damage values (Appendix E). This suggests that the currently chosen parameters (based on macroscopic cyclic performance) provide a lower estimate of the interfaces stresses and the associated driving force for delamination. It is also apparent that the model does not represent the experimental trends for all the textures and loading directions. One discrepancy is for the cyclic deformation, which shows the transition texture to be the strongest, rather than the center texture as the simulation suggests. This is attributed to the chemistry / precipitate differences evident at the center of the plate, from both the X-ray (Figure 2.3) and Auger experiments (Sections 2.1.1-3). Furthermore, these differences appear to be more pronounced during cyclic deformation, which suggests that the final stabilized microstructure differs from the initial microstructure. Macroscopically, the center region of the plate displayed less...
cyclic hardening than the other textures. Other factors that are ignored in this model are latent hardening and residual stress effects, which may be texture dependent. Modifying the current parameters is not expected to drastically improve model’s ability to represent these experimental trends and slight changes in these parameters will be investigated in a subsequent section. Nevertheless, useful observations and trends are extractable from the model.

Figure 4.3: The effect of texture on stress vs. strain for (a) monotonic and cyclic experimental results and (b) material model simulations

4.2 Single Crystal Behavior

Before discussing the current model’s implications for polycrystals, a brief investigation on single crystal deformation was conducted. It should be noted that the poly-crystal behavior is much more complex, but this exercise illustrates many trends that texture may introduce. The single crystal deformation includes the anisotropic elasticity (Figure 4.1) and FCC crystal plasticity with 12 potentially active slip systems (Section 3.5), using parameters from Figure 4.2. Only uniaxial deformation in the L-direction (1-direction) was considered for texture components presented in Table 2.4. Figure 4.4 illustrates the single crystal deformation of common texture components: Cube, Goss, Brass, Copper, and Taylor. As the figure illustrates, common single crystal deformation (stage I, II, and III) are not all reproduced with the current model. Only stage III (parabolic) deformation occurs, which is the result of the determination of material parameters from polycrystalline behavior, and the assumption of independent slip systems in the model. Modeling only stage III behavior is considered appropriate when multiple active slip systems dominate the plastic deformation, which is typical of
polycrystalline [86] and stable cyclic deformation. The material under investigation, 2099-T861, displays sub-granular strengthening mechanisms, which tend to minimize the contribution of stages I and II to the deformation.

![Figure 4.4: Single crystal stress vs. strain for common texture orientations](image)

The simulations in Figure 4.4 emphasize the importance of crystallographic orientation to the mechanical response. With the current modeling framework, the differences in axial stress for different crystallographic orientations mirror those reported in the literature [55]. For the loading chosen (L-direction uniaxial tension), the Cube is the softest, and the Copper orientation is the hardest. The Cube and Goss textures are expected to result in identical behavior because they only differ by a single rotation that is aligned with the loading direction (L-direction). Coincidentally, the range of internal crystallographic orientations bounds the bulk macroscopic deformation. It is the combination of these stress-strain differences and the boundary conditions applicable to a polycrystalline structure that will give rise to a driving force for delamination.

### 4.3 Uniform Deformation Model

To approximate the material behavior on a length scale much larger than the grain size, a uniform deformation model was utilized. This method trivially enforces compatibility between crystallographic orientations and is generally considered an upper bound estimate for maximum principal stress [109, 110]. In the context of delaminations, the orientation dependence of these local stress estimates may correlate with some critical grain misorientation. Although this method does not directly address grain-grain contact,
the overall influence of texture is enforced. Details of the uniform deformation model have been discussed in Section 3.7.

The primary purpose of the uniform deformation model is to provide an estimate of bulk polycrystalline stress-strain behavior from the grain-based material properties without the complexity of spatial discretization. For uniaxial tension, only one strain component and five stress components are specified on the macro-scale. Depending on the loading direction and texture, the uniform deformation model provides both the average axial stress response and the average strain components in the other directions. For clarity, consider room temperature uniaxial loading in the L-direction with edge ((t/8)) texture. The strain and stress components versus time are presented in Figure 4.5a-b. As expected, the only macro stress component that is non-zero is the axial component (LL). The remaining strain components (assuming orthotropic symmetry) show some variation from zero, especially in the normal, NN, and transverse, TT, directions due to the Poisson effect and plastic incompressibility. The material anisotropy is evident by comparing the TT and NN response, where the NN component is softer than the TT. This trend corresponds to the ovaling observed experimentally in large strain compression (Section 2.3.1). The corresponding axial (σLL) stress-strain response is presented in Figure 4.5c, illustrating the transition from elastic to plastic deformation for both the initial monotonic loading and subsequent cyclic behavior. Points A-J are labeled at regions of interest including: bulk elasticity (A, B), monotonic plasticity (C, D), elastic unloading (E, H), and cyclic plasticity (F, G, I, J), for subsequent discussion. It should be noted that the cyclic behavior is stable and points D and J are identical.

Figure 4.5: Uniaxial cyclic simulation in the L-direction of the edge texture illustrating (a) strain components versus time, (b) stress components versus time, and (c) axial stress versus strain.
In addition to the bulk polycrystalline response, stress-strain behavior for individual crystallographic orientations can be obtained from the uniform deformation model. An initial presentation of the local stress behavior will utilize a modification of Rodrigues space presented for texture analysis (Section 2.1.1.2). Instead of the intensity indicating relative likelihood of various texture components, the intensity is indicative of a chosen stress component relative to the depicted crystallographic orientation in Rodrigues space [35, 148]. Figure 4.6 displays the axial stress, $\sigma_{LL}$, in Rodrigues space for the L-direction cyclic simulation of the edge texture. Points A-J correspond to the macroscopic stress-strain points introduced in Figure 4.5. Points that only deform elastically, such as initial loading (A-B) or unloading (D-E and G-H), show very little change in the orientation dependence of the axial stress intensity. Only the magnitude of stress changes significantly at these points. This observation reinforces the critical role of plastic deformation to the development of relatively high stresses for “hard” orientations. By comparing the tensile reversal point (D, J) and the compressive reversal point (G), one notices that they have inverted color schemes, due to the sign change in the axial stress. If only the magnitude of stress were considered, then the orientation dependence is identical for the two endpoints. In other words, the “hard” orientations in tension (red at Point D) correspond to “hard” orientations in compression (blue at Point G).

The axial stress results may also be presented in a statistical format, which was previously considered by utilizing the average to represent the bulk deformation. The statistical analysis of the axial stress, $\sigma_{LL}$, is presented for the L-direction cyclic simulation of the edge texture in Figure 4.7a-b. As before, points A-J correspond to those previously defined. Figure 4.7a illustrates the cumulative probability with respect to axial stress and Figure 4.7b illustrates the corresponding histogram, or the derivative of probability with respect to axial stress. No probability density function has been assumed or should be implied for this representation. The results indicate that there is much less statistical variation in the elastic regime (Points A, B) than after bulk plastic deformation occurs. The statistical variation increases as more plastic deformation occurs (Points C, D), resulting in an axial stress range of 450 to 600 MPa at the reversal point. The cumulative probability illustrates that the highest stress range (575-600 MPa) is still relatively common, occurring for approximately 15% of the orientations that characterize
the texture. Elastic unloading from the reversal point (Points D-E and G-H) shows significant changes in stress magnitude, but the stress range (150 MPa) remains constant. This supports the observation inferred with the Rodrigues space, which suggests purely elastic deformation has much less affect on the orientation stress dependence than bulk plastic flow. The statistical presentation (Figure 4.7) at the tensile reversal points (D, J) and the compressive reversal point (G) show a mirrored trend, similar to the observations inferred from Figure 4.6.

Figure 4.6: Axial stress in Rodrigues space of the L-direction cyclic simulation for the edge texture demarking points A-J.
Although the axial stress of the current simulation (L-direction uniaxial cycling of the edge texture) is the only non-zero component on average, other stress-states are potentially useful on the grain scale. The ensuing discussion will focus on stresses resolved on the elongated grain boundary interface. The method of resolving the stress components on the elongated grain boundary interface was described previously in the bicrystal modeling section (Section 3.8). For the material under investigation, the grain boundary interface is on the N-plane; thus the normal stress is described by, $\sigma_{NN}$, and the shear stress resolved on the grain-boundary is described by:

$$\tau = \sqrt{\sigma_{LN}^2 + \sigma_{TN}^2}.$$  \hfill (4.4)

This shear definition is appropriate for single point considerations; however, direction may be significant for cyclic loading, particularly for non-proportional loading.

First consider the normal stress, whose tensile strength was experimentally measured to be relatively strong (~500 MPa). Figure 4.8 illustrates this normal stress in Rodrigues space and statistically. Both the orientation and statistical dependence are direction dependent as their sign inverts for the compressive vs. tensile endpoints. The normal stress does not change during elastic unloading (points D-E and G-H), as the average remains constant (zero) and the range depends on prior plastic deformation. For the cyclic range considered (±1% strain), the normal stress varies from ±130 MPa. Only the positive stresses are likely to contribute to the damage associated with subsequent delamination. With this interpretation, the Shear1-cube orientations (center of N-face to the origin) is the most damaging during tension and the P-orientation (center of T-face) is
most damaging during compression. Both these critical orientation regimes correspond to relatively low magnitude axial stresses (Figure 4.6), or “soft” axial grains. This observation suggests that grains with the highest axial stresses are not those most likely to have high grain boundary normal stresses. It should be noted that the monotonic tensile strength is approximately four times larger than the largest normal stress observed at 1% strain, which is a loading where cyclic delaminations were observed. Therefore, the normal stresses alone do not drive delamination failure.

Figure 4.8: Grain-boundary normal stress of the L-direction cyclic simulation for the edge texture illustrating Rodrigues space (points D and G), the cumulative probability and histogram with demarcated points A-J

The resolved shear stress at the grain boundary interface is defined without directional specification and is strictly a magnitude representation as described in Eq. 4.4. Figure 4.9 illustrates both the Rodrigues space at the endpoints (D and G) and the statistical representation at all time points (A-J). The resolved shear stress’s orientation dependence is not significantly affected by tension or compression. There is a noticeable difference in maximum stress from point D to G, which is attributed to texture asymmetry and a very slight asymmetry of the applied loading (1% vs. -0.99% strain). The statistical character of the shear stress indicates a fairly uniformly distribution,
showing equal probability of grains with low shear stresses (< 50 MPa) to those with high shear stresses (> 50 MPa). The maximum shear stress (~105 MPa) is on the same order of magnitude as the maximum normal stress (~130 MPa). However, since the shear strength (225 MPa) is much weaker than the normal strength (500 MPa), the shear stress is expected to dominate the damage leading to delamination. It is also significant to notice that the “hard” orientations in resolved shear stress (Brass-like corners) do not correspond to either the “hard” axial orientations or the “hard” normal stress orientations. This emphasizes that an appropriate critical stress choice must be utilized to adequately determine the critical orientations for delamination.

Damage leading to delamination is likely composed of contributions from both positive normal stress and resolved shear stresses at the grain boundary interface. It is likely that grains exhibiting both a positive normal stress and a relatively large shear stress will be the most damaging and a potentially critical orientation for the initiation of delamination. A 3D-histogram representing the likelihood of both shear and normal components at both endpoints (D and G) is presented in Figure 4.10. First it should be
recognized that the instances of the high normal stresses (100-130 MPa) correspond to relatively low shear stresses (< 50 MPa) for both endpoints. The compressive endpoint (G) displays higher tensile normal stresses than the tensile endpoint (D). However, point D has a greater probability of tensile normal stresses than point G due to the skew nature of the normal stress distribution (Figure 4.8). No particularly striking trends are clear in the shear stress distribution, as a relatively uniform distribution was previously observed for its character (Figure 4.9).

![Shear-normal stress histogram of the L-direction cyclic simulation for the edge texture illustrating points D and G](image)

**Figure 4.10: Shear-normal stress histogram of the L-direction cyclic simulation for the edge texture illustrating points D and G**

To relate the stresses on the grain boundary interface to eventual delamination initiation, shear-normal stress coupling is expected to be significant. In particular, a positive normal stress is expected to enhance the damage done by the cyclic shear stress. To account for such coupling, a Findley [147, 149], type damage parameter was considered. The classic Findley parameter is shown below:

\[
D_f = \Delta \tau + \alpha_f \sigma_n^{\text{max}},
\]

(4.5)
which relates cyclic fatigue damage to a linear combination of the cyclic shear stress amplitude, $\Delta \tau$ and the maximum normal stress, $\sigma_n^{\text{max}}$, on a critical plane. In the current investigation the critical plane is assumed to be the known delamination plane (N-plane). This assertion simplifies the calculation of both the shear stress amplitude and maximum normal stress. Specifically, the shear stress amplitude and maximum normal stress may be determined from the expressions:

$$\Delta \tau = \sqrt{\left(\tau_{L^N}^A - \tau_{L^N}^B\right)^2 + \left(\tau_{T^N}^A - \tau_{T^N}^B\right)^2},$$

$$\sigma_n^{\text{max}} = \max\left[\sigma_{NN}^A, \sigma_{NN}^B\right],$$

where $A$ and $B$ refer to the cycle’s endpoints. The parameters $D_f$ and $\alpha_f$ are typically determined experimentally for a given life; however, in this investigation sufficient fatigue experiments are not readily available. Instead, consider the monotonic strength measurements in shear (225 MPa) and N-direction tension (500 MPa) to estimate the coupling parameter, $\alpha_f$, from their ratio:

$$\alpha_f = \frac{\tau_{\text{crit}}}{\sigma_{n_{\text{crit}}}} = \frac{225}{500} = 0.45.$$

Although this is a crude estimate, it is close to that implemented in previous work studying the delamination process ($\alpha_f = 0.5$) [6]. It should be noted that a lower value of this coupling parameter may be anticipated for fatigue behavior, but was not considered as shear stress dominates the behavior even with this ratio. Furthermore, if damage were to include local stress behavior at grain boundaries, then both experiments likely include shear-normal coupling. In other words, the N-direction uniaxial tension test likely has a significant shear stress component, and similarly the interface shear strength test likely has a normal stress contribution to damage.

Because only relative damage estimates, based on crystallographic misorientation, are of interest, the damage parameter, $D_f$, is not strictly specified. However, using the experimental results as a guide, both monotonic and cyclic estimates may be forwarded for the sake of discussion. For monotonic behavior, the interface shear strength and N-tension experiments suggest a critical value around 225 MPa (ignoring experimental coupling). In contrast, using the $R = -1$ torsion cyclic experiment (again neglecting any normal stress contribution), a shear range of 600 MPa resulted in delamination in less
than 100 cycles (Figure 2.42). This difference between monotonic and cyclic damage behavior is attributed to cyclic hardening, the adoption of a range-based format (which results in as much as 2x the magnitude of the monotonic case), experimental shear-normal coupling, and statistical variation. Since cyclic deformation is of primary interest in this investigation, the later estimate is likely more appropriate for the ensuing discussion. It may be supposed that a damage values near 600 MPa would take around 100 cycles to initiate delamination. Higher damages would delaminate with even fewer cycles and a lower magnitude may still cause subsequent delaminate, but in more cycles. The damage parameter likely has a minimum value to initiate delamination, as was evident from the experiments. If one considers the R = 0 cyclic torsion experiment that resulted in no delamination as a guide (Figure 2.40), a minimum damage threshold value of 150 MPa is an appropriate lower bound for cyclic loading.

Returning to the L-direction uniaxial cycling of the edge texture presented throughout this section, the Findley based damage parameter may be determined for cyclic deformation at various reversal endpoints. The Rodrigues space and statistical representation of this damage parameter are presented in Figure 4.11 for fully reversed loading with endpoints corresponding to points B, C, and D. First consider cyclic point D, where both the Rodrigues space and statistical representations closely follow the previously presented shear stress component (Figure 4.9). This similarity emphasizes the significance of the shear stress on the delamination interface. The most notable differences are the magnitude, which is roughly double that of the shear stress, and the increased likelihood of larger values. The Rodrigues space shows only slight deviation from the shear stress alone, where again a corner orientation (similar to brass) shows the largest damage. As X-ray results illustrate (Figure 2.10), this texture component is present in this material.

The Findley-based damage parameter is also presented for cyclic reversal points before bulk plastic deformation (Point B) and after moderate plasticity (Point C) in Figure 4.11. The stress response of cycling in the elastic regime (Point B) shows very little ‘damage’ at the grain boundary interface, with less than 10 MPa or 5% of the damage threshold for nearly all orientations. This model characteristic supports the experimental observation that noticeable bulk plastic deformation is required to promote
delamination failures. In contrast, the simulation after moderate plasticity (Point C) displays significantly larger ‘damage’, with values exceeding 95 MPa, or nearly ten times more damaging than the elastic case (Point B). The reversal at 1% strain (Point D) displayed twice as much ‘damage’ as the reversal at Point C.

![Figure 4.11: Findley based damage parameter for symmetric L-direction cyclic loading reversed at Points B, C, and D for the edge texture](image)

The Findley-based damage is displayed versus the axial strain in Figure 4.12 for various cumulative probabilities (max, 99%, 90%, 70%, and 50%) of the L-direction, Edge texture, uniform deformation simulation. The transition from nominal elastic to plastic deformation is evident in this presentation, showing a distinct increase in the slope of the damage parameter after 0.5% strain. This trend emphasizes the importance of
plastic deformation on the accumulation of damage leading toward delamination. It should be noted that this trend is also apparent for both the normal and resolved shear stress components. The probability threshold does not change this elastic-plastic trend and simply lowers the damage-strain slope for decreasing probability percentage.

Figure 4.12: Damage at various percentages versus axial strain for L-direction fully-reversed cyclic loading using the uniform deformation model

4.4 Bi-Crystal Deformation Model

To consider specific neighboring grain orientations in the investigation of delamination, the bi-crystal model was employed. Each bi-crystal consists of a pair of crystallographic orientations whose grain boundary is initially aligned with the N-plane normal. The orientations were chosen based on a random sampling of the representative ‘bulk’ texture (Edge, Transition, or Center). To avoid extensive computational overhead and maintain compatibility on length scales ranging from the orientation pairs to the bulk material response, the uniform deformation model was utilized to determine the displacement boundary conditions. These boundary conditions trivially maintain compatibility everywhere and are anticipated to maintain the upper bound features of the uniform deformation model. However, since the grain boundary interface was stipulated to be in equilibrium by ensuring equal interface stresses ($\sigma_{NN}$ and $\tau$) at the orientation interface, stresses are expected to decrease in magnitude (on average) compared to the uniform deformation model. For more specific details on the bi-crystal model, refer to Section 3.7 in the text.

Much like the uniform deformation model, the results from the bi-crystal model may be represented utilizing either Rodrigues space or statistics for various
measurements, which include the normal stress, $\sigma_{NN}$, the resolved shear stress, $\tau$, and the Findley-based damage parameter, $D_f$. In this analysis, the Rodrigues space representation is restricted to specific grain pairs (i.e. Cube, Shear1, and Brass pairing illustrated in Figure 4.13). The location of the Cube and Shear1 orientation are depicted in the figure with a black square and triangle respectively. Such a representation requires one orientation to be specified, while the other is uniquely presented in Rodrigues space. Alternatively, one could choose to illustrate the stress differences for specific grain-pair misorientations. However, misorientation space is not unique, where multiple stress states are expected for identical misorientations. This behavior is clearly forwarded by the uniform deformation model, where multiple stress values are observed for equivalent misorientations, which are all trivially equal to the identity.

Perhaps the most appropriate representation for the results of the bi-crystal model is through the use of statistics. Unlike the Rodrigues space, a statistical representation of the interface behavior (stress or damage) may be collectively interpreted without restriction. As with the uniform deformation model, both the cumulative probability and its derivative with respect to the selected parameter are considered (see Figure 4.13). The statistical approach is limited by the intrinsic modeling assumptions (i.e. uniform deformation boundary conditions, N-plane grain boundary orientation) and the randomly sampled pairing assumption adopted in this investigation. For each simulation 10,000 grain-pairs were chosen from the 1,000 representative orientations stipulated by the X-ray experimental results. This number of grain-pairs was deemed sufficient to obtain statistically significant and sufficiently representative results. Beausir has suggested that an improved statistical representation may be achieved by considering the material’s grain misorientation distribution to select the grain-pairs [150].

First consider the normal stress results from the cyclic uniaxial loading of the edge texture in the L-direction. A few specific grain-pairings were chosen to represent the orientation dependence in Rodrigues space. Specifically, Figure 4.13 illustrates the results of Cube, Shear1, and Brass orientation pairings. As shown, the influence of orientation appears to be independent of the specific adjacent orientation pair, indicating that misorientation is not driving large changes in normal stress. All cases show a maximum normal stress at the L and N-faces and a minimum normal stress at the T-face,
as is consistent with uniform deformation model results. In contrast, the magnitude of normal stress is very dependent on the adjacent orientation pair. For the tensile loading up to 1% strain, the Shear1 pairing is the largest followed by Cube and Brass pairings. This trend mirrors the uniform deformation model, where the Shear1 orientation resulted in the highest normal stress. For cyclic loading, the sign of these magnitudes invert, making the T-face of the Brass-Pairs most damaging.

The statistical representation of the bi-crystal normal stress is compared to the uniform deformation model results in Figure 4.13. As expected from the uniform deformation upper bound property, the bi-crystal model results in slightly lower normal stress magnitudes. Nevertheless, the overall trend between the two models is very similar, rarely deviating by more than 20 MPa. This observation indicates that the normal stress resulting from specifying orientation pairs is a consequence of each orientation’s independent normal stress character. This relatively weak coupling is attributed to the unidirectional property of the normal stress, and suggests that an averaging scheme to predict normal stresses of bi-crystal pairings may be appropriate.

![Figure 4.13: Bi-crystal results for uniaxial cyclic loading of the Edge texture in the T-direction illustrating the normal stress, $\sigma_{NN}$, with Cube, Shear1, and Brass pairs in Rodrigues space and a comparison of the statistical results with the uniform deformation model](image)
Figure 4.14: Bi-crystal results for uniaxial cyclic loading of the Edge texture in the T-direction illustrating the resolved shear stress, $\tau$, with Cube, Shear1, and Brass pairs in Rodrigues space and a comparison of the statistical results with the uniform deformation model.

The shear stress resolved on the grain boundary interface is presented in Rodrigues space (Cube, Shear1, and Brass pairs) and statistically in Figure 4.14. Much like the normal stress case, the orientation dependence is very similar to the uniform deformation results, where only the ranges differ for the three specified pairings. The magnitude of shear stress follows the same trend as the uniform deformation model (Brass > Shear1 > Cube), but unlike the normal stress, the differences are clearly not proportional. The overall statistical representation illustrates that the bi-crystal resolved shear stress is much lower (on average) than the uniform deformation model predicts. This characteristic is expected, based on the uniform deformation model’s upper bound character and increased constraint. However, the sensitivity to the resolved shear stress direction also contributes to this drop, which was not the case for the normal stress. In contrast, the peak shear stress is very similar for both cases, and they would be identical if millions of grain pairings were simulated. For the case presented in Figure 4.14, the shear stress exceeds 60 MPa only 5% of the time for the bi-crystal model, but 35% of the time for the uniform deformation. The differences in the statistics imply that the uniform deformation model predicts more grains with high shear stress than the bi-crystal model.
Figure 4.15: Bi-crystal results for uniaxial cyclic loading of the Edge texture in the T-direction illustrating the damage parameter, $D_f$, with Cube, Shear1, and Brass pairs in Rodrigues space and a comparison of the statistical results with the uniform deformation model

The Findley-based damage parameter results are presented in Figure 4.15 for the same bi-crystal simulation previously presented with respect to the normal stress (Figure 4.13) and shear stress (Figure 4.14). For the most part, the orientation dependence and comparison with the uniform deformation model closely follows the trends presented from the shear stress alone. One slight deviation is the orientations subtle sensitivity to specific orientation pairings. Specifically, the Cube, Shear1, and Brass pairs show minor differences that were not evident from either the normal or shear stress representations alone. This sensitivity is attributed to the combination of these features and the non-linearity of their relative magnitudes. On the other hand, the maximum damage parameter is approximately the same for both cases ($\sim 225$ MPa), and corresponds to approximately 3/5 of the critical cyclic damage for failure in less than 100 cycles observed from experiments ($\sim 600$ MPa). This ratio is reasonable considering that the uniaxial experiments delaminated after approximately 5,000 cycles. The lower frequency of high damage pairings suggests that imminent delamination will be less frequent than the uniform deformation model indicates. For example, if one were to consider a critical threshold at 150 MPa ($\sim 70\%$ of $D_f^{\text{max}}$), the bi-crystal model predicts only 5\% of pairings
will exceed this value, whereas the uniform deformation model predicts 30%. For the typical L-direction cyclic experiment, there are approximately 500 grains through the cross-section. After cyclic failure, 3-5 delaminations were commonly observed (Figure 2.30), which is about 1% of the grain boundary interfaces. Hence, the bi-crystal model’s statistics are likely more realistic than the uniform deformation model because they suggest very damaging grain boundary pairs only 1-2% of the time.

Non-linearity of the damage parameter, with regard to the axial strain, is presented in Figure 4.16. The maximum threshold and the trend of increasing slope after bulk plastic deformation (~0.5% strain) is very similar to the uniform deformation model (Figure 4.12). Lower percentages of the damage parameter probability are much lower than the uniform deformation model. For instance, the 90% bi-crystal threshold is very similar to 50% of the uniform deformation model. As before, the elastic-plastic transition increases the accumulation of damage with respect to the applied uniaxial strain. However, this trend is increasingly subtle for lower probability percentages. Nevertheless, the damage relationship to axial strain remains consistent with other observations of the bi-crystal model.

![Figure 4.16: Damage at various percentages versus axial strain for L-direction fully-reversed cyclic loading using the bi-crystal model](image)

As previously noted, a distinct advantage of the bi-crystal model is the ability to query the most damaging pairs of a statistically representative set of pairings. Figure 4.17 illustrates the 100 most damaging pairs, which represent the top 1% of pairs most likely to delaminate. These damage values correspond to the upper plateau of the cumulative probability in Figure 4.15. In Figure 4.17, each symbol appears twice, once for each
grain pair, where blue represent the top 0.1% and red the instances between 0.9-1% (other colors are intermediate probabilities). It should be noted that some of the most damaging pairs are often relatively close in orientation, which is a consequence of the uniform deformation assumption, and the texture representation. In general, S-like orientations (just inside the missing corners) most frequently occur as part of the critical pairings. These observations are consistent with those observed by Tayon et. al. [53], whom studied crystallographic orientations in the proximity of delaminations caused by a crack-tip field.

![Diagram](image)

**Figure 4.17:** The 1% most damaging Bi-crystal pairs (100 pairs) presented in Rodrigues space for cyclic loading of the Edge texture in the T-direction

The ability of the bi-crystal model to query specific orientation pairs was utilized to compare damage parameter of random combination with specific choices determined from EBSD experimental results. Recall the EBSD experimental investigation of cyclic uniaxial delaminated fracture surfaces (Section 2.2.1.3). The cumulative probability of L-direction uniaxial fully reversed deformation of the Transition texture is illustrated in
Figure 4.18. A set of three specific grain pairings, determined from the EBSD results in Figure 2.35, are also illustrated. Specifically, the grain pairs are demarked as follows: A) closest to the fracture surface (bottom) of the low magnification image, B) Further up the same delamination where the grain on the right-hand-side appears to have a thin sub-grain orientation, and C) the tip of another smaller delamination from the high magnification image that was measured elsewhere on the same specimen. All three of these orientation pairs showed relatively large damage parameters, greater than 75% of the probable combinations representative of the texture. Furthermore, the orientation pair A shows very high damage, in the 98% percentile of the probable grain pairing. Although this impressive correlation is somewhat surprising, it is not unexpected very near the fracture surface. A uniaxial cyclic experiment provides a substantial statistical sampling of potential grain pairings where delamination may initiate. For the experiment considered, as many as 10,000 grains are present within the specimen’s gage section, resulting in more than 30,000 grain-pairs with interfaces in the N-direction. In contrast other delamination tests (such as torsion, fracture, and shear tests) provide inferior statistics for experimentally measuring critical grain pairs due to their inherent large stress gradients.

Figure 4.18: Cumulative probability vs. the damage parameter for L-Direction uniaxial cycling of the transition texture (1% max), with grain pairs corresponding to the EBSD investigation (Figure 2.35)
Although the bi-crystal model provides a more complete avenue toward predicting stresses at the grain boundary interface, the previous presentation indicates that the uniform deformation model illustrates many trends with significant computational savings. Specifically, the uniform deformation model is more amenable to illustrate the orientation dependence through the use of Rodrigues space, without the complexity of stipulating a specific orientation for one of the pairs. Furthermore, the orientation dependence is consistent with that observed for the bi-crystal model, where only the statistical distribution is significantly different. The maximum magnitude of the normal stress, \( \sigma_{NN} \), the resolved shear stress, \( \tau \), and the Findley-based damage parameter, \( D_f \), are similar for both models. While the uniform deformation model can identify a critical grain orientation, only the bi-crystal model can ascertain the critical orientation pairings. Despite this critical advantage, the uniform deformation model’s computational efficiency and overall mirroring of trends make it more amenable to investigate many of the modeling nuances.

4.5 Bulk Texture and Loading Direction

Much of the previous discussion has been limited to L-direction uniaxial cyclic loading of the Edge texture. However, experimental results suggest that delamination may be significant in other loading cases with varying texture and directions. In this investigation, the effect of texture for uniaxial loading on the current model is studied by considering the three characteristic plate regimes (Edge, Transition, and Center) observed through X-ray diffraction (Section 2.1). The modeling results are compared with each other and experimental results to determine if the model is appropriately reproducing the desired trends. Both macroscopic axial stress-strain behavior and local grain boundary interface values (normal stress, resolved shear stress, and damage) are included to determine the effect of texture and loading direction on macroscopic behavior, crystallographic orientation, and statistical variation.

Figure 4.19 illustrates the macroscopic uniaxial stress-strain response of the uniform deformation model for each texture and loading direction considered in this investigation. If one compares the effect of texture for a given loading direction, then the axial stress at a given strain changes with texture as follows: Edge < Transition < Center.
The stress differences are commonly 5-15% different (at 1% axial strain), with the L-direction being the most sensitive and the N-direction the least. The hardening differences are subtle, where distinguishable differences are only apparent for the N-direction. It should be emphasized that the observed effect of texture is consistent with the experimental observations from larger strain compression tests (Figures 2.48-2.50) and tension tests (Figure 2.62) at approximately 1% strain. This trend was also observed for the initial yield behavior (plastic hardening $> E$) as illustrated in Figures 2.30-2.32. However, the stable cyclic deformation at 1% strain does not follow the model’s texture dependence (Edge $< \text{Transition} < \text{Center}$). Specifically, the Center texture was experimentally observed to result in lower axial stresses at 1% strain than both the Edge and Transition textures. Recall that the center of the plate is associated with a change in plate chemistry (Figure 2.3), which may account for this modeling discrepancy. Furthermore, this difference suggests that cyclic deformation emphasizes the subtle changes that are related to the hardening mechanisms in this material. It may be concluded that such mechanism changes would require adjustments to the modeling effort beyond simply changing the texture (or the orientation distribution function).

Next consider the effect of loading direction on the macroscopic response of the current model for each texture. Figure 4.19 illustrates that loading direction results in the following trend on the macroscopic axial stress for a 1% strain: $N < T < L$. The N-direction is typically 5-10% lower (in axial stress at 1% strain) than either the L or T-directions. L and T-directions are only significantly different for the Center texture, where L is 5% higher than T. As before, the direction appears to only subtly change the hardening character (shape of stress-plastic strain response), with the N-direction trending toward saturation more quickly than L or T-directions. Also, the effect of loading direction is consistent with the large strain compression and tension testing results discussed previously. Additionally, the directional dependence on the modeling behavior is consistent with the cyclic response. However, it should be emphasized that L and T-directions are very similar in both modeling and experiment and the N-direction was not experimentally investigated under cyclic deformation. The consistent correlation of the directional dependence with experiments is somewhat surprising considering that the grain aspect ratio is not considered in the uniform deformation model. This
emphasizes the greater significance of the grain orientation rather than its aspect ratio, at least for the macroscopic stress-strain response.

The local orientation dependent grain boundary components (normal stress, resolved shear stress, and damage) are useful to distinguish which grain orientations will most likely lead to delamination and their relative probability. Texture and loading direction dependence of local properties will highlight potential changes in both the critical orientation and the relative frequency of potentially damaging orientations. Unlike the macroscopic stress-strain behavior, the local behavior cannot be directly compared with the available experimental results. Instead, only relative information is obtained and comparison to other simulations and observations of delamination are discussed.

A summary of the normal stress component is presented in Figure 4.20. Nine potential combinations of the three textures (Edge, Transition, and Center) and three uniaxial loading directions (L, T, and N) are included to compare both the orientation dependence (Rodrigues space) and probability. As illustrated by the Rodrigues space representation, the texture has a small affect on the most damaging orientation. This is expected since the texture does not significantly change the macroscopic strain (or applied uniform deformation). Some slight deviation to this trend is illustrated for the Center texture. However, this texture is highly concentrated near the missing corners.
(Figure 2.10), and limited orientation information is available for the other locations. The effect of texture on the magnitude of normal stress is clearly texture dependent with changes on the order of 20% commonly observed for 1% axial strain. Furthermore, texture dependence consistently displays the following trend: Center < Transition < Edge. This trend is opposite of the macroscopic results and reiterates that the normal stress magnitude tends to increase for decreasing axial stress with constant applied uniform deformation.

Figure 4.20: Texture and Direction dependence of uniaxial cyclic loading (peak at 1% strain) of the normal stress, $\sigma_{NN}$, illustrating the Rodrigues space and statistics
Unlike the relatively subtle differences observed by changing the texture, the loading direction (in Figure 4.20) shows a significantly different sensitivity, particularly in the N-direction. For instance, the orientation dependence changes significantly with changing loading direction. Specifically, the L and T-directions show large compressive normal stresses on the T and L-faces respectively and large tensile normal stress on the N-face. In contrast, the N-direction loading shows maximum stresses on the edges between L and T-faces with minimum stresses on the N-face. It should be noted that for symmetric cyclic loading, the tensile and compressive character of the L and T-directions reverses, but the magnitude of normal stress for N-direction loading does not change. The magnitude of normal stress is relatively insensitive to the L and T-directions, but is much higher for the N-direction. This behavior is not surprising since loading in the N-direction does not require the average normal stress to be zero, as is stipulated for L and T-directions. This difference causes the N-direction loading to result in normal stresses centered at the macroscopic stress-strain response at 1% axial strain (or ~500 MPa). In other words, the magnitude and statistics of the N-direction sensitivity should be treated separately from the L and T-directions. Consequentially, the effect of loading direction on the normal stress appears to be more significant than the effect of changing texture.

A corresponding presentation is available in Figure 4.21 for the shear stress resolved on the elongated grain boundaries. This representation shows many of the same trends as the normal stress case. Specifically, the effect of texture again follows the opposite trend of the macroscopic axial stress (Center < Transition < Edge). Also, changing the texture does not change the orientation dependence (Rodrigues space) except for the Center texture, which again has limited orientation statistical variability. The orientation dependence is very sensitive to the loading direction and the N-direction again appears to have special characteristics. Despite these similarities, the resolved shear stress displays several unique features relevant to the delamination process. In particular, the orientation dependence appears to be minimal near cube and is most critical near the removed corners (brass-like) for all loading directions and textures. The magnitude of shear stress, which does not change for cyclic behavior, is much more sensitive than the normal stress, varying by as much as 50 MPa or 50% of the maximum value. Furthermore, the effect on the resolved shear stress magnitude from changes in
loading direction displays a clear trend: N < T < L, which happens to show the same trend as the macroscopic results. Interestingly, the effect of texture on the resolved shear stress shows the opposite trend of the macroscopic stress-strain results. This observation differs with the inverse relationship to the macroscopic axial behavior that dominated the normal stress results.

Figure 4.21: Texture and Direction dependence of uniaxial cyclic loading (peak at 1% strain) of the resolved shear stress, \( \tau \), illustrating the Rodrigues space and statistical representation
Finally, consider a combination of the normal and shear stress components with a Findley-based damage parameter, as illustrated in Figure 4.22. As for the normal and shear stresses, the results are most easily categorized into two groups: L and T-direction and the N-direction. For the L and T-directions, the damage behavior closely mirrors the resolved shear stress, as is expected when shear stresses are relatively high. Both the trends of texture (Center < Transition < Edge) and loading direction (T < L) correlate well with the delamination observations from cyclic experiments (Figures 2.30-2.32).
Furthermore, the magnitude of maximum damage is approximately 225 MPa, as was stipulated previously for the L-edge case. In contrast, the N-direction more closely mirrors the behavior of the normal stress. This indicates that the normal stress in the N-direction is the primary driving force for subsequent delamination, or in this case mode I crack initiation. The N-direction loading mirrors the general trend in texture for the maximum damage (Center < Transition < Edge). This trend does not match the experimental tendency for failures to occur at the center of the plate during N-direction tensile loading (Figure 2.61). However, the simulation’s trend inverts at probabilities less than 50%. Additionally, the Center texture may decrease the normal strength due to the subtle change in chemistry. Another interesting result that is apparent from the N-direction simulation involves the shear-normal coupling previously established. Recall that the shear-normal stress coupling were determined assuming no shear stress during N-direction axial loading, and no normal stress during pure nominal shear loading. These simulations indicate that the effect of normal stress was likely over-estimated from the nominal N-direction tensile experiment. As the simulation indicates, significant resolved shear stress is present during nominal N-direction uniaxial deformation. This suggests one should account for these potential shear stresses during the determination of the normal stress ratio. However, direction measurement of these shear stresses is quite difficult and was not attempted in this investigation. Alternatively, the current modeling effort (N-direction bulk uniaxial loading) could provide an avenue toward improving the proposed shear-normal coupling. However, such an avenue toward representing damage was not employed in the current investigation.

4.6 Shear Deformation

In this section consider the effect of an alternative nominal deformation, simple shear. In this case, the nominal stress was enforced to be composed of only one shear component (either LT, LN, or TN) while all other components were required to be zero (on average). The uniform deformation model was utilized to determine the deformation up to 1% engineering shear strain (\(\gamma\)). It should be noted that applying both symmetric and skewed uniform shear deformation was also investigated with remarkably similar results. The nominal shear stress-strain relationship of the Edge texture is illustrated in Figure 4.23 for each shearing direction: LT, LN, and TN. The nominal shear stress is
directionally dependent showing the following trend: LT < LN < TN, where as much as 20 MPa difference is observed on the macroscopic trend at 1% shear strain. The shear stress-strain behavior is very similar to the Nadai approximations [68] from the torsion experiments (Figure 2.42), although with slightly higher stresses, similar to the difference observed for uniaxial deformation (Figure 4.3). The shear stress magnitudes are considerably higher than the maximum values measured from the interface shear strength experiments (Figure 2.66), so it is expected that the predicted damage parameters will be relatively large. The grain-pairing statistics for the two experiments and relative texture dependence are not equivalent. Specifically, the torsion experiment is subjected to significant averaging of loading direction and variations in texture, where as the shear strength experiment was measuring shear in a single direction (LN or NL) of relatively few grain pairings. Several other nuances may have contributed to this apparent discrepancy. For instance, the interface shear strength experiments included a macroscopic normal stress based on FEM simulation [77], which was not reported previously. Also, the torsion experiments did not fail catastrophically like the interface shear strength tests due to the adjacent elastic core, which may contribute to over estimating the torsional shear strength.

![Macroscopic shear stress versus shear strain for each shear direction for the Edge texture](image)

**Figure 4.23:** Macroscopic shear stress versus shear strain for each shear direction for the Edge texture.

The Rodrigues space and probability of the normal stress component is presented in Figure 4.24 for each shear direction. The orientation dependence is very different from the uniaxial deformation. Specifically, larger normal stress magnitudes (either positive or
negative) are observed for rotations about the face perpendicular to both the shear direction and plane from a cube orientation. For example, the rotations about the L-direction result in positive normal stress for TN shear. The statistical character of the shear stress has many expected attributes, including that both the average and most frequent normal stress are zero. Furthermore, the distribution of normal stresses is symmetric around the origin where the maximum values are direction dependent following the same trend as the nominal behavior ($LT < LN < TN$). The maximum normal stress magnitude is relatively small ($< 35$ MPa) for all cases (compared to uniaxial deformation). With the proposed coupling, the normal stress would contribute less than 5% to the damage estimate and can likely be neglected for torsion experiments.

![Diagram](image1.png)

**Figure 4.24:** Shear direction effect for cyclic loading of the Edge texture (peak at $\gamma=1\%$) of the normal stress, $\sigma_{NN}$, illustrating the Rodrigues space and statistics

Next consider the shear stress resolved on the grain boundary interface for each shear loading direction, as illustrated in Figure 4.25. Since the grain boundary interface is aligned with the N-plane, one may expect that the LN and TN nominal shear deformations to have particularly large resolved shear stresses. In fact, this is the case, as Figure 4.25 shows two distinct behaviors, one for LT and one for LN and TN directions. First consider the LT case, which exhibits a relatively low magnitude (less than 40 MPa)
resolved shear stress. Although this magnitude seems insignificant (only 20% of the nominal behavior), it is twice the maximum normal stress for the LT case (20 MPa), and may be as high as 80 MPa in range for fully reversed cyclic deformation. The orientation dependence shows maximum shear stresses near Brass-like corner orientations somewhat similar to the uniaxial dependence.

The LN and TN directions result in resolved shear stresses on the order of the nominal response. The directions are fairly similar, but follow the macroscopic trend of LN < TN. The magnitude of shear stress has a significant range from 200-300 MPa. For these loading directions, the orientation dependence is also very different from most of the cases explored in this investigation. The maximum shear stress occurs for Cube orientated grains and rotations about the shear plane or shear direction axes. In other words, TN shear deformation is a maximum at cube and practically any rotation about the N or T-directions. Hence, for the torsion specimen utilized, having a different axis of the specimen (in the N-plane, i.e. L, T, or LT45°) would minimally affect the elongated grain boundary shear stresses.

Figure 4.25: Cyclic shear deformation of the Edge texture (peak at γ =1%), illustrating the orientation and statistical dependence of the shear stress, \( \tau \)
Figure 4.26: Cyclic shear deformation of the Edge texture (peak at $\gamma =1\%$), illustrating the orientation and statistical dependence of the damage, $D_f$

The Findley-based damage is illustrated in Figure 4.26 for fully reversed cycling at 1% shear strain for each direction. As is expected with very small normal stress values, the damage reproduces the trends of the resolved shear stress (Figure 4.25). However, due to the cyclic application and the very high shear stresses in the LN and TN directions, the damage reaches very high values (up to 600 MPa). The shear stress range for these simulations is similar to that observed in the fully reversed torsion experiment (Figure 2.41). Like for uniaxial tension, the uniform deformation and bi-crystal models have different statistical distribution, but similar maximum and minimum values. At moderate probabilities, the bi-crystal model has lower stress values (i.e. at 0.6 probability LN is 560 MPa for uniform deformation model and only 500 MPa for the bi-crystal). The difference is much less severe near the most damaging pairs than the uniaxial test, but the trend of a smaller number of grain pairs at very damage is preserved. The interpretation of damage was established utilizing nominal stress-strain behavior. When the nominal shear stress (at 1% strain) is multiplied by two (for fully reversed loading with normal stress neglected) and compared to the local statistical response, a corresponding probability between 40% and 60% is apparent for the uniform deformation.
and bi-crystal models respectively. This suggests that the critical damage value determined from the nominal behavior of a torsion experiment may only be valid if a ~50% probability is appropriate. However, in most instances, the critical pairs that initiate delamination are those occurring at higher cumulative probability, which causes the nominal value to underestimate the actual local phenomenon. Therefore, when establishing a local damage criterion, the nominal experimental data should be interpreted with a local approach.

4.7 Plane Strain Cyclic Deformation

One slight modification to bulk uniaxial deformation is plane strain deformation. In this case, the loading strain component is specified with another component stipulated to be exactly zero, and the other components remain stress free (on average). Such a scenario increases constraint relative to uniaxial boundary conditions and may be most applicable to specimen geometries with one relatively large dimension perpendicular to the loading axis. One may expect the added constraint to increase the stress response relative to the uniaxial behavior (on average). This is indeed the case for both TT and NN plane strain boundary conditions for nominal L-direction loading of the edge texture, as shown in Figure 4.27. Furthermore, the figure illustrates that the NN constraint results in higher stresses than the TT constraint, for the specified texture. It should be noted that NN constraint could be appropriate for specialized geometries such as machined pockets into the plate thickness or estimations around a crack-tip.

![Figure 4.27: Macroscopic axial stress-strain response for L-direction loading of the Edge texture for uniaxial and plane strain boundary conditions](image)
Despite the constraint’s similar effect on the macroscopic stress-strain response, the response on the elongated grain boundary interface is expected to be quite different. First consider the normal stress component, whose orientation dependence and probability are presented in Figure 4.28 at 1% axial strain. As illustrated, the normal stress for the uniaxial and TT-constrained cases are quite similar, ranging from -150 to 80 MPa. In contrast, the NN-constrained case shows much higher normal stresses, ranging from 160 to 280 MPa, which is expected for constraint aligned with the normal direction of the elongated grains. The orientation dependence (Rodrigues space) is remarkably similar for all three cases, with N-rotated cube orientations producing the most positive normal stresses. Upon full reversal of the deformation (at -1% strain), the signs would switch and the uniaxial and TT-constrained case would find the largest positive normal stress. In contrast, the NN-constrained case would not result in any positive normal stresses during compressive axial loading. It should be reiterated that the nominal stresses on the N-normal grain boundary are examined for all simulations, as this is the stress normal to the potential delamination plane.

Figure 4.28: Uniaxial versus plane strain boundary conditions for L-direction cyclic loading of the Edge texture (peak at 1% strain) of the normal stress, $\sigma_{NN}$, illustrating the Rodrigues space and statistics
Unlike for the normal stress, which is expected to be different for NN constraint, the shear stress resolved on the elongated grain boundary does not have an obvious dependence on the constraint. The resolved shear stress is illustrated in Figure 4.29 for all three cases at 1% axial strain in the L-direction of the Edge texture. The orientation dependence shows very similar behavior with the maximum shears stresses occurring near the removed corners, or brass-like orientations. Furthermore, the statistical variation of shear stress due to constraint in either the TT or NN components is minimal. Less than 10 MPa difference is detected for a given cumulative probability between the three cases.

![Shear Stress Distribution](image)

**Figure 4.29:** Uniaxial versus plane strain boundary conditions for L-direction cyclic loading of the Edge texture (peak at 1% strain) of the resolved shear stress, \( \tau \), illustrating the Rodrigues space and statistics

The Findley-based damage parameter is presented in Rodrigues space and statistically in Figure 4.30, for the L-direction loading of the Edge texture at 1% axial strain. The orientation dependence follows a similar trend to the resolved shear stress, with a significant variation in magnitude for the NN-constrained case. This is expected due to the increased normal stress for the NN constrained case over the uniaxial and TT constrained cases, even considering that the TT constrained case has its maximum normal stress in compression. These observations will be revisited for the crack-tip discussion.
Figure 4.30: Uniaxial versus plane strain boundary conditions for L-direction cyclic loading of the Edge texture (peak at 1% strain) of the damage, $D_f$, illustrating the Rodrigues space and statistics

4.8 Deformation near a crack-tip

Much of the work that motivated this investigation involved the observation of delamination during fracture toughness testing. Such delaminations occur in two basic configurations: crack-divider and crack-turner. These configurations are named for the orientation of elongated grain boundaries (potential delaminations) relative to the primary crack front. The crack-divider configuration, whose potential delaminations split the primary crack front, occurs when loading a mode I crack in the L or T-direction while the N-direction is aligned with the crack width. The crack-turner configuration, whose potential delaminations turn the primary crack direction 90°, also occurs when loading a mode I crack in the L or T-direction, but the N-direction is aligned with the primary crack. For both configurations, it has been shown that after the delamination nucleates, the driving force for continued propagation significantly increases as the continuum shear component of deformation increases [6]. In contrast, the nucleation process is more complex and probably requires a local approach similar to the one taken for other loading cases during this investigation.
In order to study the initiation of delamination with the current investigation’s modeling tools (uniform deformation model or bi-crystal model), the nominal stress or deformation behavior near a crack-tip must be adequately specified. Unlike the previous cases (uniaxial, shear, plane strain), the deformation near a crack-tip has a significant stress-strain gradient, which complicates the use and interpretation of the current models. Specifically, the assumption that constraint around a particular grain orientation is adequately described by the surrounding nominal stress-strain behavior is increasingly suspect as the gradient encompasses a length-scale of the grain size. This difficulty may be overcome by involving spatial discretization (i.e. FEM) with appropriate crystallographic dependent mechanical response. However, completing a statistically representative study of even a single cracked specimen is exceedingly expensive, and not practical for the current investigation. Alternatively, if the average behavior of many potential grains in the vicinity of a crack is considered, then the nominal behavior may simulate reasonable constraint for a specific grain boundary.

To obtain a deformation field in the vicinity of a crack-tip, the well-known Hutchinson-Rice-Rosengren (HRR) elastic-plastic solution was adopted [151-153]. The HRR solution is appropriate for a thin crack in an infinite medium loaded in mode I. Additional assumptions include that the distance from the crack-tip must be large enough to avoid crack blunting (on the order of the crack height) and small enough such that plastic deformation dominates the strain response, because incompressibility is assumed for the plane strain stress calculation. This results in an over estimate of pressure, when significant compressible elastic deformation occurs. Despite these drawbacks, the HRR solution was chosen to provide a tractable elastic-plastic deformation field to investigate the trends of delamination near a crack-tip.

The HRR solution estimates the monotonic plastic deformation with a power law relationship. The stress–total strain relationship is shown below:

\[
\varepsilon = \mathcal{E}^e : \sigma + \frac{3}{2} k \left( \frac{\sigma_{eq}}{\sigma_o} \right)^{n-1} \mathcal{K} : \sigma
\]  

(4.9)

where \( n \) is the hardening exponent, \( k \) is the hardening coefficient, \( \sigma_o \) is a reference stress, \( \mathcal{E}^e \) is the elastic compliance tensor, and \( \sigma_{eq} \) is the equivalent or von Mises stress. The
material parameters were chosen to adequately simulate the tensile experimental mechanical response, which resulted in a relatively high value for the exponent \((n = 8)\). The HRR normalized stress behavior is presented in Figure 4.31 for the L-direction nominal loading of the crack-divider and crack-turner configurations. The continuum normal and shear stress components resolved on the elongated grain boundaries are included along with the coupled Findley-based damage estimate. The equivalent stress is included to estimate the magnitude of plastic deformation, which is coupled to the resolved shear stresses for a given crystallographic orientation.

![Figure 4.31: The HRR solution for the crack-divider and crack-turner configurations for a hardening exponent of \(n = 8\)](image)

From the HRR solution, several angles (relative to the primary crack direction) were chosen for subsequent investigation using the uniform deformation model. Specifically, angles 0°, 20°, 28°, and 90° were investigated to characterize the local grain boundary stresses. The angles 20° and 28° were chosen because they maximize the nominal damage parameter for the crack-divider and crack-turner configurations respectively. The 0° and 90° angles were specified for completeness, but the 90° direction has the added benefit of being near the maximum equivalent stress, which occurs at 85°. The magnitude of deformation, quantified by the \(J\) integral, was stipulated to be approximately half the critical energy release rate (18.6 N/mm) or \(J = 9.3\) N/mm for the material under consideration [154]. A distance of \(r = 1\) mm from the crack-tip was specified to ensure adequate distance to mitigate the effect of crack blunting while considering a length scale of 1 (T-direction) to 10 (N-direction) grains from the crack-tip. It should be noted that the analysis is insensitive to the distance from the crack-tip due to
the high hardening exponent. The tensorial stress and strain values are summarized in Table 4.1 for both crack configurations, where the 1, 2, and 3 components correspond to the L, T, and N-directions respectively. These strain values were used as the boundary conditions for the uniform deformation model. The only texture considered is the set of statistically representative crystallographic orientations that characterize the Edge region. The crack simulations will be compared to previous loading cases using three criteria: orientation dependence, magnitude of stress or damage, and statistical variation.

**Table 4.1: Stress and strain determined from the HRR solution for the crack-divider and crack-turner configurations at half the fracture load**

<table>
<thead>
<tr>
<th>Crack Divider</th>
<th>Stress (MPa)</th>
<th>Strain (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>θ = 0°</td>
<td>[1470 0 0]</td>
<td>[0 0.18 0]</td>
</tr>
<tr>
<td></td>
<td>[0 1030 0]</td>
<td>[0 0 0.61]</td>
</tr>
<tr>
<td></td>
<td>[0 0 1250]</td>
<td>[1.03 0 0]</td>
</tr>
<tr>
<td>θ = 20°</td>
<td>[1270 230 0]</td>
<td>[0.64 0.45 0]</td>
</tr>
<tr>
<td></td>
<td>[230 1240 0]</td>
<td>[0.45 0.59 0]</td>
</tr>
<tr>
<td></td>
<td>[0 0 1260]</td>
<td>[0 0 0.61]</td>
</tr>
<tr>
<td>θ = 28°</td>
<td>[1120 220 0]</td>
<td>[0.35 0.43 0]</td>
</tr>
<tr>
<td></td>
<td>[220 1380 0]</td>
<td>[0.43 0.87 0]</td>
</tr>
<tr>
<td></td>
<td>[0 0 1250]</td>
<td>[0 0 0.61]</td>
</tr>
<tr>
<td>θ = 90°</td>
<td>[820 -340 0]</td>
<td>[-0.85 0.23 0]</td>
</tr>
<tr>
<td></td>
<td>[-340 710 0]</td>
<td>[0 0 0.37]</td>
</tr>
<tr>
<td></td>
<td>[0 0 760]</td>
<td>[-340 0 0.85]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Crack Turner</th>
<th>Stress (MPa)</th>
<th>Strain (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>θ = 0°</td>
<td>[1470 0 0]</td>
<td>[1.03 0 0]</td>
</tr>
<tr>
<td></td>
<td>[0 1250 0]</td>
<td>[0 0.61 0]</td>
</tr>
<tr>
<td></td>
<td>[0 0 1030]</td>
<td>[0 0 0.18]</td>
</tr>
<tr>
<td>θ = 20°</td>
<td>[1270 0 230]</td>
<td>[0.64 0 0.45]</td>
</tr>
<tr>
<td></td>
<td>[0 1260 0]</td>
<td>[0 0.61 0]</td>
</tr>
<tr>
<td></td>
<td>[20 0 1240]</td>
<td>[0.45 0 0.59]</td>
</tr>
<tr>
<td>θ = 28°</td>
<td>[1120 220 0]</td>
<td>[0.35 0 0.43]</td>
</tr>
<tr>
<td></td>
<td>[0 1250 0]</td>
<td>[0 0.61 0]</td>
</tr>
<tr>
<td></td>
<td>[220 0 1380]</td>
<td>[0.43 0 0.87]</td>
</tr>
<tr>
<td>θ = 90°</td>
<td>[820 0 -340]</td>
<td>[0.50 0 -0.85]</td>
</tr>
<tr>
<td></td>
<td>[-340 0 710]</td>
<td>[0 0 0.37]</td>
</tr>
<tr>
<td></td>
<td>[0 0 0]</td>
<td>[-340 0 0.85]</td>
</tr>
</tbody>
</table>

Before examining the local stress components, a brief discussion on the characteristics of the nominal loading conditions presented in Table 4.1 is useful. Examination of the principal diagonal (particularly for the 20° cases) reveals that the relatively high stress magnitudes are the result of a significant contribution from hydrostatic pressure. Since the pressure is expected to act identically for all crystallographic orientations, it is advantageous to consider the deformation without this contribution to compare each case with the behavior previously investigated. First consider the configurations at 0°, where only principle strain components are applied. With the pressure contribution removed, the crack-divider and crack-turner deformations are similar to L-direction uniaxial deformation with plane strain constraint in the N and
T-directions respectively (Section 4.7). This observation suggests the crack-divider case (at 0°) will have higher normal stress than the crack-turner case, but both will mirror uniaxial deformation results with increased normal stress and damage. The cases at 20° result in nearly pure shear deformation in the LT and LN directions for the crack-divider and crack-turner configurations respectively (Section 4.6). This suggests that very little normal stress variation will be observed and the crack-divider case will have very little resolved shear stress on the elongated grain boundary compared to the crack-turner configuration. The LT shear for the 20° crack-divider case will potentially drive plasticity in the grains, but does not directly load the grain boundary interface of interest. The cases at 28° result in a mix of shear and uniaxial deformation. For this angle (28°), the crack-divider configuration will exhibit only small variations in normal and shear stress due to small contributions from both the shear and uniaxial deformations. In contrast, the shear component of deformation for the crack-turner configuration likely dominates pressure independent behavior due to the NL direction’s alignment with the elongated grain boundary. Lastly consider the deformation at 90°, where the shear component of deformation is negative and much larger in magnitude than the remaining strains on the principle diagonal. In this case, the character of the pressure independent response is expected to mirror negative shear deformation previously discussed (Section 4.6). The resulting behavior will likely mirror the cases at 20°, but with a larger shear component (twice the strain) and a smaller pressure contribution (nearly half). The deformation at 90°, will likely lead to increased plasticity, which will increase the statistical variation and resolved shear stress for both configurations.

Both the orientation dependence and statistical measures of the normal stress, resolved on the elongated grain boundaries, are illustrated in Figure 4.32 for each of the configurations and angles previously specified. As expected, the orientation dependence is minimal for cases where hydrostatic pressure dominates the behavior, as is the case for crack-divider (0°, 20°, and 28°) and the crack-turner (20°). Each of these cases exhibit less than 50 MPa variation in normal stress despite a magnitude near 1200 MPa. Consequentially, these curves lie on top of each other in the statistical representation. The crack-turner configuration at 0° shows slightly more variation with decreased pressure (~950 MPa) and is very similar to the L-direction uniaxial or plane strain tension
case (Figure 4.28) as suggested by the deformation. The crack-divider at 90°, and the crack-turner at 28° and 90° display similar trends to those observed for shear deformations in the –LT, LN, and –LN directions respectively (Figure 4.24). The notation, –LT, signifies an opposite shear loading than was previously discussed and inverts the trends in normal stress. Due to the increased plasticity and larger shear strains, each of these cases result in a larger range of normal stress variation (up to 150 MPa). In general, both crack configurations have larger normal stresses than any deformation case discussed previously, which is attributed to the constraint associated with the HRR deformation field. The crack-turner configuration results in higher normal stresses than the crack-divider configuration, which is consistent with the normalized continuum estimate present in Figure 4.31. The normal stress magnitude may be partially attributed to the use of the HRR model, whose over-constraint likely elevates the pressure. Hence, theses estimates are considered an upper bound on the normal stress.

![Diagram showing normal stress distribution for different crack configurations](image)

**Figure 4.32:** L-direction mode I loading near a crack-tip based on the HRR solution for the normal stress, $\sigma_{NN}$, illustrating the Rodrigues space and statistics
Next consider the resolved shear stress, whose orientation dependence and statistical behavior are illustrated in Figure 4.33. The orientation dependence and statistical variation are consistent with the trends anticipated based on the pressure independent nominal deformation. In short, the cases at 0° behave similar to plane strain tension (Figure 4.29), the crack-divider cases (20° and 90°) closely resemble LT shear, and the crack-turner cases (28° and 90°) are similar to LN shear deformation (Figure 4.25). Unlike the normal stress, the shear stress magnitude is not dictated by hydrostatic pressure. As a result, the magnitude of the shear stress is similar to the cases previously investigated (uniaxial and shear). Furthermore, cases with relatively little plasticity or no applied shear strain in the LN or TN directions (crack-divider at 0°, 20° and 28° and crack-turner at 0°) display low resolved shear stresses with little variability (< 50 MPa). For the crack-divider cases this is expected due to the lack of N-direction gradient, and for the 0° crack-turner case, it is due to symmetry. In contrast, the remaining cases, which had larger plastic strains (90°) or applied LN shear deformation (crack-turner at
20° and 28°) were typically found to have larger shear stresses and significant statistical variation. Unlike the normal stress, which exhibits a similar magnitude for all cases, the shear stresses are much higher for the crack-turner configuration. This is attributed to the nominal LN shear rather than LT shear. Not surprisingly, the maximum shear stress for both configurations occurs at 90°, which corresponds to the approximate location of both the maximum nominal shear and magnitude of plastic deformation. One other interesting result is evident from the crack-turner configuration at 20°. In this case, large shear stresses were predicted with significant statistical variation, but negligible variation was found for the normal stress. This reinforces the notion that the shear and pressure deformation are decoupled in their affect on the shear and normal stresses respectively.

Lastly consider the Findley-based damage parameter for tension (R = 0) cyclic loading. The orientation dependence and statistical character are illustrated in Figure 4.34. As for nearly every case investigated, the orientation dependence follows the trends presented for the shear stress (Figure 4.33). This is true despite the magnitude of damage being dominated by the normal stress contribution for all cases expect 90°, where the shear and normal stress contributions are nearly equal. This normal stress dominance shows the importance of accurately quantifying the shear-normal coupling to predict delamination near a crack-tip. Since the magnitudes are much larger than for the other cases considered in this investigation, the normal stress contribution may seem to be over estimated by the 0.45 ratio stipulated. However, limitations of the HRR solution may be responsible for the high normal stresses. Nevertheless, the damages for the crack-turner configuration are very high, suggesting that loading up to as little as half the critical load would result in imminent cyclic delamination. The failure mode of fracture specimens test for this material [154] display crack turning. In other words, the material’s capability to resist delamination is overcome at lower nominal loads than the threshold required to drive the primary mode I crack. For such high damages, the crystallographic orientation is unlikely to play a critical role, unlike for the cases previously considered. As a consequence, delamination will likely occur at the most favorable pairing within a close proximity of the crack-tip. For more moderate loadings, especially those approaching the delamination threshold, the orientation is expected to affect where certain crack locations may lead to delamination while others will simply grow the primary crack.
Figure 4.34: L-direction mode I loading near a crack-tip based on the HRR solution for the damage, $D_f$, illustrating the Rodrigues space and statistics

Unlike the crack-turner configuration, which appears to be critically driven by relatively equal contribution of shear and normal stresses, the damage for the crack-divider orientation appears to be driven almost entirely by the resolved normal stress. Furthermore, the normal stress dependence is relatively insensitive to the local crystallographic orientations due to the contribution of pressure. This indicates that there is a weak correlation with critically damaging grain boundary pairs. This weak correlation is consistent with the experimental observation, as the crack-divider orientation tends to occur geometrically through the specimen thickness (i.e. along the center plane $t/2$, then $t/4$ and $3t/4$, followed by $t/8$, $3t/8$, $5t/8$ and $7t/8$, etc…) [3]. This observation suggests that for sufficiently high normal stresses, it may be possible to initiate delamination without bulk plasticity or significant resolved shear stresses. The character of the crack-divider constraint provides an interesting scenario to test such an assertion. However, it is possible that the low shear stress is a result of ignoring the large
stress gradient near the crack-tip. If this is true, the crack-divider configuration may require spatial discretization to predict shear stresses and local plastic behavior that leads to the nucleation of delaminations.

In addition to the damage estimates, the HRR crack-tip investigation provides insight on the implementation of both the uniform deformation and bi-crystal local models to study the delamination phenomenon. As shown, the deformation from continuum elastic-plastic modeling may be utilized to estimate the statistical nature of the stresses at grain boundary interfaces of interest. The inability to account for the significant stress-strain gradients persists, but this drawback is negligible when specific grain orientations are unspecified. Furthermore, the local damage appears to correlate very well with the continuum estimates. This suggests that the most damaging deformation (or nearly the most damaging) may be determined by the continuum model’s stress estimates. By employing such a modeling procedure, the critical deformation may be estimated by the method of choice (i.e. FEM). Then the deformation may be applied to a local crystallographically dependent model (i.e. the uniform deformation or bi-crystal model) with an appropriate statically representative texture. This process would result in an estimate of the probability to initiate delamination within a specific number of cycles. Alternatively, the simulation could indicate that the loading causes interface stresses below a given threshold; thus delamination may be suppressed in the absence of an initiated crack. With such an approach, it is conceivable to safely design around the delamination phenomenon.

4.9 Summary of Results

The uniform deformation and bi-crystal models provide similar estimates for the stresses on the elongated grain boundary interface that is susceptible to delamination. A Findley-based damage parameter, which couples normal and shear contributions, was utilized to relate these interface stresses to the delamination process. This damage parameter scaling is consistent with many of the experimental trends observed for delamination and is expected to provide a method to predict the initiation of delamination as a cyclic process. The results illustrate several useful observations that are categorized
below as: modeling characteristics, characteristics of damage, and correlation with experiment.

**Modeling Characteristics:**

- Plastic deformation is required for significant resolved shear stresses to develop on the elongated grain boundary interface (for loading other than TN and LN shear), which leads to more realistic damage values, and dominates the orientation dependence.

- Hydrostatic pressure may increase the resolved normal stress, which contributes to damage, but this contribution is independent of crystallographic orientation.

- Both the uniform deformation and bi-crystal models have very similar maximum and minimum values for the normal stress, shear stress, and damage parameter; however, their statistical nature is different.

- The orientation dependence of the bi-crystal model follows the trends outlined by the uniform deformation model, where the most damaging orientations result in the maximum damage when paired with a specific neighboring orientation.

**Characteristics of damage:**

- A normal-shear coupling of 0.45 was estimated using N-direction and LN-shear monotonic experiments while neglecting local coupling. However, this coupling is non-trivial on the local stress response, particularly for N-direction uniaxial loading, where shear stresses contribute as much as 30% to the damage parameter.

- The damage parameter, which is dominated by nominal shear stress, may be linked to an approximate cyclic lifetime through comparison with torsion experiments. For instance, a damage value of 600 MPa corresponds to a short lifetime (~100 cycles) before the onset of delamination.

- The damage parameter appears to have a minimum critical value, below which the accumulation of delamination damage is slower than classical fatigue failure. Limited torsional experimental results indicate that this value is approximately 150 MPa, suggesting that damage values above this threshold will lead to delamination after sufficient cycles.
Correlation with experiment:

- The local damage estimates from the modeling reflect the trends of a wide range of experimental observations on delamination, which include: uniaxial cyclic loading, torsional cyclic loading, and fracture experiments.

- The bi-crystal model distinguishes the damage of specific orientation pairs, which showed excellent correlation with the delaminated pairs that were observed with EBSD.

- The range of bulk crystallographic textures that are representative of the material considered has a relatively small impact on both the statistical range and critical orientation of the damage. However, its inclusion successfully reproduces the experimental trends for both the macro-scale stress-strain behavior (except at Center) and the tendency to delaminate (Edge > Transition > Center).

- Shear deformation is relatively independent of local normal stress, highlighting the utility of torsion experiments for tuning the damage parameter to be capable of predicting delamination.

- Plane strain boundary conditions have little impact on the estimates of damage compared to the corresponding uniaxial case, except for N-direction constraint, which increases damage due to increased normal stress.

- By using the damage parameter with continuum stress-strain behavior, the crack solution indicates that the most likely location for subsequent delamination may be identified. The local damage may then be established by utilizing the continuum deformation as a boundary condition for either local model.

- The crack-divider configuration leads to orientation independent, geometrically determined delamination driven primarily by normal stress near the crack-tip.

- The crack-turner configuration results in higher damage values than the crack-divider configuration and is composed of nearly equal contributions from both shear and normal stresses.

Both the uniform deformation model and bi-crystal model provided useful local stress estimates that are relevant to the delamination process. Specifically, if a local grain
orientation undergoes local plastic deformation that leads to resolved stresses (damage) that are sufficiently high, then the delamination process will likely initiate after some number of cycles.
5 Conclusions and Recommendations

The current investigation was inspired by the delaminations observed during fracture toughness testing of the 2099-T861 aluminum alloy under investigation. Subsequent experiments showed delamination failures also occurred for cyclic uniaxial deformation at temperatures less than 100°C. A modeling framework was developed to estimate the local stress state on the grain length scale, and was utilized to systematically relate local stresses to the initiation of delamination for a variety of nominal loadings. The major developments of this investigation and complementary recommendations are outlined in the following subsections.

5.1 Conclusions

The current document has characterized many of the aspects of the delamination phenomenon. Delamination was observed to occur along the elongated grain boundary interface. This elongated interface, or N-plane, is a consequence of the pancake-like grain structure, whose dimensions are approximately 12 : 9 : 1 in the L : T : N directions respectively, with some variation with plate location (thru-thickness). Mechanically, this elongated interface was more sensitive to shear loading (~225-300 MPa) than normal loading (~500-550 MPa), based on nominal shear and axial tests. Delamination is only expected to occur in materials with a sufficiently weak elongated grain boundary interface compared to other potential failure modes.

The apparently weak grain boundary interface is a consequence of several potential factors that may be categorized by the observation length scale. The literature [13] recognizes the presence of precipitates (δ’, θ’, T₁) that likely contribute to the material’s strengthening. On a relatively small length-scale (1 μm), this investigation utilized Auger spectroscopy to measure the chemistry on the delamination surface. The results indicate that Cu-rich precipitates (likely T₁) are preferentially located near the grain boundary and are adjacent to thin precipitate-free zones. These clusters of precipitates likely contribute to increased local stresses and decreased ductility at the grain boundary interface. On a slightly larger length scale (1-10 μm), the delamination process was determined to occur concurrently with a localized phenomenon, slip banding. Such localized behavior may cause increased stresses at the grain boundary
interface, due to the discontinuity created by the local plastic slip system mismatch. This
mechanism’s link to the delamination phenomenon is supported by the nominal strain-
rate insensitivity, which coincides with the temperature / strain-rate regime where cyclic
delamination was observed (Section 2.2.1). Strain-rate insensitivity likely contributes to
the localization phenomenon by accommodating potential instabilities rather than
dampening them, as would be the case for positive strain-rate sensitivity. For a length
scale on the order of the grain-size (10-100 µm), the local crystal structure of adjacent
grain pairs result in a deformation mismatch that is constrained by the mechanical
response of the bulk texture. This constraint potentially leads to increased stresses, which
occur locally on the grain boundary interface by activating the mechanisms on smaller
length scales.

To complement the experimental observations of delamination, a modeling
framework was developed to study the grain boundary stresses on the grain-size length
scale. To account for the rate insensitivity, crystallographic orientation dependence, and
interest in cyclic deformation, a cyclically stable crystal plasticity model with rate
independent kinematic hardening on uncoupled crystallographic slip systems was
developed. Due to the rate insensitivity, the traditional visco-plastic strain-strain
behavior used for many crystal plasticity models was inappropriate. To overcome this
obstacle, the kinematic hardening model was restructured to maintain rate insensitivity,
while maintaining numerical stability. Finite deformation was adopted to accommodate
potentially localizations, although this feature was not fully utilized due to its inherent
need for spatial discretization.

The grain-size length scale was incorporated into the basic crystal plasticity
framework by utilizing both a uniform deformation and bi-crystal model. The uniform
deformation model prescribes identical deformation on a set of crystallographic
orientations representative of the bulk texture. The result of such a boundary condition is
an upper bound on the local stress response. The same deformation is applied to the bi-
crystal model, which incorporates a pair of adjacent crystallographic orientations whose
interface is aligned with the elongated grain boundary (or N-plane). This added freedom
relaxes the constraint imposed by the uniform deformation model, providing alternate
estimates of the stress on the grain boundary interface. The bi-crystal model also allows
specific orientation pairings to be investigated, which were compared to local orientation measurements in the region of delamination with EBSD. Using either of the proposed local stress models, it is possible to study a statistically significant number of potential orientations (or pairs) for subsequent analysis. Consequentially, local stress estimates were analyzed by considering both their orientation dependence and statistical nature. To visually highlight the orientation dependence, Rodrigues space was scaled by the local stress or damage quantities rather than orientation probability. Because the bulk texture was specified, the statistical nature of the local stresses or damage is expected to mirror their occurrence in the bulk material.

By employing either model, the local stress state can be estimated for a specified deformation. This local stress may be resolved into the shear and normal components relative to the weak elongated grain boundary interface, which are the components that likely contribute to delamination. A Findley-based damage parameter was adopted to quantitatively account for the shear-normal coupling, where the range of shear stress is combined with the maximum normal stress during a cycle. The shear-normal coupling was roughly estimated from bulk monotonic deformation as 0.45 (Eq. 4.8). The damage parameter may be related to a fatigue based ‘lifetime’ from macroscopic fatigue experiments. Specifically, the short life fatigue torsion experiment, which delaminated in less than 100 cycles, exhibited a nominal damage parameter of approximately 600 MPa. Similarly, the long life torsion experiment, which did not delaminate within $10^6$ cycles, exhibited a nominal damage parameter of 150 MPa. Consequentially, a damage parameter less than 150 MPa is not expected to nucleate delamination before other fatigue failure mechanisms. Since these damage bounds were established with nominal stress, they serve as a lower bound for the local damage behavior.

The results from the uniform deformation and bi-crystal models follow similar trends in the crystallographic orientation dependence. In other words, the most damaging orientation (i.e. brass-like) paired with a specific orientation (i.e. cube) in the bi-crystal model follows the trend indicated by the uniform deformation model (i.e. brass-like is most damaging). This tendency indicates that the orientation dependence is most efficiently specified by the uniform deformation model, where each orientation is independent and uniquely distinguished in Rodrigues space. Both models also share
similar maximum and minimum shear stresses, normal stresses, and damage values for the specified deformation, indicating that predictive capabilities of the uniform deformation model may be sufficient to conservatively determine a potential maximum damage. Despite these similarities, the uniform deformation and bi-crystal models exhibit different statistical distributions, where the bi-crystal model typically predicts a lower frequency of highly damaging states of stress. However, only the bi-crystal model is capable of predicting the response of specific orientation pairs. The EBSD measured crystallographic pair that likely initiated a delamination was in the top 2% of the statistically predicted orientation pairs for cyclic uniaxial loading.

Simulations were conducted for several nominal loading, including uniaxial cyclic loading, torsional cyclic loading, and fracture. Uniaxial experimental results were utilized to confirm that the effect of texture and loading direction were adequately accounted for in the material model. The results showed agreement in all the experimental trends, except near the center of the plate where different local precipitates were observed with Auger spectroscopy and X-ray diffraction. This verifies that the crystal plasticity framework, with independent slip systems is adequate to simulate the proportional cyclic response at relatively small plastic deformations. It should be noted that for larger deformations or non-proportional loading, latent hardening would probably need to be incorporated. Shear simulations, which were compared with cyclic torsion tests, exhibit a relatively small normal stress contribution to the damage parameter. This reinforces the notion that shear stresses alone are capable of driving delamination. For these simple loading cases, shear stresses dominated the damage parameter, and plasticity was required for the grain boundary stresses to exhibit significant orientation dependence.

The Hutchinson-Rice-Rosengren (HRR) [151-153] elastic-plastic crack field solution proved to be a useful exercise that highlights the procedure to estimate local delamination damage from a classical continuum modeling of a hypothetical complex geometry. The continuum estimate of damage (resolved on the N-plane, which corresponds to the elongated grain boundary) provides an appropriate method to distinguish the location of potential delamination nucleation sites. Furthermore, it shows that the continuum deformation at this critical location may be applied to the local stress models to obtain an improved estimate to the damage. This procedure also distinguishes
which orientations and the probability of delamination for the prescribed deformation. Employing the HRR field to the uniform deformation model resulted in reasonable correlation with the experimental trends observed from fracture experiments. Specifically, the crack-divider delamination configuration was shown to be relatively insensitive to crystallographic orientation and is expected to be a consequence of high N-direction constraint near the crack-tip. The damage for this configuration is driven by normal stresses resulting from the hydrostatic stress inherent to the crack-tip field. Normal stresses resulting from hydrostatic pressure were shown to display minimal orientation dependence. This assertion is consistent with the experimental observations that the crack-divider delaminates in geometric intervals through the plate thickness. The crack-turner configuration was confirmed to be more damaging than the crack-divider orientation. The tendency for crack turning is driven by nearly equal shear and normal contributions that are likely to occur without crack growth for monotonic and high amplitude fatigue cycling near a mode I crack-tip. The increased shear contribution coincided with the higher orientation dependence of this case.

5.2 Recommendations

As with all ongoing research, the current investigation would benefit from additional research related to the delamination phenomenon. Perhaps the most beneficial progress would result from clarifying many aspects of the damage parameter. For example, the estimation of the shear-normal coupling may be improved by coupling the local stress model to the nominal experimental measurements. The coupling may be dependent on the number cycles to failure and may be clarified by conducting cyclic fatigue experiments in torsion, N-direction uniaxial, and a mixed mode case such as L-direction uniaxial. With three such loading cases, a series of load levels that result in delamination after cycling for a given life (i.e. ~100, ~1000, ~10000, etc… cycles) would be performed. With these experiments the predictive capabilities of the local stress model may increase dramatically. It should be emphasized that if the loadings are chosen to be small enough, the threshold for delamination may be tightly defined, providing a powerful design tool. Although delamination may be of primary interest, measuring non-delamination failure attributes would also be useful. If one were to consider a range of
temperatures, strain rates, and loading conditions, then it may be possible to construct a failure mechanism map that highlights loadings with a tendency to delaminate.

Although this proposed research direction would improve the model’s predictive capabilities, it may be limited to proportional loading. To account for applications that are loaded non-proportionally, the plasticity model would likely benefit from introducing latent hardening effects. To determine these effects, one may tune the model based on other single crystal observations or tune it to capture the trends observed for non-proportional deformation. Regardless of approach, non-proportional predictive capabilities would require non-proportional testing. These experiments should be examined to determine that both the damage / delamination lifetime predictions are consistent and the nominal mechanical response is adequately reproduced by the local models. If one were successful in matching the non-proportional behavior, design considering delamination may become feasible for nearly any application.

Another feature of the current investigation that may benefit significantly from further research is the quality of the local stress estimates on the grain boundary interface. To study this assumption, spatial discretization (i.e. FEM) of a representative grain field may be modeled to estimate the stresses at the grain boundary interface. The material model should be consistent with the local stress model (i.e. rate independent crystal plasticity). Completing such simulations for a broad range of crystallographic orientations, grain field sizes, and nominal loading conditions may quantify the limitations and quality of the local stress modeling approach. Both 2D and 3D simulations would be required, however a logical first step would be 2D modeling with plane strain stipulated in the 3rd direction. Furthermore, such a study may be capable of highlighting the model’s potential inadequacy in the vicinity of large stress gradients, perhaps even providing a method for estimating the local stress model’s error as a function of magnitude of stress gradient.
List of References


Appendices

A. True Stress Conversion

In this investigation, axial small strain and large strain tests are combined to obtain compressive material properties. A ‘true’ or Cauchy stress-strain space, applicable to both small and large strain regimes, should be implemented. The traditional true strain conversion defines the differential of true strain, \( d\varepsilon^{\text{true}} \), as the ratio of instantaneous change in length, \( dL \), over current length, \( L \):

\[
d\varepsilon^{\text{true}} = \frac{dL}{L}
\]  \hspace{1cm} (A.1)

This form is easily integrated from an initial length, \( L_o \), to \( L \) resulting in the following expression:

\[
\varepsilon^{\text{true}} = \ln \left( \frac{L}{L_o} \right) = \ln \left( 1 + \frac{\Delta L}{L_o} \right)
\]  \hspace{1cm} (A.2)

The engineering strain, \( \varepsilon^{\text{eng}} \), is traditionally defined as the ratio of change in length, \( \Delta L \), over original length:

\[
\varepsilon^{\text{eng}} = \frac{\Delta L}{L_o}
\]  \hspace{1cm} (A.3)

Resulting in the traditional conversion to true strain:

\[
\varepsilon^{\text{true}} = \ln \left( 1 + \varepsilon^{\text{eng}} \right)
\]  \hspace{1cm} (A.4)

which is valid for homogeneous axial deformation over the gage length.

True stress computations are not so simple. If one defines true stress as the ratio of load, \( P \), over current homogeneous cross sectional area, \( A \), then the ratio relative to the original cross sectional area, \( A_o \), relating the engineering stress applies:

\[
\sigma^{\text{true}} = \frac{P}{A} = \frac{A_o}{A} \frac{P}{A_o} = \frac{A_o}{A} \sigma^{\text{eng}}
\]  \hspace{1cm} (A.5)

A derivative or instantaneous form of true stress could be defined, but since both engineering and Cauchy stresses are directly proportional to load, the proposed expression is equivalent. The ratio of areas can be decomposed into volume, \( V \), and length quantities for homogeneous deformation:
Conveniently the ratio of lengths is specified from Eq. A.2 and A.4:

\[
\frac{L}{L_o} = 1 + \varepsilon^{eng}
\]  

(A.7)

A common assumption is the conservation of volume during plastic deformation (as is the case for most plastic deformation involving slip). This implies that any change in volume can be attributed to isotropic elastic axial deformation:

\[
\Delta V = V_o (1 - 2\nu) \varepsilon^{eng} \Rightarrow \frac{V_o}{V} = \frac{1}{1 + (1 - 2\nu) \varepsilon^{eng}}
\]  

(A.8)

where \( \nu \) is Poisson’s ratio. If the elastic strain is assumed to be a linear decomposition of total strain, Eq. A.4 can be manipulated to find the relation between true and engineering elastic strain:

\[
\varepsilon^{eng} = \varepsilon^{true} - 1
\]  

(A.9)

When Eq. A.5 through A.9 are combined, a non-linear expression for true stress results:

\[
\sigma^{true} = \sigma^{eng} \frac{1 + \varepsilon^{eng}}{1 + (1 - 2\nu)(\varepsilon^{true} - 1)}
\]  

(A.10)

where, the true elastic strain is obtained from the stress relationship:

\[
\varepsilon^{true} = \frac{\sigma^{true}}{E}
\]  

(A.11)

Equation A.10 can be solved using successive substitution until convergence is achieved. For typical elastic and strength properties of engineering materials, the true stress calculation, including the elastic volume change, is a small correction over the traditional form, which ignores volume changes, (apply \( \varepsilon^{eng} = \varepsilon^{true} = 0 \) or \( \nu = 0.5 \)); thus convergence is rapid.

To show the magnitude of the correction on small strain deformation, a zoomed in view of the reversal point of an incremental step test is shown in Figure A.1. The figure illustrates that the difference between engineering and true definitions (~1%) is greater than the discrepancy introduced by ignoring elastic volume changes. Despite the
minimal effect, this correction was implemented throughout this experimental investigation for completeness.

Figure A.1: Reversal point of a typical incremental step test illustrating the difference of engineering stress, true stress with elasticity, and typical true stress.

B. Machine Stiffness

In this investigation, large strain compression specimens are quite stout, to avoid bucking, and are not amenable to the installation of an extensometer. During such a test, displacement is measured from a Linear Variable Displacement Transducer (LVDT) within the actuator. Due to the location of this measurement, some correction was necessary to account for the finite stiffness of the machine and grips.

First, assume the LVDT measurements can be decomposed into specimen and machine deformations. By assuming series elements, the following stiffness relation results:

\[ \frac{1}{K_{LVDT}} = \frac{1}{K_{Spec}} + \frac{1}{K_{Mach}} \]  

(B.1)

where, the stiffness is defined as the change in load over the change in displacement:

\[ K = \frac{\Delta P}{\Delta x} \]  

(B.2)

Using this definition, the stiffness measured with the LVDT can be calculated from the following expression:

\[ K_{LVDT} = \frac{P - P_0}{X_{LVDT} - X_0^{LVDT}} \quad , \quad X_{LVDT} \neq X_0^{LVDT} \]  

(B.3)
The specimen stiffness was approximated using an uncapped cylindrical compression sample (Figure B.1a). Due to specimen dimensions and anticipated loads, a dual strain gauged specimen was practical to measure deformation. The average strain within the specimen can be computed using the following equation:

\[ \varepsilon = \frac{1}{2} \left( \varepsilon^A + \varepsilon^B \right) \tag{B.4} \]

where, the strains, \( \varepsilon^A \) and \( \varepsilon^B \), are obtained from strain gages on opposite sides of the specimen. These strains were within 1% of being identical, indicating minimal bending or buckling of the sample. Converting engineering strain to displacement using the standard expression:

\[ x_{\text{spec}} = \varepsilon L_0 \tag{B.5} \]

Using Eqs. B.2, B.4 and B.5, the specimen stiffness can be determined at each data point:

\[ K_{\text{Spec}} = \frac{2}{L_0} \left( \frac{P - P_0}{\left( \varepsilon^A + \varepsilon^B \right) - \left( \varepsilon^A_0 + \varepsilon^B_0 \right)} \right), \quad \left( \varepsilon^A + \varepsilon^B \right) \neq \left( \varepsilon^A_0 + \varepsilon^B_0 \right) \tag{B.6} \]

Lastly, the machine stiffness can be computed from Eq. B.1 as shown below:

\[ K_{\text{Mach}} = \frac{K_{\text{LVDT}} K_{\text{Spec}}}{K_{\text{Spec}} - K_{\text{LVDT}}} \tag{B.7} \]

Figure B.1b illustrates typical results, where machine stiffness versus applied load is plotted. It should be noted that the machine stiffness should be determined for each machine used to conduct large strain compression tests. Additionally for the tests setup with the hydraulic grips inside the temperature chamber, the stiffness also displays temperature dependence. For tests on other frames, such as the high temperature frame, the temperature of the hydraulic fluid is carefully controlled by the cooling fluid and is only marginally affected by testing temperature. After initial loading, the machine stiffness is nearly constant.
Figure B.1: (a) 2024 aluminum strain gage specimen (b) Machine stiffness vs. load at room temperature for temperature chamber test frame.

C. Coordinate Rotations

When dealing with anisotropic material models and finite deformations, transforming between various orientations is often necessary. A unique method of demarking the coordinate frame for specific tensorial components is adopted in this discussion. For a given tensor, $Z$, the components may be written utilizing the following notation:

$$ [Z]^{oc} = [Z]^{oc} = Z^{oc}_{ij} $$

Where the brackets, [ ], are often dropped for indicial notation but represent that the tensor has been evaluated to rotate between frames associated with the upper indices, $o$ and $c$. It should be noted that applying an inverse requires the generalized upper indices to switch. For clarity the inverse of tensor, $Z$, can be equivalently written:

$$ ([Z]^{oc})^{-1} = Z^{oc}_{ij} = [Z^{-1}]^{oc}_{ij}. $$

Notice that for the shorthand notation, the upper indices always represent the behavior of $Z$ (without an inverse).

In this formulation, the generalized upper indices $(oc)$ can be permuted with the following: the initial lab-frame ($o$), previous Cauchy-frame ($p$), current Cauchy-frame ($c$), and the crystal-frame ($x$), and are each potentially employable depending on the application. These frames are illustrated in Figure C for clarification. It should be noted that the inverse of rotation $R$ at $t = 0$ is defined as the lab to crystal rotation:
\[ \mathbf{g}^{\alpha} = \left( [\mathbf{R}^{(\alpha)}]^{\text{C}} \right)^T. \]  

(C.3)

The possible rotations used in this formulation are listed below for each transformation:

- **Lab to Crystal:**
  \[ g^{\alpha}_{ij} \]
  \[\text{(C.4)}\]

- **Crystal to Previous:**
  \[ R_{ij}^{(i)} \]
  \[\text{(C.5)}\]

- **Crystal to Current:**
  \[ R_{ij}^{(i)(c)} \]
  \[\text{(C.6)}\]

- **Lab to Previous:**
  \[ R^{(i)}_{ik} g^{\alpha}_{kj} \]
  \[\text{(C.7)}\]

- **Lab to Current:**
  \[ R^{(i)(c)}_{ik} g^{\alpha}_{kj} \]
  \[\text{(C.8)}\]

- **Previous to Current:**
  \[ R^{(i)(c)}_{ik} R^{(i)(p)}_{jk} \]
  \[\text{(C.9)}\]

Only the first three rotations are independently defined, since they are the most convenient for the current investigation.

**Figure C.1: Coordinate rotation between various reference frames.**

For completeness, the rotation rules for various tensors utilized in this analysis are summarized below:

- **0th Order Tensor (Scalar):**
  \[ a = a \]
  \[\text{(C.10)}\]

- **1st Order Tensor (Vector):**
  \[ x_i^X = \ell_{ij}^{XX} X_j^X \]
  \[\text{(C.11)}\]

- **2nd Order Tensor:**
  \[ \sigma_{ij}^X = \ell_{ij}^{X\alpha} \sigma_{\alpha\beta}^{\alpha\beta} \]
  \[\text{(C.12)}\]

- **4th Order Tensor:**
  \[ C_{ijkl}^{X\alpha} = \ell_{ij}^{X\alpha} \ell_{kl}^{X\beta} C_{\alpha\beta\gamma\delta}^{\alpha\beta\gamma\delta} \]
  \[\text{(C.13)}\]

where \( \ell_{ij} \) is any rotation in an orthogonal reference frame (mostly likely one previously specified). These coordinate rotations are utilized during the solution technique and post-processing as necessary throughout this investigation.
D. **Elastic Anisotropy**

The anisotropic elastic modeling utilized throughout this investigation benefits from a few clarifications presented in this appendix. First, the imposed cubic symmetry is confirmed for the elastic strain energy density. Next, the stress dependence on the bulk modulus is specified while maintaining a unique relationship between stress and elastic strain. Lastly, the modeling sensitivity to the elastic assumption (large anisotropic, small anisotropic, large isotropic, and small anisotropic elastic strains) is quantified for cyclic uniaxial tension in the L-direction of the Edge texture.

D.1 **Elastic Strain Energy Density**

To illustrate that the chosen anisotropic elastic strain energy density is consistent with cubic symmetry, first consider the strain energy density based on the Green-strain:

\[
\Psi^e = \frac{1}{2} \mathbf{C}^{Ge} : \mathbf{\varepsilon}^e : \mathbf{E}^{Ge} = \frac{1}{2} \left( \mu \left( E_{kk}^{Ge} \right)^2 + \frac{2}{3} \left( 2\mu + 3\kappa + 2\xi \right) E_{kk}^{Ge} E_{kl}^{ Ge} \right) + \xi \left( E_{11}^{Ge^2} + E_{22}^{Ge^2} + E_{33}^{Ge^2} \right) \]

which clearly exhibits cubic symmetry as \( E_{kk}^{Ge} \) and \( E_{kl}^{Ge} \) are invariants. Alternatively, if one were to consider the elastic right Cauchy-Green tensor, \( \mathbf{C}^{Ge} \), then the internal elastic work can be rewritten as shown:

\[
\Psi^e = \frac{1}{8} \left( \mathbf{C}^{Ge} - \mathbf{I} \right) : \mathbf{\varepsilon}^e : \left( \mathbf{C}^{Ge} - \mathbf{I} \right) = \frac{1}{8} \left( \mu \left( C_{kk}^{Ge} \right)^2 + \left( 13\mu + 6\kappa + 7\xi \right) \left( 1 - \frac{2}{3} C_{kk}^{Ge} \right) \right) + \frac{2}{3} \left( 2\mu + 3\kappa + 2\xi \right) C_{kk}^{Ge} C_{kl}^{Ge} + \xi \left( C_{11}^{Ge^2} + C_{22}^{Ge^2} + C_{33}^{Ge^2} \right) \]

where,

\[
\mathbf{C}^{Ge} = \mathbf{U}^{eT} \mathbf{U}^e
\]

Again, the cubic symmetry is apparent, and it is concluded that the cubic character of the anisotropic elastic strain energy density is preserved for either strain definition.

D.2 **Elastic Stress Dependence**

Elastic stress dependence in aluminum may play a role at small strains and at reversals during cyclic deformations. In this investigation, uniaxial experiments indicate a slight linear stress dependence on the axial elastic modulus (Section 2.2.1.1). Although such a phenomenon is rarely reported, other researchers have found a similar trend for
high strength polycrystalline steel [54]. Additional effort is required to implement stress
dependence into the 4th order stiffness tensor. When hyper-elasticity is assumed, several
researchers have discussed the limitations on the available stress-dependent forms for
isotropy and transverse isotropy [140-141].

Based on the experimental observations, it is sufficient for the stress dependence
to be isotropic and dependent on only the first invariant of engineering stress, $S_{kk}^e$.
Furthermore, a linear stress dependence on the derivative of engineering stress with
respect to elastic Green strain is appropriate:

$$\frac{dS^e}{dE^e_{Ge}} = 2\mu H + \left(3\kappa + 3\kappa_\alpha S_{kk}^e\right)J + \zeta K$$

(D.4)

where $\kappa_\alpha$ controls how the bulk modulus varies with stress. This form is easily invertible
and takes the following form for the derivative of elastic Green strain.

$$\frac{dE^e_{Ge}}{dS^e} = \frac{1}{2\mu} H + \left(\frac{1}{3\kappa + \zeta + 3\kappa_\alpha S_{kk}^e} + \frac{\zeta}{2\mu(\zeta + 2\mu)}\right)J + \frac{-\zeta}{2\mu(\zeta + 2\mu)} K$$

(D.5)

Integrating either expression to solve for stress and strain (where $S^e = 0$ implies $E^e_{Ge} = 0$)
results in the following unique relationship between stress and elastic strain

$$S^e = \mathcal{E}^e : E^e_{Ge} + \frac{3\kappa + \zeta}{27\kappa_\alpha} \left(\exp\left(9\kappa_\alpha E^e_{Ge}\right) - 9\kappa_\alpha E^e_{Ge} - 1\right)\delta$$

(D.6)

$$E^e_{Ge} = \mathcal{E}^{-1} : S^e + \frac{1}{27\kappa_\alpha} \ln\left(1 + \frac{9\kappa_\alpha S_{kk}^e}{3\kappa + \zeta} - \frac{S_{kk}^e}{9\kappa + 3\zeta}\right)\delta,$$

(D.7)

where the first invariant of stress and elastic strain can be related as follows:

$$S_{kk}^e = \frac{3\kappa + \zeta}{9\kappa_\alpha} \left(\exp\left(9\kappa_\alpha E^e_{Ge}\right) - 1\right)$$

(D.8)

$$E^e_{kk} = \frac{1}{9\kappa_\alpha} \ln\left(1 + \frac{9\kappa_\alpha S_{kk}^e}{3\kappa + \zeta}\right).$$

(D.9)

This stress-dependent elastic relationship was only employed to compute the elastic
constants from the experimental data, and was not utilized to run subsequent modeling
simulations.

D.3 Sensitivity to Elasticity Assumption

Throughout the modeling development, large strain anisotropic elasticity was
adopted to accommodate the potentially large stresses at relatively small nominal strains.
After subsequent analysis of the material under investigation (Section 4.1), the elastic anisotropy was determined to be quite small, even by aluminum’s standards. One may expect that elastic isotropy would not be an unreasonable assumption, even at small nominal strains and relatively large stresses. Similarly, small strain elasticity is commonly considered an appropriate assumption for most engineering metals. To quantify the effect of assuming elastic isotropy/anisotropy and small/large strain elasticity, uniform deformation simulations to 1% strain in the L-direction for the Edge texture were completed. Not surprisingly, the macroscopic stress showed negligible variation on the order of 1-2% between the four cases (Figure D.1).

![Figure D.1: Macroscopic stress-strain response of four elastic assumptions](image)

The statistical variation on the normal and shear stress resolved on the grain boundary interface were also examined, as illustrated in Figure D.2. In this case, the derivative of the cumulative probability was selected to highlight the differences most clearly. The normal stress (Figure D.2a) is very small and is on the order of 1-2 MPa difference between cases, where the maximum difference occurs for positive normal stresses. Similarly, the shear stress (Figure D.2b) also shows a small effect on the statistics. Particularly the difference between the small and large strain assumption at low shear stress. At higher shear stresses, the small strain assumption results in a 2 MPa lower maximum shear stress than the large strain assumption. The anisotropic vs. isotropic elasticity models shows a 2-3 MPa difference at both low and high shear stresses. However, at low shear stresses (10 - 20 MPa) the isotropic case displays a
greater probability (Figure D.2b), but near the maximum shear stress it displays a lower frequency. This difference is attributed to the interplay of elastic anisotropy and plastic deformation. For a more anisotropic material, such as copper or gold, the differences due to anisotropy would be much more pronounced. It should be emphasized that these results indicate at worst, a 5% difference in damage is expected for any of the four cases with different elastic assumptions. Thus, any choice is relatively insignificant compared to other modeling sensitivities explored in this investigation. In spite of the relative insensitivity of the modeling to the elastic assumptions, the anisotropic large elastic strain case was utilized for all of the simulations (unless otherwise specified). This was in part due to its straightforward implementation within the general solution framework.

![Figure D.2: Sensitivity of the normal and shear stress histograms for uniaxial loading of the Edge texture in the L-direction to elasticity assumptions: large strain elasticity vs. small strain elasticity and anisotropic vs. isotropic](image)

**E. Sensitivity to Plasticity Parameters**

The effects of texture, loading direction, and loading type have been covered in the previous sections. The components of deformation with the most potential for variation are the plastic slip system properties. Such properties include variation in hardening slopes, $\theta_{(i)}$, hardening threshold, $\tau_{(i)}$, and latent hardening effects. Only the effects of changes in the hardening threshold are considered in this investigation, due to similar behavior expected from the hardening slope and a significant increase in complexity involved in introducing latent hardening.
Figure E.1: Sensitivity of L-direction uniaxial loading to a 10 MPa drop in pseudo-saturation stress through a sample of plastic slip parameters

The sensitivity to changes in the hardening threshold may be split into two categories: a 10 MPa decrease in the slip system saturation stress, and a 10 MPa delay in the hardening threshold. First consider the 10 MPa decrease in slip system saturation stress, as illustrated in Figure E.1. It should be noted that the ‘Base’ case uses the slip parameters specified in Figure 4.2, and Cases I-V are permutations specified in Figure E.1 that result in this 10 MPa decrease in local saturation. Observation of the macroscopic stress-strain behavior illustrates that the 10 MPa decrease in local saturation stress results in approximately a 20 MPa decrease in the bulk axial response at 1% strain. This observation is evident for the cases when the modified parameters achieved saturation (Cases I-III), and proportionally for Case V. Closer observation suggests that Cases I and II are negligibly different, which is a result of the hardening slopes $\theta_{(3)}$ and $\theta_{(1)}$ both being greater than the elastic stiffness and significantly larger than $\theta_{(2)}$. Case III displays a small difference from the Base at strains below 0.5%, but quickly mirrors
Cases I-II at larger strains. Similarly Case IV is nearly identical to the base up to 0.9% strain, which emphasizes the delayed effect of changing the threshold values of hardening slope parameters that dominate the later deformation process. It should be noted that lower hardening slopes tend to dominate deformation at higher strains. In all cases, the statistical representation of the local Findley-based grain boundary damage maintains its Base character and changes on the same order as the perturbation (10 MPa). As illustrated, lowering the higher hardening slope threshold parameters \( r(y) - r(2) \) tends to increase the maximum damage parameter by up to 10 MPa for the same applied axial strain (1% in this case). This tendency is due to the other threshold parameters \( r(3), r(4) \) not saturating by 1% axial strain. One may conclude for this loading case (L-direction uniaxial loading) that if slip is easier, then damage will increase for identical deformation.

Next consider a sample of hardening shift variations as presented in Figure E.2. The permutations forwarded do not change the overall saturation stress. As before, a 10 MPa local decrease results in a 20 MPa macroscopic stress decrease and a 10 MPa local damage increase. The seven cases presented in Figure E.2 may be categorized into three distinguishable responses thanks to the significantly higher hardening slopes associated with \( r(y), r(1), \) and \( r(2) \). The first is the Base and Case VI response, which are nearly identical, and emphasize that shifting between \( r(y) \) and \( r(1) \) does not change the stress-strain behavior or damage. Next consider Cases VII and IX, which show a tendency for earlier yielding, but quickly approach the Base case stress by 1% strain. In contrast, Cases VIII, X and XI are also similar thanks to the indistinguishable character of \( r(y), r(1), \) and \( r(2) \). They display significantly less plastic hardening similar to the 10 MPa drop observed for Cases I-III in Figure E.1. These observations further emphasize that the threshold \( r(3) \) is not achieved during the simulation up to 1% strain. As before, the statistical damage is very similar for shifts in the threshold stress. The largest variations are on the order of a 10 MPa decrease and are evident in the cases where later hardening occurs (Cases VIII, X, and XI).
Figure E.2: Sensitivity of L-direction uniaxial loading to a hardening shift through a sample of plastic slip parameter pairs
Author’s Biography

Russell and his twin sister Carrie were born, on November 5, 1979. Eighteen years later he graduated from Moline High School, and began studying at the University of Illinois in the field of Mechanical Engineering. In 2001, he took an hourly position as a grader for Dr. Peter Kurath. Discussions with Dr. Peter Kurath about non-grading related topics nurtured an interest in material behavior that lead to Russell’s employment as an undergraduate lab assistant, where he first learned to conduct experiments. Shortly after, Russell received his Bachelor of Science (2002) and subsequently his Master of Science (2004) degrees in Mechanical Engineering, while working under the guidance of Dr. Peter Kurath. After briefly considering employment in industry, Russell was drawn back to academia by the allure of continuing his education under the guidance of both Dr. Peter Kurath and Prof. Armand Beaudoin. So, his work began on the delamination of Aluminum-Lithium that developed into his dissertation research toward completing his Doctoral degree. In fall of 2008, Russell was honored with a departmental teaching fellowship to teach ME 430: Failure of engineering materials. Upon completion of his Doctoral dissertation, Russell will begin a Post-Doctoral position with Prof. Darrell Socie and will be actively pursing an academic career.