Multi-Scale Modelling of Texture Evolution and Surface Roughening of BCC Metals During Sheet Forming

by

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Abstract

This thesis examines the qualitative and quantitative variation in local plastic deformation and surface roughening due to crystallographic texture in body-centered cubic materials, specifically interstitial-free steel sheet and molybdenum foil and sheet. Complex forming operations currently used in industrial manufacturing lead to high material failure rates, due in part to the severity of the applied strain path.

A multi-scale model was developed to examine the contribution of mesoscopic and local microscopic behaviour to the macroscopic constitutive response of bcc metals during deformation. The model integrated a dislocation-based hardening scheme and a Taylor-based crystal-plasticity formulation into the subroutine of an explicit dynamic FEM code, LS-DYNA.

Numerical analyses using this model were able to predict not only correct grain rotation during deformation, but variations in plastic anisotropy due to initial crystallographic orientation. Simulations of molybdenum foil under uniaxial tension supported the existence of bending due to local variations in plastic anisotropy, confirmed with good quantitative agreement by experimental measurements of surface roughening.
A series of two-stage strain-path tests were performed, revealing a prestrain-dependent softening of both the steel and molybdenum samples when an orthogonal secondary strain path is applied. Numerical analyses of these tests overestimate macroscopic work hardening during complex loading, due in part to the dynamic nature of the FEM code used.
Acknowledgements

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Contents

Abstract

Acknowledgements

Contents

List of Tables

List of Figures

Abbreviations

Nomenclature

Chapter 1: Introduction

1.1 Research Scope

1.2 Thesis Outline

Chapter 2: Literature Review

2.1 Development of Surface-Roughening Models
2.2 Development of Finite-Element Models to Capture Local Work Hardening ........................................... 9
   2.2.1 Overview of Integrated Work-Hardening Models .............. 12
2.3 Capturing Transient Constitutive Behaviour ................................................................. 15
   2.3.1 Numerical Representation of Transient Effects ...................... 17
2.4 Research Objectives .......................................................................................... 23

Chapter 3: Development of a Multi-Scale Model ................................................... 31
   3.1 Crystal-Plasticity Formulation ................................................................. 31
      3.1.1 Taylor Ambiguity ........................................................................ 35
   3.2 Finite-Element Modelling in LS-DYNA ................................................... 36
      3.2.1 Construction of a Crystal Plasticity umat ................................. 36
   3.3 Validation of the Multi-Scale Model .......................................................... 42
      3.3.1 Single-Element Analyses ............................................................. 43
      3.3.2 Multiple-Element Analyses ......................................................... 53
   3.4 Summary .............................................................................................. 56

Chapter 4: Molybdenum Foil Tensile Testing .................................................. 75
   4.1 Material Selection ...................................................................................... 76
   4.2 Sample Preparation .................................................................................... 77
   4.3 Experimental Testing and Characterization ............................................... 78
      4.3.1 Local Texture Measurements ....................................................... 79
      4.3.2 Surface Profilometry .................................................................... 80
   4.4 Numerical Analyses ................................................................................. 80
   4.5 Analysis of Numerical and Empirical Data .............................................. 82
   4.6 Summary .............................................................................................. 86

v
Chapter 5: Two-Stage Strain Path Analyses ...

5.1 Experimental Data for Model Calibration
   5.1.1 Monotonic Shear Tests
   5.1.2 Orthogonal Strain-Path (Cross) Tests
   5.1.3 Reverse Strain-Path (Bauschinger) Tests

5.2 Conventional Cross-Test Studies
   5.2.1 Data Acquisition

5.3 Assessment of the Three-Tier Model under Strain-Path Change

Chapter 6: Discussion

6.1 Qualification of LS-DYNA within the Three-Tier Model
   6.1.1 The Development of Texture-Based Anisotropy
   6.1.2 Inertial Effects and the Courant Condition

6.2 Qualification of an Integrated Taylor-Based Crystal Plasticity Model in LS-DYNA

6.3 Qualification of Mesoscopic Hardening Theory in a Multi-Scale Model
   6.3.1 Isotropic Hardening under Monotonic Strain Paths
   6.3.2 Analyses of Complex Two-Stage Strain-Path Behaviour

6.4 Contributions to the Field

Chapter 7: Conclusions and Recommendations

7.1 Conclusions

7.2 Recommendations for Future Work

References
List of Tables

2.1 Slip reversal conditions arising during plastic deformation. 25

3.1 List of \{111\}\langle110\rangle slip systems for fcc crystal structures. 57

3.2 List of \{110\}\langle111\rangle slip systems for bcc crystal structures. 58

3.3 List of \{112\}\langle111\rangle slip systems for bcc crystal structures. 59

3.4 List of \{123\}\langle111\rangle slip systems for bcc crystal structures. 60

3.5 Test matrix implemented for model validation (bcc structure). 61

3.6 Active slip systems for \{110\}\langle111\rangle slip, compared to the results of Chin and Mammel. Taylor factors $M$ calculated by the model for specific orientations in each region (shown below) are given. 62

3.7 Active slip systems for \{112\}\langle111\rangle slip, compared to the results of Chin and Mammel. Taylor factors $M$ calculated by the model for specific orientations in each region (shown below) are given. 63

3.8 Active slip systems for mixed \{110\}\langle111\rangle and \{112\}\langle111\rangle slip. Taylor factors $M$ calculated by the model are compared to the results of Chin and Mammel. 64

4.1 Parameters used as input for Mo foil simulations. 87
5.1 Experimental test matrix for calibration of the mesoscopic hardening model. .......................................................... 124

5.2 Chemical composition (wt %) of the investigated IF steel. .......... 125

5.3 Experimental test matrix for conventional cross-test analyses. ....... 126

5.4 Material parameters for IF steel used in the three-tier model, compared to those of Peeters. .................................................. 127

A.1 Variation of strain ratio from elasticity ($\beta_{L,el}$) to the onset of plasticity ($\beta_L$) due to changes in the proportionality constant $m$. ............ 195

B.1 Ratio $\kappa$ of the longitudinal strain of the outermost element to that of the innermost element along the tensile axis, under a total applied strain of 25%. ................................................................. 215
List of Figures

1.1 Tube pre-bending and hydroforming process commonly used in the automotive industry. Above: placement of a pre-bent steel tube into a hydroforming die. Below: morphology of the tube cross-section as a result of the hydroforming process. ........................................ 6

2.1 Ridging mechanism proposed by Chao. ........................................ 26
2.2 Cellular dislocation structure formed during Stage II hardening. .... 27
2.3 Stages of work hardening. ............................................................. 28
2.4 Experimental measurements of an IF steel during two-stage strain-path tests. Above: Cross effects after primary applied strains of 10 and 20 %. Below: Bauschinger effects after primary applied strains of 10 and 30 %. ................................................................. 29
2.5 Above: TEM micrograph of an IF steel subjected to 20 % tensile strain along the axis specified. Below: Schematic representation of the microstructure as outlined in the Peeters hardening model. ............... 30

3.1 Flow diagram illustrating the integration of the crystal plasticity umat and LS-DYNA. ................................................................. 65
3.2 Conditional statements governing the selection of active slip systems.

3.3 Contours of $M$ obtained from Chin and Mammel. Dashed boundaries delineate regions within which a specific set of slip systems are active. 
(a) Case of $\{110\}<111>$ slip. (b) Case of $\{112\}<111>$ slip. (c) Case of $\{123\}<111>$ slip. (d) Case of mixed slip on $\{110\}<111>$, $\{112\}<111>$, and $\{123\}<111>$.

3.4 Grain rotation paths of orientations in a standard stereographic triangle. (a) Tensile behaviour of fcc material under axisymmetric deformation, superimposed by X-ray goniometer measurement of polycrystalline copper subjected to wire drawing. (b) Tensile behaviour of fcc material predicted by the umat. (c-g) Compressive behaviour of bcc material predicted by the umat: (c) $\{110\}<111>$ slip; (d) $\{112\}<111>$ slip; (e) $\{123\}<111>$ slip; (f) combined $\{110\}<111>$ and $\{112\}<111>$ slip; and (g) combined $\{110\}<111>$, $\{112\}<111>$, and $\{123\}<111>$ slip.

3.5 Grain rotation paths for a bcc structure. (a) Solutions for axisymmetric compression produced by LS-DYNA, mixed $\{110\}<111>$ and $\{112\}<111>$ slip. (b) Solutions for axisymmetric tension produced by LS-DYNA, mixed $\{110\}<111>$ and $\{112\}<111>$ slip. (c) Rotation field predicted by Calnan and Clews for axisymmetric compression under $\{112\}<111>$ slip.

3.6 Evolution of $\beta_{L,i}$ and $\beta_{L,t}$ for a single-element CE-oriented grain under uniaxial tension.

3.7 Evolution of $\beta_{L,i}$ and $\beta_{L,t}$ for a single-element CF-oriented grain under uniaxial tension.
3.8 Evolution of $\beta_{L,i}$ and $\beta_{L,t}$ for a single-element CC-oriented grain under uniaxial tension. ........................................ 72
3.9 Grain rotation paths for a bcc structure under uniaxial compression:
   (a) assuming axisymmetric deformation, combined $\{110\} \langle 111 \rangle$ and $\{112\} \langle 111 \rangle$
   slip; (b) assuming plane-stress, combined $\{110\} \langle 111 \rangle$ and $\{112\} \langle 111 \rangle$
   slip; and (c) assuming plane-stress, combined $\{110\} \langle 111 \rangle$, $\{112\} \langle 111 \rangle$, and $\{123\} \langle 111 \rangle$ slip. ........................................ 73
3.10 Banded texture model results: (a) mesh construction, highlighting 15x3-element regions of polycrystalline material with similar orientation and direction of loading (plot of Euler angle $\Phi$ shown – CF = blue, CE = red); and (b) plot of through-thickness strain after an applied strain of 20% along the x-axis. ........................................ 74
4.1 ECC images of Mo foil (a) before and (b) after vacuum annealing at 1873 K for 1 h. Of note, the difference in magnification from (a) to (b) is roughly 10 x. .......................... 88
4.2 Incomplete pole figures of Mo foil (a) before and (b) after 1873-K anneal for 1 h. ........................................ 89
4.3 True stress-strain behaviour of Mo foils A and B under uniaxial tension. Values are given in terms of both total strain and plastic strain ($\epsilon_p$). ........................................ 90
4.4 Gold location marker viewed under a SEM at (a) 50x, and (b) 100x magnification (locations not coincident). Carbon burns resulting from texture scans are visible to the left of the marker at higher magnification. 91
4.5 Texture maps acquired using OM of undeformed Mo foil specimens: (a) Foil A, and (b) Foil B. Green areas represent non-indexed regions. 92
4.6 Texture maps acquired using OM of deformed Mo foil specimens: (a) Foil A, and (b) Foil B. Green areas represent non-indexed regions.

4.7 Comparison of pole figures determined from (a) bulk texture measurements using XRD with local texture data acquired using EBSD for (b) foil A and (c) foil B. The tensile direction is aligned with the vertical axis of each plot.

4.8 Surface profile of Mo foil A prior to deformation: (a) using a large colour table; and (b) using a small colour table.

4.9 Surface profile of Mo foil B prior to deformation: (a) using a large colour table; and (b) using a small colour table.

4.10 Surface profile of Mo foil A after deformation: (a) using a large colour table, showing loading direction; and (b) using a small colour table.

4.11 Surface profile of Mo foil B after deformation: (a) using a large colour table, showing loading direction; and (b) using a small colour table.

4.12 Example of crystallographic input for the multi-scale model, illustrated using the Eulerian angle Φ: (a) unrefined OM data of foil B prior to deformation; (b) refined OM data using CHANNEL 5 software; and (c) finite-element mesh containing the refined orientation data in (b).

4.13 Plastic work-hardening behaviour for Mo foil B, compared with results from the multi-scale model. Fluctuations in the experimental curve are due in this case to time-dependent noise in the source hydraulics.

4.14 Surface roughness of foil A after deformation: (a) the experimental roughness profile; and (b) the simulated through-thickness strain.
4.15 Surface roughness of foil B after deformation: (a) the experimental roughness profile; and (b) the simulated through-thickness strain. Terminal values of the colour table in (b) have been reduced to decrease the influence of inertial/boundary effects on the overall contour plot.

4.16 Correlation between $\beta_L$ and surface profile.

4.17 Plastic bending phenomenon suggested by Wright.

4.18 Refined texture maps of Mo foil A (a) prior to and (b) after 10 % deformation, and Mo foil B (c) prior to and (d) after 15 % deformation. Low-angle grain boundaries ($< 10^\circ$) are black, while all higher-angle boundaries are green.

4.19 Experimental (110) and (200) discretized pole figures of Mo foil A (a) prior to and (b) after 10 % deformation, and Mo foil B (c) prior to and (d) after 15 % deformation.

4.20 Comparison of discrete-point pole figures for foil A (a) via EBSD prior to deformation, (b) via EBSD after deformation, and (c) simulated using the multi-scale model after deformation.

4.21 Comparison of discrete-point pole figures for foil B (a) via EBSD prior to deformation, (b) via EBSD after deformation, and (c) simulated using the multi-scale model after deformation.

5.1 A typical constitutive response for IF steel sheet under extreme cases of strain path change. Above: cross tests after 10 and 20 % tensile pre-strain, compared to monotonic loading behaviour. Below: Bauschinger tests after preshear values of $\gamma = 0.1$ and $\gamma = 0.3$. 

xiv
5.2 Planar simple shear device. *Clockwise from top-left:* mounting of the rig in a hydraulic tensile apparatus; detail of the rig highlighting mobile (left in the figure) and immobile (right in the figure) parts; and mounted camera for image acquisition during analyses. 129

5.3 Small-scale Mo specimens subjected to simple shear (units shown are cm). *From left to right:* an unprepared sample, a sample after the application of a white latex paint and black line along the SPN to monitor the total applied shear strain, and a sample after 40% shear strain is imparted. 130

5.4 Constitutive response of IF steel and Mo to in-plane simple shear, with SD parallel to the RD and the SPN parallel to the TD. 131

5.5 Schematic detailing the large-scale tensile specimen geometry (dimensions in inches). 132

5.6 Large-scale tensile apparatus used for primary deformation of cross tests. 133

5.7 Extraction of secondary simple shear specimens from a deformed large tensile sample. 134

5.8 Constitutive response of IF steel sheet under a two-stage cross test, compared to monotonic simple shear (upper and lower bounds represent standard deviations from the average data). 135

5.9 Constitutive response of Mo sheet under a two-stage cross test, compared to monotonic simple shear (upper and lower bounds represent standard deviations from the average data). 136

5.10 Large-scale planar shear device, mounted within a hydraulic tensile apparatus. *Left:* mounting of the rig. *Right:* detail of the rig with mounted LVDT (top-left in figure). 137
5.11 Exploded view of the large-scale shear device, presenting the outer fixed grips (top-left, top-right) which clamp the ends of the sample, while the mobile grip (bottom center) clamps the center of the sample. A specimen deformed using the device is shown still clamped to the mobile grip. Arrows indicate the direction of relative displacement during deformation. ............................................. 138

5.12 Schematic detailing the large-scale shear specimen geometry (dimensions in inches). ............................................. 139

5.13 Shear strain distribution over the gauge zone in an IF steel sheet sample: (a) $\gamma = 0.1$; and (b) $\gamma = 0.3$. ............................................. 140

5.14 Constitutive response of IF steel sheet under a two-stage reverse test (upper and lower bounds represent standard deviations from the average data). ............................................. 141

5.15 Constitutive response of Mo sheet under a two-stage reverse test (upper and lower bounds represent standard deviations from the average data). 142

5.16 Schematic of the specimens used for primary strain-path tests in conventional cross-test studies (dimensions in inches). .............................. 143

5.17 Setup used for the primary strain-path tests in conventional cross-test studies. $A$: data acquisition system. $B$: high-intensity lights for image capture. $C$: image capture via digital camera or video. $D$: wide-grip mounts. ............................................. 144

5.18 Small-scale tensile specimens used for secondary strain-path tests in conventional cross-test studies: (a) extraction scheme using the pre-deformed specimen; and (b) schematic of the extracted tensile sample (dimensions in inches). ............................................. 145
5.19 Constitutive response of (a) IF steel and (b) Mo sheet during application of the secondary strain path in conventional cross-test analyses. . . . 146

5.20 EBSD scan of a representative IF steel sample used for two-stage strain-path tests. A comparison of pole figures for the local (complete, bottom left) and bulk (incomplete, bottom right) textures is provided. . . . . 147

5.21 Mo sheet texture scans: (a) unrefined local texture scan using a 4-µm step size; (b) local texture scan using a smaller 0.3-µm step size, refined using CHANNEL 5 software to predict non-indexed orientations (low-angle grain boundaries in light blue, boundaries with misorientations > 10° in black); (c) incomplete bulk texture pole figures for the Mo sheet; and (d) incomplete bulk texture pole figures for the Mo foil. . . 148

5.22 Comparison of experimental calibration data for IF steel with numerical results, upon activation of $I, R, I^{wd},$ and $R^{wd}$. . . . . . . . . . 149

5.23 Simulated behaviour of cross tests using the original Peeters model, with (a) no activation of recovery effects associated with non-currently generated CBB’s, (b) activation of $R_{ncg}$, and (c) activation of $R_{ncg}, \beta_1$ and $\beta_2$. . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 150

5.24 Simulated behaviour of the three-tier model, with increasing values of $R_{ncg}$ ($\beta_1 = \beta_2 = 0$). . . . . . . . . . . . . . . . . . . . . . . . . . . . 151

6.1 Comparison of $\beta_L$ for (a) CE-oriented grains and (b) CF-oriented grains under uniaxial tension, using constant nodal velocity $v_n$ and nodal acceleration $a_n$ profiles (see Appendix A). . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 169
6.2 Comparison of (a) a solution of the original Peeters model for an IF steel under monotonic loading with (b) a solution of the three-tier model with and without active $I_{wd}$ and $R_{wd}$ parameters. . . . . . . . . . 170

6.3 Comparison of (a) cross-test data of IF steel sheet presented by Peeters with (b) data acquired from tests at LPMTM of a similar material. . 171

A.1 Evolution of (a) total strain and (b) $\beta_L$ for a single-element, CE-oriented grain under uniaxial tension with a constant nodal velocity $v_n$. . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 196

A.2 Evolution of (a) applied strain, and (b) transverse and through-thickness strains for a single-element, CE-oriented grain under uniaxial tension, with varying levels of constant $v_n$. . . . . . . . . . . . . . . . . . . . . . . . . . . . 197

A.3 Evolution of (a) incremental $\beta_L$ and (b) total $\beta_L$ for a single-element, CE-oriented grain under uniaxial tension, with varying levels of constant $v_n$: $\epsilon_{RD} = 0.275$. . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 198

A.4 Evolution of (a) applied strain, and (b) transverse and through-thickness strains for a single-element, CE-oriented grain under uniaxial tension, with varying timestep (dt): $v_n = 2.44E-8 \text{ m/s}$. . . . . . . . . . . . . . . . . . . . . . . . . . . 199

A.5 Evolution of (a) applied strain, and (b) transverse and through-thickness strains for a single-element, CE-oriented grain under uniaxial tension, with varying levels of constant $\dot{\epsilon}$. . . . . . . . . . . . . . . . . . . . . . . . . . . . 200

A.6 Evolution of (a) incremental $\beta_L$ and (b) total $\beta_L$ for a single-element, CE-oriented grain under uniaxial tension, with varying levels of constant $\dot{\epsilon}$: $\epsilon_{RD} = 0.275$. . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 201
A.7 Evolution of (a) applied strain, and (b) transverse and through-thickness strains for a single-element, CE-oriented grain under uniaxial tension, with varying timestep (dt): $\dot{\varepsilon} = 3.0E-2$ s$^{-1}$. ........................................ 202

A.8 Evolution of (a) applied strain, and (b) transverse and through-thickness strains for a single-element, CE-oriented grain under uniaxial tension, with varying levels of constant $a_n$. ........................................ 203

A.9 Evolution of (a) incremental $\beta_L$ and (b) total $\beta_L$ for a single-element, CE-oriented grain under uniaxial tension, with varying levels of constant $a_n$: $\epsilon_{RD} = 0.275$. ........................................ 204

A.10 Comparison of (a) applied strain, and (b) transverse and through-thickness strains for a single-element, CE-oriented grain under uniaxial tension, using initial conditions as shown in Figure A.8, and under a shortened test run. ........................................ 205

A.11 Comparison of (a) incremental $\beta_L$ and (b) total $\beta_L$ for a single-element, CE-oriented grain under uniaxial tension, using initial conditions as shown in Figure A.8, and under a shortened test run. ........................................ 206

A.12 Comparison of (a) strain evolution, and (b) $\beta_L$ for a single-element, CE-oriented grain under uniaxial tension, using original and optimized velocity profiles. ........................................ 207

A.13 Comparison of (a) strain evolution, and (b) $\beta_L$ for a single-element, CF-oriented grain under uniaxial tension, using original and optimized velocity profiles. ........................................ 208

A.14 Comparison of (a) strain evolution, and (b) $\beta_L$ for a single-element, CC-oriented grain under uniaxial tension, using original and optimized velocity profiles. ........................................ 209
B.1 1x3-element mesh used to analyze $\beta_L$ at the onset of plasticity (plot of Euler angle $\Phi$ shown – CF = blue, CE = red). 216

B.2 Mesh scale effects: contour plots of transverse strain after an applied strain of 20% along the x axis (interpolation suppressed to discretize solution). Results are given for models under varying refinement: (a) 1x3-element mesh; (b) 1x9-element mesh; and (c) 1x15-element mesh sizes. 217

B.3 Effects of constant-acceleration velocity profiles in multi-element solutions. Contour plots of the longitudinal strain in (a) a 3x1-element CE mesh, (b) a 5x1-element CE mesh, (c) a 7x1-element CE mesh, and (d) a 9x1-element CE mesh, subjected to a total strain of 25% along the x axis. 218
Abbreviations

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>IF</td>
<td>Interstitial-free</td>
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<tr>
<td>CP</td>
<td>Crystal plasticity</td>
</tr>
<tr>
<td>FC</td>
<td>Full constraint</td>
</tr>
<tr>
<td>FE(M)</td>
<td>Finite element (method)</td>
</tr>
<tr>
<td>EBSD</td>
<td>Electron backscatter diffraction</td>
</tr>
<tr>
<td>OM</td>
<td>Orientation mapping</td>
</tr>
<tr>
<td>SEM</td>
<td>Scanning electron microscope</td>
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<tr>
<td>TEM</td>
<td>Transmission electron microscope</td>
</tr>
<tr>
<td>bcc</td>
<td>Body-centered cubic</td>
</tr>
<tr>
<td>fcc</td>
<td>Face-centered cubic</td>
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<tr>
<td>Abbreviation</td>
<td>Description</td>
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<td>-------------</td>
<td>--------------------------------------------------</td>
</tr>
<tr>
<td>CE</td>
<td>Cube-on-edge</td>
</tr>
<tr>
<td>CF</td>
<td>Cube-on-face</td>
</tr>
<tr>
<td>CC</td>
<td>Cube-on-corner</td>
</tr>
<tr>
<td>CB</td>
<td>Cell boundary</td>
</tr>
<tr>
<td>CBB</td>
<td>Cell-block boundary</td>
</tr>
<tr>
<td>NCG</td>
<td>Non-currently generated</td>
</tr>
<tr>
<td>RD</td>
<td>Rolling direction</td>
</tr>
<tr>
<td>TD</td>
<td>Transverse direction</td>
</tr>
<tr>
<td>ND</td>
<td>Normal direction</td>
</tr>
<tr>
<td>SD</td>
<td>Shearing direction</td>
</tr>
<tr>
<td>SPN</td>
<td>Shear plane normal</td>
</tr>
<tr>
<td>LPMTM</td>
<td>Laboratoire des Propriétés Mécaniques et Thermodynamiques des Matériaux</td>
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</table>
Nomenclature

\[ x \quad \text{Scalar} \]
\[ \mathbf{x} \quad \text{Tensor} \]
\[ x_{ij} \quad \text{Components of a } 2\text{nd-rank tensor} \]
\[ \dot{x} \quad \text{Time derivative of } x \]
\[ \mathbf{A} \quad \text{Tensor representing the crystallographic orientation of a single crystal} \]
\[ b \quad \text{Magnitude of the Burgers vector} \]
\[ \mathbf{d} \quad \text{Slip direction} \]
\[ E \quad \text{Young’s modulus} \]
\[ f \quad \text{Volume fraction of dislocation sheets} \]
\[ G \quad \text{Shear modulus} \]
\[ I \quad \text{Immobilization coefficient associated with the randomly distributed dislocation density } \rho \]
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<tbody>
<tr>
<td>$I^{wd}$</td>
<td>Immobilization coefficient associated with density of CBB dislocations, $\rho^{wd}$</td>
</tr>
<tr>
<td>$I^{wp}$</td>
<td>Immobilization coefficient associated with the polarized dislocation density, $\rho^{wp}$</td>
</tr>
<tr>
<td>$K$</td>
<td>Tensor comprising orientation data for potentially active slip systems</td>
</tr>
<tr>
<td>$M$</td>
<td>Taylor factor</td>
</tr>
<tr>
<td>$n$</td>
<td>Slip plane normal</td>
</tr>
<tr>
<td>$R$</td>
<td>Recovery coefficient associated with the randomly distributed dislocation density $\rho$; Lankford coefficient</td>
</tr>
<tr>
<td>$R_{ncg}$</td>
<td>Recovery coefficient associated with the dislocation density in non-currently generated CBB’s</td>
</tr>
<tr>
<td>$R_{rev}$</td>
<td>Recovery coefficient associated with the change in polarized dislocation density $\rho^{wp}$ due to the reversal of flux $\Phi^{wp}$</td>
</tr>
<tr>
<td>$R_{sat}$</td>
<td>Saturation value of the randomly distributed dislocations</td>
</tr>
<tr>
<td>$R^{wd}$</td>
<td>Recovery coefficient associated with density of CBB dislocations, $\rho^{wd}$</td>
</tr>
<tr>
<td>$R^{wd}$</td>
<td>Recovery coefficient associated with the polarized dislocation density, $\rho^{wp}$</td>
</tr>
<tr>
<td>$R_2$</td>
<td>Recovery coefficient associated with the change in dislocation density $\rho$ due to re-mobilized polarity dislocations</td>
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<tr>
<td>Symbol</td>
<td>Definition</td>
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<tr>
<td>--------</td>
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</tr>
<tr>
<td>$R_t$</td>
<td>Total surface roughness</td>
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<tr>
<td>$t$</td>
<td>Sample thickness</td>
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<tr>
<td>$u_i^w$</td>
<td>Unit vector perpendicular to the $i^{th}$ family of CBB’s</td>
</tr>
<tr>
<td>$u_s^b$</td>
<td>Unit vector assigned to the slip direction of slip system $s$</td>
</tr>
<tr>
<td>$W_T$</td>
<td>Plastic work</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>Dislocation interaction parameter</td>
</tr>
<tr>
<td>$\beta_1, \beta_2$</td>
<td>Fitting parameters for microband cut-through</td>
</tr>
<tr>
<td>$\beta_L$</td>
<td>Plastic strain ratio</td>
</tr>
<tr>
<td>$\epsilon$</td>
<td>Plastic strain</td>
</tr>
<tr>
<td>$\epsilon_p$</td>
<td>Plastic strain</td>
</tr>
<tr>
<td>$\epsilon_{VM}$</td>
<td>Equivalent von Mises plastic strain</td>
</tr>
<tr>
<td>$\Phi_i^{wd}$</td>
<td>Flux of mobile dislocations coplanar to the $i^{th}$ family of CBB’s meeting these CBB’s</td>
</tr>
<tr>
<td>$\Phi_i^{wp}$</td>
<td>Flux of mobile dislocations non-coplanar to the $i^{th}$ family of CBB’s meeting these CBB’s</td>
</tr>
<tr>
<td>$\gamma$</td>
<td>Crystallographic slip; shear strain</td>
</tr>
<tr>
<td>$\dot{\gamma}_s$</td>
<td>Dislocation slip rate along slip system $s$</td>
</tr>
</tbody>
</table>

xxv
\( \dot{\Gamma}_i \)  Total slip rate on the slip system with the \( i^{th} \) highest slip

\( \dot{\Gamma}_{\text{new}} \)  Total combined slip rate on the two slip systems with the highest slip activity, \( \dot{\Gamma}_1 + \dot{\Gamma}_2 \)

\( \phi_1, \Phi, \phi_2 \)  Euler angles

\( \kappa \)  Longitudinal strain ratio between outermost and innermost finite elements

\( \rho_{\text{bausch}} \)  Re-mobilized polarity dislocation density

\( \rho_s \)  Global dislocation density on slip system \( s \)

\( \rho_{\text{sat}} \)  Saturation value of the randomly distributed dislocation density \( \rho \)

\( \rho_{\text{wp}}^{\text{sat}} \)  Saturation value of the polarized dislocation density \( \rho_{\text{wp}} \)

\( \rho_{\text{wd}} \)  Density of immobile dislocations stored in CBB’s

\( \rho_{\text{wp}} \)  Density of directionally moveable (or polarized) dislocations

\( \sigma \)  Macroscopic flow stress

\( \tau \)  Microscopic flow stress

\( \tau_0 \)  Initial critical resolved shear stress

\( \tau^{\text{CB}} \)  Local shear resistance in cell-block interiors

\( \tau^{\text{CBB}} \)  Local shear resistance in cell-block boundaries

\( \tau_s \)  Resolved shear stress on slip system \( s \)
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\tau_s^c$</td>
<td>Critical resolved shear stress on slip system $s$</td>
</tr>
<tr>
<td>$\tau_{\text{sat}}$</td>
<td>Saturation value of the shear resistance $\tau$</td>
</tr>
<tr>
<td>$\tau^{\text{wd}}$</td>
<td>Local shear resistance due to the dislocation density $\rho^{\text{wd}}$ in CBB’s</td>
</tr>
<tr>
<td>$\tau^{\text{wp}}$</td>
<td>Local shear resistance due to the directionally movable dislocation density $\rho^{\text{wp}}$</td>
</tr>
<tr>
<td>$\psi$</td>
<td>Flux switch parameter</td>
</tr>
<tr>
<td>$\mathbf{d}\omega$</td>
<td>Incremental crystal rotation tensor</td>
</tr>
</tbody>
</table>
In recent years considerable effort has been made to develop accurate numerical models to predict sheet metal forming behaviour for complex loading scenarios. The challenges facing modellers are great: discretization issues related to relatively small through-thickness dimensions, localization issues such as shear-band formation, and verification issues due to complexities in experimental data acquisition (e.g. through-thickness strain readings) are some of the most formidable problems at hand [1]. Nevertheless, the predictive capability of these models continues to improve.

A new area of concern in the simulation of sheet metal plasticity is the evolution of surface roughness as a function of applied strain. Many analytical models currently used to study plasticity assume the sheet material experiences homogeneous deformation, which is prohibitive to analysing surface roughening behaviour. During the early development of such models, separate studies were underway to examine inhomogeneous ridging in ferritic stainless steels [2–4]; at the time, however, macroscopic, strain-induced surface roughening was studied in an attempt to eliminate the poor aesthetic quality resulting from deep drawing applications. As a consequence,
the results from this early work have only recently been applied to multi-path sheet forming operations.

Decades of research concerning the ridging behaviour found in ferritic stainless steel have led to conclusions applicable to a variety of sheet metals; of note, macroscopic surface roughening can be directly related to the crystallographic texture of the material. The texture – in many cases, comprising bands or clusters of similarly oriented grains – has been shown to also contribute to heterogeneous deformation within the material due to texture-specific differences in work hardening [3]; it cannot be assumed, however, that accounting for texture alone will accurately predict constitutive behaviour and failure events. Yamaguchi et al. [5] have shown that forming limits for sheet metals increase when surface roughness – not texture – is removed from the material, implying a geometric effect.

The aforementioned challenges in numerical analyses of sheet metal formability are further compounded when considering complex loading operations. The application of multiple forming operations to parts comprising sheet material are commonly used in the automobile industry. Figure 1.1 illustrates an example where steel tube product is subjected to axial bending followed by a hydroforming process – such processes are typical in the construction of automotive frames [6]. In this case, two completely different strain paths are imposed sequentially; this introduces the potential for additional work-hardening effects unique to multiple-path operations. Consequently, conventional plasticity models must not only simulate deformation during simple monotonic loading, but they must also account for material behaviour once a new strain path is applied. These features comprise the current objectives of predicting sheet metal formability: to produce a model that utilizes the crystallographic texture of the material to predict heterogeneous work-hardening behaviour, thereby facilitating
the analysis of surface roughness evolution during complex loading procedures.

1.1 Research Scope

The study presented herein focuses on the development and validation of a numerical model capable of simulating inhomogeneous material deformation and the evolution of surface topography under a variety of loading scenarios. The greatest advancement to current predictive capabilities is realised via a detailed study of body-centered cubic (bcc) material such as steel sheet product, since the majority of related data published is for this crystalline structure, allowing for an accurate and thorough assessment of the proposed model. Both Mo and interstitial-free (IF) steel sheet have been selected as candidate materials; furthermore, analyses of Mo foil are performed to examine the influence of through-thickness texture on model accuracy. The objectives that follow outline the numerical and experimental targets that are specific to the thesis work presented herein:

- Characterize local surface roughness and crystallographic texture, and compare these trends to bulk material properties;
- Develop a process to ensure coincidence in local measurements taken prior to and after specimen deformation;
- Develop a multi-scale model capable of using local texture measurements as input to predict heterogeneous plastic behaviour;
- Validate the components of the multi-scale model using published theory and empirical data, in regards to both texture evolution during deformation and texture-based anisotropy;
• Assess the numerical accuracy of the model by comparing the predicted surface roughness and texture of Mo foil deformed under uniaxial tension to experimental results;

• Capture the constitutive response of bcc materials subjected to a variety of two-stage strain-path tests;

• Assess the suitability of the numerical model for providing solutions to complex forming operations.

This research represents the first attempt to evaluate heterogeneous material deformation during two-stage loading scenarios, focusing on surface roughness as a means of validation. Analyses of Mo foil and sheet product will also be addressed, as only IF steel sheet has been previously studied during limited two-stage strain-path tests [7]. Additional loading schemes will be studied that have not been examined previously using similar modelling approaches, and are more representative of common industrial forming operations. This additional work will prove the versatility of the multi-scale model such that industrial applicability may be realised. Furthermore, successful prediction of surface roughening behaviour in the material has significant benefits, as it will prove the model is capable of predicting such inhomogeneous behaviour from the undeformed local texture scans of the material exclusively.

1.2 Thesis Outline

The body of this thesis is presented via the following chapters:

Chapter 2 provides a summary of theory and experiment related to texture
effects, surface roughening, and complex strain-path behaviour, as found in the literature;

Chapter 3 elucidates the development of a three-tier multi-scale model, with validation of its core functionality using theoretical benchmarks;

Chapter 4 presents experimental data and numerical analyses pertaining to monotonic deformation of Mo foil specimens;

Chapter 5 contains the collective two-stage strain-path experiments for Mo and IF steel sheet specimens, along with calibration and validation studies;

Chapter 6 elaborates on important aspects of the research observed in previous chapters and includes a discussion of the contributions to the field that arise as a result of this work;

Chapter 7 provides a summary of key findings and primary recommendations for further study of related issues.
Figure 1.1: Tube pre-bending and hydroforming process commonly used in the automotive industry (adapted from [6]). Above: placement of a pre-bent steel tube into a hydroforming die. Below: morphology of the tube cross-section as a result of the hydroforming process.
Chapter 2

Literature Review

This chapter reviews the advances made in predicting both the constitutive response of materials under a variety of loading conditions, and the development of deformation-induced surface roughening. Much of the past research into work hardening and surface roughening has been developed separately; therefore, accounts of this work have been divided herein for clarity. Subsequent combination of the two characteristics are then addressed in a detailed overview of the hardening model that is to be incorporated into the present work. Much of the recounted material in the following sections examines the behaviour of body-centered cubic (bcc) crystal structures, although some mention is made of work regarding face-centered cubic (fcc) studies where pertinent advances have been made.

2.1 Development of Surface-Roughening Models

When addressing surface roughening, it is important to first identify the length scale of interest. As the current focus is on the relationship between this roughening behaviour
and local work-hardening characteristics, micron-scale macroscopic roughening events such as orange-peel and ridging/roping effects are considered, whereas microscopic events such as slip band formation and surface cracks are not.

Much of the early theoretical work in identifying the cause of surface roughening was performed on ferritic stainless steels, most notably Fe 17% Cr. Studies by Takechi et al. [2] and Chao [3] were the first to relate the presence of deformation-induced ridges in these steels to the crystallographic texture produced during sheet fabrication. Realising that the crystallographic orientation of a grain in a material affects the associated work-hardening rate, it was believed that groups or colonies of similarly oriented grains existed within cold-rolled sheet materials, such that the deformation in one area of the material was noticeably different from another area, leading to the formation of a corrugated surface profile. An example of Chao’s hypothesis is presented in Figure 2.1: here, the orientation-dependent variation in the Lankford coefficient $R$ causes a divergence in the strain normal to the sheet surface, leading to the development of surface roughness.

Unfortunately, the ribbed profiles predicted by Chao were not observed in the ferritic stainless steels analysed. Early theoretical models were also grossly oversimplified, as they relied on large clusters of similarly oriented grains existing within the material to produce the observed ridges – an assumption that was later proven incorrect. Subsequent models developed by Wright [4] and Harase et al. [8] do not require such large clusters; instead, the authors assumed the corrugated behaviour of the material resulted from the warping or plastic bending of bands of different texture. The reduced cluster size and corrugated surface quality was closer to observed data than in previous work, but there was still considerable deviation. The most recent work in these sheet materials has been reported by Bethke et al. [9] and Brochu
et al. [10]; the models developed in this work utilize electron backscatter diffraction (EBSD) techniques to examine specific orientations of grains over a large region of the material, both on the normal surface and through the thickness of the sample, along rolling and transverse directions. Consideration of through-thickness texture-based inhomogeneity similar to that observed on the surface has led to the development of models that qualitatively describe the roughening phenomena and also provide a reasonable level of quantitative accuracy.

Using the work of ferritic stainless steels as a foundation, research into roping/ridging behaviour has spread into other materials, notably Al sheet. Work by Beaudoin et al. [11], Baczynski et al. [12], Wu et al. [13], and Bennett et al. [14] apply the texture-based theory developed in bcc steel to fcc aluminum. Of particular importance is the work of Wu et al., who have shown good qualitative agreement between numerical solutions of roping behaviour with experimental results of Al sheet under a variety of simple loading scenarios. Solutions were obtained using a two-dimensional plane-stress finite-element (FE) model, relying on through-thickness deformation of the surface grains to account for the predicted roughening behaviour. It may be inferred from this work that a FE approach for predicting the evolution of surface roughness during deformation warrants further investigation.

2.2 Development of Finite-Element Models to Capture Local Work Hardening

Currently, FE analyses have been implemented using both crystal plasticity and continuum mechanics to describe the constitutive response of a material under deforma-
tion. Continuum mechanics allows for an average response over a discrete volume of material, which implies that the predicted behaviour is homogenous in nature. Heterogeneous behaviour, due to mesoscopic and microscopic influences, has been identified as the cause for such macroscopic events as surface roughening [15]; hence, continuum models are inappropriate to accurately simulate local variations in constitutive response necessary for this research.

The most frequently implemented crystal-plasticity model is the full constraint (FC) Taylor model [16]. The model assumes the strain-rate tensor applied to each crystal in a polycrystalline aggregate is equivalent to the macroscopic strain-rate tensor. As such, strain compatibility across the specimen is ensured, although force equilibrium across grain boundaries is violated. Bishop and Hill [17, 18] further extended this work, modifying some of the base assumptions used in FC Taylor models. One such modification is Hill’s Maximum Work Principle [19], which states that of all stress states permitted by the yield locus of the crystal, the one that maximizes the external plastic work is correct. For this reason, the Taylor-Bishop-Hill (TBH) model has been referred to as an upper bound model. By contrast, an earlier model developed by Sachs [20] satisfies neither compatibility nor equilibrium conditions, but assigns proportional (not uniform) loading to each grain in the aggregate. The correct solution in this treatment is that which produces a minimization of external work, and as such, it is termed a lower bound model.

Several crystal-plasticity models have been developed that attempt to satisfy both equilibrium and compatibility to varying extents. Two of the more popular are relaxed constraint (RC) Taylor models and self-consistent models. RC Taylor models,

---

1A detailed description of the FC Taylor model and its implementation within a FE code is presented in Chapter 3.
such as the one developed by Van Houtte [21], apply the same constraints as in the FC Taylor model with some slight modifications. The model is advantageous for application-specific processes such as metals subject to rolling operations, where appropriate shear terms in the prescribed strain-rate tensor are left free, leading to more realistic predictions of constitutive response. Self-consistent models create the overall aggregate response from analysis of the known properties of the constituent grains and the interaction of these grains with their environment, which is assumed to be a homogeneous medium for each grain [22, 23]. The model allows for strain compatibility and force equilibrium in an average sense, due to the compliant nature of the surrounding material for each grain analysed.

Many of the aforementioned crystal-plasticity models provide a solution that is non-unique (i.e. one of several sets of linearly independent slip systems that satisfy some necessary criteria are chosen arbitrarily), resulting in potentially erroneous predictions of crystal rotation during deformation that may lead to incorrect predictions of texture evolution. Such non-uniqueness stems from the inability of these models to select the appropriate set of slip systems for a given applied strain, as multiple sets of slip systems may satisfy the conditions required for deformation; the chosen set will dictate the grain rotation, and different sets can lead to an entirely different grain rotation path while resulting in the same observed deformation. A proposed solution to this non-uniqueness issue has been rate-dependent models, in particular the one developed by Asaro and Needleman [24]. What accounts for a unique solution in these models is the assumption that all slip systems are simultaneously active; unfortunately, this assumption may inaccurately predict the amount of slip on a given slip system, which may be problematic if the work-hardening model used relies on this phenomena to be quantitatively accurate.
2.2.1 Overview of Integrated Work-Hardening Models

The primary difference between the preceding models is the method by which the active slip systems are chosen. Another variable in crystal-plasticity models is the type of work-hardening model employed, which is necessary for predicting the constitutive response of the material. Establishing a physical representation of the work-hardening behaviour of metals requires a thorough understanding of dislocation theory, particularly aspects involving dislocation motion, interaction, and substructure evolution. Comprehensive reviews pertaining to various stages of work hardening and the role dislocations play in each have been presented by Honeycombe [25] and Gil Sevillano [26]. In these accounts, the importance of forest hardening is highlighted. During polycrystalline deformation, multiple sets of slip systems will activate such that dislocations will accumulate on several planes, many of which will be non-coplanar. The interactions these dislocations have with each other dictate both the evolution of the dislocation substructure and the work-hardening rate.

It is commonly understood that after a given amount of strain\(^2\), dislocations become tangled and interconnected, resulting in loose cellular structures. As the strain increases the structures become well-defined, until a definite heterogeneity is observed in the dislocation density; Figure 2.2 provides a schematic example of this cellular patterning. Additional strain causes the cell walls to become sharper, while the diameter of the cell decreases [27]; such behaviour follows the principle of similitude, as first defined by Kuhlmann-Wilsdorf [28], which proposes a direct correlation exists between the diameter of the cell and the thickness of the cell wall. Equilibrium during Stage III hardening (defined below) is maintained due to interplay between

\(^2\)The nominal strain has been identified to lie between 3 and 10 %, but the exact value is temperature-dependent [7].
the reduction in strain energy from decreasing cell wall thickness, and an increase in strain energy between the walls due to a proportionally-reduced cell diameter.

While work hardening is a direct result of dislocation interaction within the material, the level of physical representation of these effects in models is varied. For example, the model of Asaro and Needleman [24] uses a highly phenomenological approach in calculating plasticity in metals. A simple power-law relation is used between the slipping rate and the ratio of the resolved shear stress to a hardness parameter that evolves with strain. The hardness parameter is advantageous in that it describes the phenomenology of both self hardening (the increase in the critical resolved shear stress along the slip systems due to dislocations on those systems) and latent hardening (the increase in the critical resolved shear stress along a slip system due to dislocation interaction with defects on other slip systems) in the material.

In contrast, more recent quasi-static studies of dislocation behaviour by transmission electron microscopy have led to hardening models that are based on a mesoscopic length scale. The use of a more physically realistic model adds to the complexity of the analysis, as not only is the level of physical representation varied, but the applicability of the model over various stages of work hardening also comes into question. Figure 2.3 highlights the first three stages of work hardening:

- Stage I – the activation of a single slip system (achievable only in single-crystal specimens);
- Stage II – a region of linear stress-strain behaviour; and
- Stage III – parabolic behaviour, signifying the end of athermal hardening.

Stage IV and further stages of hardening have been observed [26]; however, the onset of Stage IV hardening (characterised by a thermally dependent work-hardening rate)
does not occur until significant strain (i.e. over 30%) has been introduced. Very few loading schemes allow these latter stages of hardening to occur before failure; as such, only models that are accurate over Stages II and III of work hardening are to be considered here.

One of the more accepted work-hardening models is the Kocks-Mecking-Estrin model, or the mechanical threshold stress (MTS) model [29]; versions of the MTS model have been implemented by Follansbee and Kocks [30] and Barlat et al. [31]. The model is based on a one-parameter mesoscopic analysis, with terms accounting for dislocation storage and dynamic recovery, for Stages II and III of work hardening. It uses the concept of the mechanical threshold stress of the material, and is advantageous over other models in that temperature and strain-rate effects may be decoupled and their influence on the flow stress viewed separately. Unfortunately, this single-parameter model cannot predict the transient behaviour during strain-path changes under investigation [7]. Multi-parameter models such as the ALFLOW model developed by Nes [27] are effective for the simulation of plasticity over a broader range of strain, up to and including Stage IV hardening. Due to the range of hardening the model is able to predict, and the use of a more complex dynamic recovery model, the Nes model uses three independent parameters to capture the material behaviour: the size of the cell/subgrain formed by dislocations during deformation, the dislocation density inside the cell, and the sub-boundary misorientation.

A third mesoscopic hardening model has been developed by Peeters [7]; the model also uses a multi-parameter approach to simulate cell evolution in bcc materials during Stage II and III hardening. The significance of this model is that while some models can simulate certain specific transient effects (e.g. a model that accounts for Bauschinger effects [32]), the Peeters model is the only published model capable
of predicting the general transient hardening/softening behaviour during changes in
strain path for bcc materials, a quality that is particularly important for the current
research. The model has since been modified and applied to the study of fcc copper
[33], and a simplified version of the model has been adapted to accurately predict the
constitutive behaviour of an AA3103 aluminum alloy by Holmedal et al. [34].

2.3 Capturing Transient Constitutive Behaviour

The work-hardening model developed by Peeters [7] highlights the key features of
Stage II and III behaviour. Several dislocation density terms have been identified to
mimic the evolution of a cellular substructure in the material, while storage and recov-
ery terms are included to represent dynamic recovery. The model uses a dislocation
density $\rho$ to account for both the dislocations in the cell walls and the statistically
stored dislocations within the interior of the cells. As both dislocation types con-
tribute equally to the isotropic hardening of the material, no distinction is necessary
for the desired analysis.

The key advantage of the Peeters model lies in the ability to predict transient
work-hardening behaviour inherent in many changes in strain path. Transient effects
have been observed in the early works of Basinski and Jackson [35–37], and more
recently by Bate [38]; in these studies, the contribution of alien dislocations to the
transient behaviour is identified. Alien dislocations are defined as dislocations that
are formed during an initial application of strain, which are then non-coplanar to
dislocations formed during subsequent deformation in a new direction. The afore-
mentioned studies were performed on fcc materials that included copper and alu-
minum, and showed a decrease in work-hardening rate due to softening attributed to
the recovery of these alien dislocations. In contrast, studies by Peeters on IF steel sheet revealed the transient constitutive response varies depending upon the two-stage loading scheme applied [39]. Two of the most influential effects observed lay the foundation of simulated transient effects in the Peeters model: cross effects and Bauschinger effects.

Cross effects are observed in materials subjected to significant changes in strain-path orientation. In the IF steel sheet tested by Peeters, pre-strain via uniaxial tension followed by an orthogonal shear strain displays a sharp increase in the yield stress upon the change in strain path, followed by a transient reduction in the work-hardening rate, when compared to that observed under the same degree of monotonic loading (see Figure 2.4). Another physical characteristic that developed during testing was the formation of microbands in the material; such behaviour has also been observed in other low-carbon ferritic steels [38]. The Peeters model has incorporated terms to account for this microband formation, with parameters that are curve-fit to the transient behaviour observed experimentally (discussed further in Section 2.3.1).

Bauschinger effects are unique in that the dislocations responsible for transient work-hardening behaviour are not alien, i.e. they are coplanar after the change in strain path. The resultant transient behaviour arises from a reversal of strain path, such that uninhibited dislocations travel along identical slip planes in the opposite direction. Bauschinger effects are signified (Figure 2.4) by a reduction of the yield stress in the initial few percent of applied strain after load reversal, followed by work hardening behaviour similar to that of monotonic loading (i.e. yield asymmetry with no persistent offset).

To account for the Bauschinger and cross effects requires some parameterization of the evolving material substructure. Peeters idealized this substructure (Figure 2.5)
into dislocation sheets or cell-block boundaries (CBB’s). CBB’s evolve in a manner similar to the isotropic cellular structures defined by Nes [27], including adherence to the principle of similitude [28]. The key feature of these characteristics lies in the inherent anisotropy observed in TEM micrographs; CBB’s form along the most active slip systems in preferred directions, based on the direction of the applied strain path. This anisotropy aids in the development of heterogenous deformation associated with local work hardening. To define these effects, two parameters are introduced: a dislocation density associated with the dislocation sheet \( (\rho_{wd}) \) and a dislocation density associated with polarized dislocations \( (\rho_{wp}) \). Polarized dislocations are those dislocations of similar Burgers vector that accumulate on either side of the CBB, as shown schematically in Figure 2.5. These dislocations account for the Bauschinger effect observed during load reversal; that is, continued loading in the original direction of applied strain causes these dislocations to attempt travel through the CBB where resistance is high, while load reversal causes the dislocations to travel through the relatively dislocation-free cell interior where resistance is considerably lower, causing the material to appear softer in a macroscopic sense.

2.3.1 Numerical Representation of Transient Effects

The integration of a work-hardening model into a crystal-plasticity formulation requires the solution of the latter to provide identification of the active slip systems, the amount of slip on those systems, the stresses produced, and the evolution of the crystallographic texture in the material due to grain rotations. The slip derived from this model may then be utilised in work-hardening formulae to predict substructure evolution and subsequent alteration of the critical resolved shear stresses on active
systems. The derivation of the critical resolved shear stress \( \tau_s^c \) on a slip system \( s \) is the sum of several terms dependent on the dislocation density of the system:

\[
\tau_s^c = \tau_0 + (1 - f)\tau_{\text{CB}} + f \sum_{i=1}^{6} (\tau_{is}^{\text{wp}} + \tau_{is}^{\text{wd}})_{\text{CBB}},
\]

(2.1)

where \( \tau_0 \) represents stresses in the system not included in the internal variables considered (e.g. solid solution, initial grain size) and \( f \) the volume fraction of CBB’s. The remaining terms are defined as follows:

\[
\tau_{\text{CB}} = \alpha Gb\sqrt{\rho_{i}}; \quad (2.2)
\]

\[
\tau_{is}^{\text{wd}} = \alpha Gb[\sqrt{\rho_{i}^{\text{wd}}abs(u_b^s \cdot u_w^i)}]; \quad (2.3)
\]

\[
\tau_{is}^{\text{wp}} = \alpha Gb[\sqrt{abs(\rho_{i}^{\text{wp}})u_b^s \cdot u_w^i \text{sign}(\rho_{i}^{\text{wp}})}]. \quad (2.4)
\]

Here, the three dislocation density terms driving the work-hardening model are found: \( \rho \) (randomly distributed dislocations), \( \rho_{\text{wd}} \) (CBB dislocations), and \( \rho_{\text{wp}} \) (polarized dislocations, which lie along CBB’s but are mobile during strain-path reversal). Furthermore, \( \alpha \) is a dislocation interaction parameter, \( \tau_{is}^{\text{wd}} \) the shear stress contribution due to dislocations forming the \( i^{th} \) family of CBB’s, \( \tau_{is}^{\text{wp}} \) the shear contribution due to polarized dislocations along the \( i^{th} \) family of CBB’s, \( u_b^s \) the unit vector assigned to the slip direction of the current slip system \( s \), and \( u_w^i \) the unit vector normal to the \( i^{th} \) family of CBB’s.
Randomly Distributed Dislocations

Statistically distributed random dislocations ($\rho$) are the primary contributors to isotropic hardening within a material [7]. It is these dislocations that are involved in the construction of cell blocks (CB’s – see Figure 2.5) on the active slip planes, or $s$-planes. Using the Kocks evolution equation [40] as a foundation, the density evolution ($\dot{\rho}$) is described via:

$$\dot{\rho} = \frac{1}{b}(I\sqrt{\rho} - R\rho) \sum_{s=1}^{n} |\dot{\gamma}_s|, \quad (2.5)$$

where $I$ is the dislocation immobilization coefficient associated with the construction of CB’s – resulting in both self and latent hardening – and $R$ the dislocation recovery coefficient. The sum $\sum_{s=1}^{n} |\dot{\gamma}_s|$ represents the combined slip rate on all active slip systems. While Equation 2.5 is the only one required to calculate $\rho$ during monotonic loading, an alternate equation must be considered during a reversal of slip. In such cases, an increase in CB dislocation annihilation has been observed [7], attributed to re-mobilization of the polarized dislocations near the CBB’s ($\rho_{wp}$); therefore, a second term is added to Equation 2.5:

$$\dot{\rho} = \frac{1}{b}(I\sqrt{\rho} - R\rho) \sum_{s=1}^{n} |\dot{\gamma}_s| - \Psi R_2 \rho \frac{\rho_{\text{mauch}}}{\rho_{\text{sat}}} \sum_{s=1}^{n} |\dot{\gamma}_s|. \quad (2.6)$$

The coefficient $R_2$ is used to identify additional recovery due to the transformation of polarized dislocations $\rho_{wp}$ into randomly distributed dislocations $\rho$, and $\rho_{\text{sat}}$ represents the saturation density of polarized dislocations. Depending on the condition of the flux $\Phi_{wp}^i$ along the two most active slip systems\(^3\), three conditions may occur as

\(^3\)Further explanation of $\Phi_{wp}^i$ is provided in the following section on Polarized Dislocations.
outlined in Table 2.1. The switch parameter $\Psi$ consequently triggers slip reversal effects, and $\rho_{\text{bausch}}$ (the re-mobilized dislocation density) depends on the number of systems experiencing slip reversal.

**Immobile (CBB) Dislocations**

As with the randomly distributed dislocation density evolution, immobilization of dislocations within a CBB ($\rho^{\text{wd}}$) is assumed to follow a Kocks-type relationship:

$$\dot{\rho}_i^{\text{wd}} = \frac{1}{b} (I^{\text{wd}} \sqrt{\rho_i^{\text{wd}} - R^{\text{wd}} \rho_i^{\text{wd}}} \hat{\Gamma}_i),$$  \hspace{1cm} (2.7)

where $I^{\text{wd}}$ and $R^{\text{wd}}$ are used to identify immobilization and recovery of $\rho^{\text{wd}}$, and $\hat{\Gamma}_i$ represents the total slip rate on the $i^{\text{th}}$ highest slip system. Unlike the case with random dislocations, slip over all active systems is not additive due to the asymmetric hardening of dislocation sheets, leading to the inherent directionality observed in CBB’s.

Similar to the simulation of $\dot{\rho}$, changes to $\dot{\rho}_i^{\text{wd}}$ on a given slip system may occur once a change in strain path is experienced; in this case however, changes to the density evolution equation must be allowed only when new slip systems are activated, causing dislocation sheets to form on these systems. Once the new systems are activated, the evolution behaviour of the currently generated CBB’s will follow the behaviour described by Equation 2.7. As for the CBB’s that have been previously constructed, these non-currently generated (NCG) entities will experience a gradual annihilation due to two factors, each requiring a separate term. The first involves homogeneous
CHAPTER 2. LITERATURE REVIEW

annihilation of old CBB’s due to dislocations now active on new systems, such that:

\[ \dot{\rho}_{wd}^{\text{ncg}} = -\frac{R_{\text{ncg}}}{b} \rho_{i}^{\text{wd}} \dot{\Gamma}_{\text{new}}, \tag{2.8} \]

where \( R_{\text{ncg}} \) is used as a coefficient describing the dislocation recovery within NCG CBB’s. Note that the total slip rate on the two most active systems (\( \dot{\Gamma}_{\text{new}} \)) is now used since all mobile dislocations are considered to be on non-coincident slip systems.

The second recovery method lies in the formation of microbands that cut through existing dislocation sheets. Studies by Zisman et al. [41] accredit the formation of these microbands to the accommodation of large, localised shear strains in the material through lattice rotation, as evidenced by the misorientation between the microband and the surrounding crystal. In the Peeters model, a phenomenological approach is employed to simulate this behaviour:

\[ \dot{\rho}_{i}^{\text{wd(cut-through)}} = -\sqrt{\beta_{1}} \Gamma_{\text{new}} e^{-\beta_{1} \Gamma_{\text{new}}} \rho_{i0}^{\text{wd(ncg)}} \beta_{2}, \tag{2.9} \]

where \( \beta_{1} \) and \( \beta_{2} \) are material parameters, and \( \rho_{i0}^{\text{wd(ncg)}} \) is the dislocation density of immobile dislocations on NCG CBB’s prior to microband cut-through. The combined density of CBB dislocations following a change in active slip systems is then the summation of Equations 2.7, 2.8 and 2.9.

**Polarized Dislocations**

As previously explained, dislocations of similar sign or polarity tend to accumulate on either side of a dislocation sheet that is not coplanar to the dislocation (see Figure...
2.5). The accumulation of polarized dislocations is defined in terms of the net flux:

$$\Phi_{wd}^i = \sum_{s=1}^{n} \frac{\dot{\gamma}}{b} \mathbf{u}_{s}^b \cdot \mathbf{u}_{i}^w. \tag{2.10}$$

Equation 2.10 requires that coplanar dislocations will not interfere with the CBB, as $$\mathbf{u}_{s}^b \cdot \mathbf{u}_{i}^w = 0$$ in such an instance. Once again, using a Kocks-type relationship \[40\], polarized dislocations on currently generated CBB’s can be simulated from:

$$\dot{\rho}_{wp}^i = (\text{sign}(\Phi_{wd}^i)I_{wp}^w \sqrt{|\dot{\rho}_{wp}^i|} - R_{wp}^w \rho_{wp}^i)|\Phi_{wd}^i|, \tag{2.11}$$

where $$I_{wp}^w$$ and $$R_{wp}^w$$ are coefficients representing immobilization and recovery events, respectively. Unlike other types of dislocations, polarized dislocations are affected by both a reversal in slip and a change in active slip planes.

When slip systems change, the dislocation behaviour is treated in a manner similar to immobile CBB dislocations without the cut-through effects. Equation 2.10 is used to define the behaviour of the dislocations on the new slip systems, while a solution similar to Equation 2.8 is used to identify recovery events on NCG CBB systems, such that:

$$\dot{\rho}_{wp(\text{ncg})}^i = -\frac{R_{\text{ncg}}}{b}\rho_{wp}^i \dot{\Gamma}_{\text{new}}, \tag{2.12}$$

where the term $$R_{\text{ncg}}$$ is the same value as that used in Equation 2.8. As for slip reversal, the polarized dislocations are consequently released from the CBB (i.e. they travel away from the dislocation sheet as they are not entangled), leading to two phenomena:

(i) a reversal of flux occurs as these dislocations move away from the CBB – the dislocations become mobile and polarity decreases as the number of polarized
dislocations along the boundary is reduced, thus reducing $\rho^{wp}_i$; and

(ii) the mobile dislocations interact with the random CB dislocations, causing annihilation events (previously discussed in the section on Randomly Distributed Dislocations).

The simulation of (i) is represented by:

$$\dot{\rho}^{wp}_i = -R_{rev}\rho^{wp}_i |\Phi^{wp}_i|,$$

where $R_{rev}$ is the coefficient of recovery associated with flux reversal.

Equations 2.5 to 2.13 define the dislocation evolution behaviour during both monotonic and multi-path loading conditions. Updated densities are used in Equations 2.2 to 2.4, and a new critical resolved shear stress for a given slip system is calculated via Equation 2.1; thus, the predicted dislocation evolution in the material leads to work hardening/softening in the Peeters multi-scale model.

### 2.4 Research Objectives

It is the assertion of the Peeters group, as well as the present author, that the transient behaviour defined by cross and Bauschinger effects are sufficient to calibrate a work-hardening model such that the behaviour of any arbitrary two-stage loading scheme may be predicted. In addition, the assimilation of crystal-plasticity theory into a FE model has been shown to satisfy both force equilibrium and strain compatibility; using the approach outlined by Taylor remains efficient and effective in this treatment. The research scope outlined in Section 1.1 may therefore be modified to elaborate on targets related to the development and implementation of a multi-scale model.
• Integrate the work-hardening theory developed by Peeters *et al.* into a Taylor-based crystal-plasticity framework, such that the critical resolved shear stress on each potentially active slip system for a bcc grain may be predicted during deformation;

• Unify the aforementioned framework within a FE model, whereby each element represents all or part of a single grain within a polycrystalline aggregate, satisfying force equilibrium and strain compatibility;

• Devise a means of transferring orientation and position data from local texture maps to elements within a FE mesh.

The resultant model will be able to capture plasticity at mesoscopic, microscopic and macroscopic length scales, thereby addressing the overall goals of this research, outlined in Section 1.1.
Table 2.1: Slip reversal conditions arising during plastic deformation.

<table>
<thead>
<tr>
<th>Flux condition</th>
<th>$\psi$</th>
<th>$\rho_{\text{bausch}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>No fluxes reversed</td>
<td>0</td>
<td>n/a</td>
</tr>
<tr>
<td>1 flux reversed</td>
<td>1</td>
<td>$</td>
</tr>
<tr>
<td>2 fluxes reversed</td>
<td>1</td>
<td>$</td>
</tr>
</tbody>
</table>
Figure 2.1: Ridging mechanism proposed by Chao [3].
Figure 2.2: Cellular dislocation structure formed during Stage II hardening (adapted from [27]).
Figure 2.3: Stages of work hardening [26].
Figure 2.4: Experimental measurements of an IF steel during two-stage strain-path tests [7]. Above: Cross effects after primary applied strains of 10 and 20 %. Below: Bauschinger effects after primary applied strains of 10 and 30 %.
Figure 2.5: Above: TEM micrograph of an IF steel subjected to 20% tensile strain along the axis specified. Below: Schematic representation of the microstructure as outlined in the Peeters hardening model [7].
Chapter 3

Development of a Multi-Scale Model

This chapter details the numerical analyses employed to simulate crystallographic texture evolution and texture-based anisotropic behaviour. A crystal-plasticity (CP) framework based on a full-constraints (FC) Taylor method is integrated with the finite-element (FE) code LS-DYNA. The multi-scale model is validated in single- and multi-element cases under axisymmetric and plane-stress conditions, against benchmarks found in the literature. No account of work hardening is included in this chapter as the material behaviour of interest during the validation is purely plastic.

3.1 Crystal-Plasticity Formulation

Several articles elucidate the seminal work of G.I. Taylor [16]; the work of Reid [42] and Van Houtte [21] are hereto referred because the structure of their formulae is best suited to linear programming techniques. Only analyses of polycrystalline slip
are discussed, as true single crystal deformation is not examined in this treatment.

Consider a single crystal within a polycrystalline aggregate. This crystal has an orientation relative to the sample; using texture analyses developed by Bunge [43], this orientation is expressed in terms of a rotation from the sample coordinate system to that of the crystal, given by:

\[
A = \begin{bmatrix}
\cos \phi_1 \cos \phi_2 - \sin \phi_1 \sin \phi_2 \cos \Phi & \sin \phi_1 \cos \phi_2 + \cos \phi_1 \sin \phi_2 \cos \Phi & \sin \phi_2 \sin \Phi \\
-\cos \phi_1 \sin \phi_2 - \sin \phi_1 \cos \phi_2 \cos \Phi & -\sin \phi_1 \sin \phi_2 + \cos \phi_1 \cos \phi_2 \cos \Phi & \cos \phi_2 \sin \Phi \\
\sin \phi_1 \sin \Phi & -\cos \phi_1 \sin \Phi & \cos \Phi
\end{bmatrix},
\]

(3.1)

where \(\phi_1, \Phi,\) and \(\phi_2\) are Eulerian angles [43]. Equation 3.1 allows the global plastic strain \(\varepsilon^g\) to be transformed to the local crystal system, as \(\varepsilon^c\), via:

\[
\varepsilon^g_{kl} = A_{ik} A_{jl} \varepsilon^c_{ij}.
\]

(3.2)

Using Taylor’s theory, \(\varepsilon^c\) is obtained through the activation of up to five linearly independent slip systems. For any given set of slip systems, the amount of slip on each may be determined using the relation:

\[
\varepsilon^c = K \gamma,
\]

(3.3a)

\(^1\)All references to strain in this section are assumed to be plastic, unless otherwise noted.
which can be written out in full as:

\[
\begin{bmatrix}
\epsilon^c_2 \\
\epsilon^c_3 \\
\epsilon^c_4 \\
\epsilon^c_5 \\
\epsilon^c_6
\end{bmatrix}
= \begin{bmatrix}
n_2d_1^1 & n_2d_2^2 & n_2d_2^3 & n_2d_2^4 & n_2d_2^5 \\
n_2d_3^1 & n_2d_3^2 & n_2d_3^3 & n_2d_3^4 & n_2d_3^5 \\
n_1d_3^1 + n_3d_2^1 & n_2d_3^2 + n_3d_2^2 & n_2d_3^3 + n_3d_2^3 & n_2d_3^4 + n_3d_2^4 & n_2d_3^5 + n_3d_2^5 \\
n_1d_3^1 + n_3d_1^1 & n_3d_3^2 + n_3d_1^2 & n_3d_3^3 + n_3d_1^3 & n_3d_3^4 + n_3d_1^4 & n_3d_3^5 + n_3d_1^5 \\
n_1d_2^1 + n_2d_1^1 & n_2d_2^2 + n_2d_1^2 & n_2d_2^3 + n_2d_1^3 & n_2d_2^4 + n_2d_1^4 & n_2d_2^5 + n_2d_1^5
\end{bmatrix}
\begin{bmatrix}
\gamma^1 \\
\gamma^2 \\
\gamma^3 \\
\gamma^4 \\
\gamma^5
\end{bmatrix}
\]

The tensor \( \mathbf{K} \) is comprised of slip system orientation data for the potentially active systems, utilising direction cosines\(^2\) of the slip plane normal \( n \) and slip direction \( d \) for each system. Five slip systems are considered, hence there are five variables of slip \( \gamma^s \) and five sets of orientation data; each system is identified by the superscript shown in Equation 3.3b. This equation also takes advantage of the principle of constant volume during plastic deformation, eliminating one of the redundant normal strains and reducing the number of variables in \( \epsilon^c \) to five. Consequently, \( \mathbf{K} \) is reduced to a 5x5 matrix that allows for a non-trivial solution of Equation 3.3. The amount of slip is determined through the inversion of \( \mathbf{K} \):

\[
\gamma = \mathbf{K}^{-1}\epsilon^c
\]

which is significant when determining whether a given set of slip systems are linearly independent (Section 3.2.1).

One of the fundamental assumptions of the Taylor theory is that of all the possible slip combinations which achieve the prescribed crystallographic strain, the one that produces the minimum amount of internal work is truly active. The plastic work for

\(^2\)Cosine axes are specified by the subscript.
each set of candidate slip systems is compared via:

\[ W_T = \mathbf{\gamma} \cdot \mathbf{\tau}. \]  

(3.5)

The shear stress \( \mathbf{\tau} \) for each slip system is set to the respective critical resolved shear stress \( \tau_{crss} \), as the onset of plasticity is assumed. Since no work hardening is considered in the current implementation, the material will have a constant \( \tau_{crss} \) on each slip system; hence, Equation 3.5 is simplified to:

\[ \frac{W_T}{\tau_{crss}} = \sum_{s=1}^{5} \gamma^s. \]  

(3.6)

Once the active systems have been selected for a given increment of plastic strain, the corresponding change in crystallographic stress can be determined using a stress relation similar to Equation 3.3a:

\[ \mathbf{\sigma}^c = K\mathbf{\tau}, \]  

(3.7)

where \( \mathbf{\tau} \) is a 5x1 vector containing \( \tau_{crss} \) for each system. The global stress tensor \( \mathbf{\sigma}^g \) is subsequently determined, as in Equation 3.2, using the inverse of the transformation matrix, \( \mathbf{A}^{-1} \), such that:

\[ \sigma^g_{kl} = A^{-1}_{ik} A^{-1}_{jl} \sigma^c_{ij}. \]  

(3.8)

Equation 3.8 produces the deviatoric stress tensor. Therefore, assumptions must be made about the stress state to determine the hydrostatic stress and realize the total change in the stress state of the material; this issue is addressed in Section 3.2.1.
3.1.1 Taylor Ambiguity

A common problem in the implementation of FC Taylor or Taylor-Bishop-Hill (TBH) assumptions is that of so-called “Taylor ambiguity”, where the critical resolved shear stress may be reached simultaneously on more than five slip systems [21]. For example, Chin and Mammel illustrate several orientations in a body-centered cubic (bcc) material where six or eight systems can activate simultaneously [44]. While the internal work due to the selection of any five of these slip systems is equivalent, the resultant crystallographic rotation will differ.

A novel solution to this ambiguity was proposed by Renouard and Wintenberger for use with FC Taylor theory [21, 45]. In addition to minimizing the internal work, \( W_T \), the rate of change of work with respect to the von Mises strain \( \varepsilon_{VM} \) is also minimized, thus creating a first-order selection criterion. Taking the derivative of Equation 3.5 results in:

\[
\frac{dW_T}{d\varepsilon_{VM}} = \frac{d\gamma}{d\varepsilon_{VM}} \cdot \tau + \gamma \cdot \frac{d\tau}{d\varepsilon_{VM}}. \tag{3.9}
\]

If there is no work hardening present, \( \frac{d\tau}{d\varepsilon_{VM}} = 0 \) and Equation 3.9 reduces to:

\[
\frac{dW_T}{\tau_{crs}d\varepsilon_{VM}} = \frac{d\gamma}{d\varepsilon_{VM}}. \tag{3.10}
\]

Hence, the optimal set of slip systems produces a minimal value of \( \frac{d\gamma}{d\varepsilon_{VM}} \). This value is referred to as the rotational contribution to the rate of change of internal work; therefore, it may be said that the optimal set of slip systems are such that the amount of rotation incurred as a result of a given strain increment is minimized.
CHAPTER 3. DEVELOPMENT OF A MULTI-SCALE MODEL

3.2 Finite-Element Modelling in LS-DYNA

LS-DYNA is a general-purpose FE code designed to analyze the large-deformation dynamic response of structures [46]. The primary solver uses explicit time integration to carry out the deformation algorithm; here, this algorithm is the aforementioned crystal plasticity formulation. These analyses are integrated through the construction of a user material subroutine (umat) within LS-DYNA, the contents of which are discussed below. In addition, input files are produced to specify physical material properties, element type and size, and element-dependent information such as initial-stress tensors and crystallographic orientations. Boundary conditions, displacement gradients, and timestep size are also specified, as are desired output settings. Mention is made of these settings where necessary.

3.2.1 Construction of a Crystal Plasticity umat

This section describes the construction of umat44.f, the crystal plasticity umat for use with LS-DYNA; note that while this umat includes a mesoscopic hardening model, its treatment is not included until later analyses examining the macroscopic constitutive response of a material (Chapters 4 and 5). Figure 3.1 illustrates the interaction of LS-DYNA with the Taylor-based subroutine (umat44.f).

Initially, the components of the strain increment \( (d\epsilon_{ij})^{i=0} \) are provided to the subroutine by LS-DYNA using the prescribed physical material properties, initial stress state, and displacement-gradient data; the through-thickness strain increment \( (d\epsilon_{33})^{i=0} \) is not prescribed, rather it is initialized with a value of zero and must be determined within the subroutine (to maintain the imposed condition of plane stress). For any other time step \( i \), \( (d\epsilon_{ij})^{i} \) are determined using the stress tensor of that element...
from the previous time step \((\sigma_{ij})^{i-1}\) instead of the user-defined stress state (again, \((d\epsilon_{33})^i\) is calculated within the subroutine). To ensure there are no ill-defined matrices in subsequent calculations, the incremental strain tensor is normalized by the von Mises strain increment.

**Elastic versus Plastic Deformation**

Once the partial incremental strain tensor is provided to the umat, calculation of the incremental through-thickness strain is performed. Before this can be carried out however, it must be determined whether or not the material is experiencing elastic deformation. To accomplish this task, LS-DYNA stores the total von Mises strain imparted on a given element within an array of history variables, \texttt{hisv(*)}; this strain is compared to a user-defined yield strain, which may be based on empirical data.

Such a distinction between elastic and plastic deformation is important as it affects the determination of the through-thickness strain, as well as the method by which the global stress tensor is calculated. In the case of plastic deformation, conservation of volume is assumed and \(d\epsilon_{33}\) is found via\(^3\):

\[
\epsilon_{33} = \epsilon_{11} + \epsilon_{22}. \tag{3.11}
\]

while the global stress tensor is found using the crystal plasticity formulation outlined in Section 3.1. In the case of elastic deformation, volume conservation cannot be assumed (since the analysed material is not ideal), and a separate model must be used to calculate \(d\epsilon_{33}\) and \(\sigma_{ij}\). Fortunately, such analyses are relatively simple and computationally inexpensive compared to plasticity models; the Livermore Software

\(^3\)In the current implementation, the Cartesian coordinates used constitute principal axes, allowing for this relation.
Technology Corporation (LSTC) includes an isotropic elastic model in its supporting documentation of LS-DYNA [47], which has been included as a subroutine within the crystal plasticity umat for deformation in this regime, with minor alteration (see Appendix A). Timestep size is set in the input file to ensure several timesteps are carried out in the elastic deformation region, providing an accurate representation of incremental strain at the onset of plasticity; a strong correlation exists between the first plastic strain increment and the plastic strain ratio $\beta_L$ that has been observed.

**Matrix Reduction and Vector Formulation**

Once plastic deformation has been achieved, the crystal plasticity formulae summarized in Section 3.1 are utilized within the umat. In many cases, tensors are employed in this numerical analysis; to reduce computational expense, these tensors (and any other symmetrical matrix used) can be reduced to a vector equivalent [21], provided that the following is true:

$$D_{ii} = 0 \quad (3.12)$$

where $D$ is the tensor in question. As such, a 3x3 tensor would have five independent components that could be expressed as a vector $d$ in five-dimensional space:

$$d_1 = \frac{(\sqrt{3} + 1)D_{22} + (\sqrt{3} - 1)D_{33}}{2}; \quad (3.13a)$$

$$d_2 = \frac{(\sqrt{3} - 1)D_{22} + (\sqrt{3} + 1)D_{33}}{2}; \quad (3.13b)$$

$$d_3 = \sqrt{2}D_{23}; \quad (3.13c)$$

It is recognized that iron and other bcc materials are elastically anisotropic, which will limit the accuracy of numerical solutions that assume isotropy in this regime.
\[ d_4 = \sqrt{2} D_{31}; \]  
\[ d_5 = \sqrt{2} D_{12}. \]

In this representation the following equivalency is true:

\[ \mathbf{D} : \mathbf{D}' = D_{ij} D'_{ij} = d_p d'_p = \mathbf{d} \cdot \mathbf{d}' \]  
\[ (3.14) \]

For example, the von Mises strain is updated at timestep \( i \) within the umat via:

\[ (\varepsilon_{\text{VM}})^i = (\varepsilon_{\text{VM}})^{i-1} + \left( \frac{2}{3} \mathbf{d} \varepsilon_{ij} \mathbf{d} \varepsilon_{ij} \right)^{1/2} = (\varepsilon_{\text{VM}})^{i-1} + \left( \frac{2}{3} \mathbf{d} \mathbf{e} \cdot \mathbf{d} \mathbf{e} \right)^{1/2}. \]  
\[ (3.15) \]

Conversely, Equations 3.13 may then be inverted to acquire tensor notation; this allows for matrices to be converted to vector form for efficient manipulation and reverted to matrix format for analysis.

**Slip System Input and Selection**

Equation 3.3b demonstrates the representation of slip-system orientation in crystallographic space. For the umat to determine which set of slip systems are active for a given strain increment, data for each potential slip system must be entered in the form of a slip plane normal \( \mathbf{n} \) and a slip direction \( \mathbf{d} \). Tables 3.1-3.4 list the orientations of all possible slip systems employed in the current study. The candidate systems are hard-coded into the umat and a set of five slip systems is combined to form the \( \mathbf{K} \) tensor in Equation 3.3 through the use of nested \texttt{if} statements; thus, every potential set of slip systems is considered for any prescribed increment of strain. Figure 3.2 illustrates the set of conditions used to determine the active systems. Some points of
interest are as follows:

- To drastically reduce the number of potential slip systems, only one sense of \( \mathbf{d} \) is initially specified. Once the slip vector \( \mathbf{\gamma} \) is calculated using Equation 3.3, any negative components indicate slip is occurring in the direction opposite the specification; this is remedied by reversing the direction cosines of \( \mathbf{d} \), recalculating \( \mathbf{\gamma} \) and ensuring all slip components are positive. This check is important when finding the total internal work of the system.

- While the number of potential systems included in the selection criteria is dramatically lower once directional ambiguity is assumed, this number is still quite high; assuming only one family of slip systems to be active (e.g. the \( \{110\}\langle111\rangle \) family in bcc materials) still produces over ninety-five thousand possibilities. Code structure is set such that there are no repetitious system combinations, reducing this number to 792.

- A non-zero determinant of \( \mathbf{K} \) in the umat indicates that a set of candidate slip systems is linearly independent. This check could also be performed via matrix inversion, but it may lead to segmentation faults during analysis. Depending on the slip system families considered, as few as 284 sets of slip systems may be linearly independent. Conditions of minimal internal work \( W_T \) and minimal change of work with strain (simplified as \( \frac{d\mathbf{\gamma}}{d\mathbf{\epsilon}_{VM}} \)) further reduce the number of slip systems that are subjected to full iterations of the conditional selection criteria. The resultant computational expense, discussed in Section 3.3.1, lies within acceptable limits.

- The use of Equation 3.3 forces the assumption that five slip systems are truly
active. Examination of the relative slip on each shows this assumption to be inaccurate; if deviations of slip greater than five orders of magnitude are observed, the lesser slip systems are assumed to be inactive and a null value is assigned to the incremental slip. This modification is important for the next phase of the umat, where the global stress tensor is determined.

Output Formulation and Storage

With the active slip systems selected, the global increment of deviatoric stress imparted upon the element may be determined using Equations 3.7 and 3.8. In the analyses performed within this chapter, the value of $\tau_{crss}$ on all slip systems is assumed to be equal. If any inactive systems are present, the umat is constructed to search for null values within $\gamma$ and assign a null value to $\tau_{crss}$ of the corresponding system, thereby eliminating it from the stress tensor determination.

The corresponding total stress tensor can then be determined by assuming the hydrostatic stress is equivalent to $-\sigma_{33}^g$; the material is thus assumed to be subjected to a plane-stress condition. The validity of such an assumption is affected by the type of analysis proposed. Since the work presented herein is concerned with the deformation of metallic foil and thin sheet product, a plane-stress assumption is considered reasonable. The components of the total stress tensor are then stored in the elemental array $\text{sig}(\ast)$ within LS-DYNA, to be used for determination of the subsequent incremental strain tensor.

Consequent to the assumed stress state, a plane-stress element is used within LS-DYNA. This is specified in the model input files, along with the element thickness and number of through-thickness integration points (these variables are discussed further in Section 3.3). A favourable attribute of such elements is that they are quasi-2D,
significantly reducing computational expense relative to many other 3D elements.

A second variable for storage is the updated crystallographic orientation, $A^i$. This is found via the incremental crystal rotation, $d\omega$, caused by the occurrence of slip on active systems, given by\textsuperscript{5}:

$$d\omega = \frac{1}{2}(e_{ij} - e_{ji}),$$

(3.16)

where $e_{ij}$ is the total slip in the crystal, defined as:

$$e_{ij} = \sum_{s=1}^{5} \gamma^{s} n^{s}_{i} d^{s}_{j}.$$  

(3.17)

After adding the identity matrix to $d\omega$, the final orientation is determined from:

$$A^i = d\omega : A^{i-1}.$$  

(3.18)

At this point the umat terminates and the FE model within LS-DYNA is updated.

### 3.3 Validation of the Multi-Scale Model

As its name suggests, the multi-scale model discussed must be capable of predicting material behaviour at both crystallographic and macroscopic length scales. This section examines the analyses performed to validate this model at both length scales, with reference to published data, results from existing CP code, and experimental results. Table 3.5 outlines the test matrix implemented.

\textsuperscript{5}Since LS-DYNA uses an objective strain-rate tensor that accounts for lattice rotation (i.e. Jammann rate), this effect need not be included in the crystal rotation calculations specified in Equation 3.16.
specified:

(i) elements are initially unstressed;

(ii) elements are square (in-plane) with dimensions of 2.5 \( \mu \text{m} \), have a shell thickness of 1.0 \( \mu \text{m} \), and contain only one through-thickness integration point;

(iii) physical material properties, such as the modulus of elasticity and Poisson’s ratio, are given the accepted values for Mo (refer to Table 4.1);

(iv) a time-variant timestep is used to ensure sufficient steps are taken within the elastic region of material deformation; and

(v) velocity curves are prescribed to reduce inertial effects during loading. To allow for consistent levels of applied strain when moving from single- to multi-element test cases, these curves are adjusted accordingly.

3.3.1 Single-Element Analyses

Single-element analyses are analogous to single-crystal observations insofar as each element simulates the crystallographic deformation of no more than one grain; however, the grain is assumed to be embedded within a polycrystalline structure such that multiple slip systems must activate. This is due to the nature of the CP umat. As Table 3.5 illustrates, two types of deformation are imposed on these elements: axisymmetric and plane-stress. Plane-stress conditions are those in which the incremental strain at time \( i \) is determined by code within LS-DYNA from the plane-stress state imposed at time \( i-1 \). In contrast, axisymmetric deformation requires the umat disregard the strain increment provided by LS-DYNA for each timestep and instead
use an axisymmetric strain increment hard-coded into the umat itself. While this results in erroneous output concerning the dynamic strain behaviour, the slip system selection and crystal rotation from such analyses represent true axisymmetric behaviour. The results of both deformation types are discussed below.

**Axisymmetric Deformation, No Rotation**

The prescribed (normalized) incremental strain tensor for axisymmetric deformation is hard-coded into the umat as:

\[
\begin{pmatrix}
1.0 & 0 & 0 \\
0 & -0.5 & 0 \\
0 & 0 & -0.5
\end{pmatrix}.
\]

When normalization is to be removed (e.g. for crystal rotation analyses), the value of \(d\varepsilon_{11}\) – supplied by LS-DYNA from the prescribed nodal velocity curve – is used as the equivalent strain; hence, it is possible to observe a constant assigned strain state within LS-DYNA provided the dynamic strain response is not of interest. In these test cases, it is the slip system selection and crystal rotation due to axisymmetric deformation that are key for verifying umat functionality.

Chin and Mammel have performed extensive numerical analyses of axisymmetric flow using a FC Taylor model [44]. Specifically, plots illustrating orientation dependence on slip system activation and Taylor factor \((M)\) are produced for bcc crystals with varying sets of available slip systems; these plots are shown in Figure 3.3. Regions can be seen in each standard stereographic triangle where specific sets of slip systems are active. Tables 3.6 and 3.7 present the active systems predicted by the
umat for specific orientations that lie within the regions outlined by Chin and Mam-
mel; values of $M$ for these orientations are also included, defined by:

$$M = \sum_{s=1}^{5} \frac{\gamma_s}{\epsilon_{11}}.$$  \hspace{1cm} (3.20)

Two region types may be observed: ones where a single unique set of systems
activate, and ones where multiple sets can activate, in accordance with Taylor’s mini-
mization of internal work theorem [16]. In the cases where unique sets of slip systems
activate, the umat accurately predicts the correct systems (and direction of slip on
each plane); furthermore, the Taylor factors predicted for the orientations shown in
each table are in agreement with the contour plots in Figure 3.3. Most cases result
in the situation where more than one set of systems produce the same internal work,
which is the root cause of Taylor ambiguity. Since the umat performs a first-order
Renouard-Wintenberger analysis in such cases (Section 3.1.1), only five slip systems
are listed, but it is worth noting that all of the possible (i.e. linearly independent)
combinations of slip systems listed by Chin and Mammel for these regions produce
the same minimum internal work within the model. In almost all cases, the first-order
analysis will predict a unique set of slip systems. There are special orientations where
this does not occur, however, and two equivalent systems are possible. In such cases,
the first set of equivalent systems is selected arbitrarily. Future implementation of a
work-hardening scheme in the umat will eliminate such equivalencies after the first
time increment [48].

In addition to the treatment of \{110\}<111> and \{112\}<111> slip separately, cases of
mixed slip were also studied at orientations bounding the standard stereographic tri-
gle in Figure 3.3(d); the results are presented in Table 3.8. While Figure 3.3(d) plots
CHAPTER 3. DEVELOPMENT OF A MULTI-SCALE MODEL

the predicted behaviour for combined \( \{110\}\langle111\rangle \), \( \{112\}\langle111\rangle \), and \( \{123\}\langle111\rangle \) slip, \( M \) values at the orientations selected are not affected by the inclusion of \( \{123\}\langle111\rangle \) slip systems. This association can be made by looking at the slip systems selected by the umat, and noting the high \( M \) values associated with \( \{123\}\langle111\rangle \) slip at these orientations (relative to \( \{112\}\langle111\rangle \) slip – see Figures 3.3(b) and 3.3(c)).

**Axisymmetric Deformation, Rotation**

The preceding analyses does not account for crystal rotation due to axisymmetric flow; here, the code for orientation update within the umat is activated and results are produced for a number of cases. Figure 3.4 plots the grain rotation fields for each case.

In his work, Taylor has shown that material with a face-centered cubic (fcc) crystal structure will behave in a manner similar to material with a bcc crystal structure if the applied strain is reversed [16]. Due to the relatively large amount of research available in the literature on fcc materials in this area, these results will be used as a benchmark. Buchheit et al. [49] have produced numerical analyses of texture development in polycrystalline fcc material. Grain rotation fields for a selected number of orientations are presented in Figure 3.4(a); these fields match rotation fields outlined qualitatively by Calnan and Clews [50]. To compute a similar field using the multi-scale model developed in the current study, a set of 125 orientations were selected as model input, direction cosine data for the fcc slip systems (see Table 3.1) were hard-coded to the umat, and a series of single-element studies were carried out for each orientation. Results of these analyses are presented in Figure 3.4(b).

Comparison of the two sets of predictions in Figure 3.4 shows that while the general qualities of the fcc deformation are maintained (i.e. the rotation of crystals towards
(100) and (111), and a similar divergence of rotation paths), the precision of the umat solutions is noticeably inferior. The reason for this discrepancy lies in the CP model chosen; while the umat implements a FC Taylor model that selects five active slip systems, the model employed by Buchheit et al. implements a strain-rate-dependent CP model such as that formulated by Asaro and Needleman [24]. A strain-rate-dependent CP model requires that all slip systems are active simultaneously, which results in increased precision for the solution presented in Figure 3.4. However, while such assumptions are numerically precise in regards to predicting grain rotation, they are phenomenologically inaccurate. An alternate solution for increasing precision while maintaining accuracy is described below.

Figures 3.4(c) to 3.4(g) plot the grain rotation fields for bcc structures under compression. The results of compression when only \{110\}(111) slip is possible (Figure 3.4(c)) are identical to the rotation field for fcc structures under tension, as expected. When \{112\}(111) slip is examined (Figure 3.4(d)), a match in general trends is again observed, but two points of interest are noted:

(i) path divergence is altered relative to \{110\}(111) slip; and

(ii) rotation near (100) and (111) orientations is steady.

For \{123\}(111) slip (Figure 3.4(e)), path divergence is unaltered relative to \{112\}(111) slip, but the rotation near (100) and (111) is erratic. Furthermore, the rotation near (110) orientations is steady, compared to the indiscriminate trends observed in the previous two cases.

Steady rotation fields are indicative of a preferred set of slip systems; in unsteady cases, more than one set of systems may be selected due to slight changes in orientation, resulting in unstable behaviour. Consequently, the use of mixed slip provides
a wider range of orientations for selecting a preferred set of slip systems, and thus a steady rotation. Mixed \{110\}\langle111\rangle and \{112\}\langle111\rangle slip (Figure 3.4(f)) illustrates how \{112\}\langle111\rangle slip is dominant near \langle100\rangle and \langle111\rangle, while steady rotation from \{110\}\langle111\rangle slip is apparent near the central regions of the triangle. When these are combined with \{123\}\langle111\rangle slip (Figure 3.4(g)), further orientations near \langle110\rangle contain preferred slip systems.

By increasing the number of available slip systems, an increase in phenomenological accuracy is achieved with no loss of numerical precision. Comparison of Figures 3.4(a) and 3.4(g) validates this point, and implies that including cases of pencil glide may result in the characterisation of all orientations with a unique set of slip systems for bcc materials [44]. Unfortunately, such a vast number of available systems would create an unrealistic set of slip system combinations for analysis. In this study, a solution to single-element bcc compression (\(\epsilon_{11} = -35\%\)) with \{110\}\langle111\rangle slip takes approximately two seconds. If mixed \{110\}\langle111\rangle and \{112\}\langle111\rangle slip were considered, the solution time increases to over two minutes. Including \{123\}\langle111\rangle slip causes this time to increase dramatically to nearly 1.5 h (as there are 24 available slip systems in this set). While such an analysis may be feasible for single-element problems, multiple-element solutions require a reduced set of available slip systems; in the current study, mixed \{110\}\langle111\rangle and \{112\}\langle111\rangle slip conditions were implemented for multiple-element problems.

Figure 3.5 compares compressive- and tensile-based rotation fields for bcc structures. Observed rotations qualitatively match the expected results [51]; specifically, rotation away from \langle100\rangle and \langle111\rangle, and towards \langle110\rangle is observed under tensile loading. Note that the orientations seem to rotate towards/away from a point adjacent to the \langle110\rangle orientation; this phenomena has been documented by Calnan and Clews
[51], particularly under \{112\}(111) slip, as evident in the rotation field provided in Figure 3.5.

**Plane-Stress Deformation, No Rotation**

Prescription of an incremental strain tensor in the LS-DYNA umat eliminates dynamic strain evolution based on stress history. This section analyses the effects of allowing strain evolution to take place; consequently, the ramifications of using a plane-stress condition are also observed. Since the transverse and normal strain increments are no longer fixed, examination of texture-based anisotropy is feasible. A plastic strain ratio, $\beta_L$, is used to study the extent of this anisotropy:

$$\beta_L = \frac{\varepsilon_{TD}}{\varepsilon_{ND}}.$$  \hspace{1cm} (3.21)

An isotropic material would have a ratio of $\beta_L = 1$, where materials subject to thinning would possess $\beta_L < 1$. In these analyses, both the total ratio $\beta_{L,t}$ and the incremental ratio $\beta_{L,i}$ are examined. It must be noted that the Lankford coefficient $R$ is a specific case of $\beta_L$ found often in the literature, pertaining to analyses of uniaxial tensile tests [52]; since the dynamic nature of the model developed in this thesis allows for variation of the stress tensor, the tensor is typically not representative of uniaxial tension. The plastic strain ratio is therefore commonly designated $\beta_L$ in this thesis, with occasional reference to $R$-values where analyses of uniaxial tension are performed (mainly in the literature).

To explain the ridging phenomenon observed in certain ferritic stainless steels, Chao formulated a mechanism by which colonies of grains with specific texture components produced variations in plastic flow due to differences in the Lankford coeffi-
cient [3]. Specifically, orientations defined as cube-on-edge (CE), cube-on-face (CF),
and cube-on-corner (CC) were examined and theoretical $R$-values for each were cal-
culated. These are summarized as:

$$
\begin{align*}
\text{CE} & : \frac{\epsilon_{TD}}{\epsilon_{ND}} = \frac{-1}{2} \epsilon_{RD} \\
\text{CF} & : \frac{\epsilon_{TD}}{\epsilon_{ND}} = \frac{0}{\epsilon_{RD}} \\
\text{CC} & : \frac{\epsilon_{TD}}{\epsilon_{ND}} = \frac{2}{3} \epsilon_{RD} \\
\end{align*}
$$

$$
\Rightarrow R_{\text{CE}} = 1 \\
R_{\text{CF}} = 0 \\
R_{\text{CC}} = 2 \\
$$

$$
\Rightarrow R_{\text{CC}} = \infty
$$

Figures 3.6, 3.7, and 3.8 present umat solutions for uniaxial tension tests of single-
element grains with CE, CF, and CC orientations, respectively. Crystal rotation
is suppressed to examine the evolution of the plastic strain ratio for a given initial
orientation.

CE texture components are isotropic in nature [3]. As shown in Figure 3.6, the
umat solution produces a consistent $\beta_L$ through the test duration. It can also be
shown that this variable is affected by the input strain increment due to the nature
of the CE orientation; transformation of the global strain increment to the crystal
system produces:

$$
\begin{bmatrix}
\frac{d\epsilon_{RD}}{} & 0 & 0 \\
0 & \frac{d\epsilon_{TD}}{} & 0 \\
0 & 0 & \frac{d\epsilon_{ND}}{}
\end{bmatrix}^c = \begin{bmatrix}
\frac{d\epsilon_{RD}}{} & 0 & 0 \\
0 & \frac{1}{2}(d\epsilon_{TD} + d\epsilon_{ND}) & 0 \\
0 & 0 & \frac{1}{2}(d\epsilon_{TD} + d\epsilon_{ND})
\end{bmatrix}^c.
\tag{3.22}
$$

Normalisation of this tensor with the incremental von Mises strain produces the tensor
shown in Equation 3.19, which is used for axisymmetric deformation solutions based
on the assumption of inherent isotropy. The nature of the orientation is therefore one
that will produce an isotropic response despite the global strain increment applied; the isotropic global stress tensor at time $i-1$ will produce an identical strain increment at time $i$ and that applied at time $i+1$. Hence, it is necessary that the strain increment be isotropic at the onset of plasticity.

This requirement poses difficulties as the transition from elastic to plastic deformation signifies a change in deformation mechanisms; specifically, the theoretical conservation of volume for plastic deformation is not upheld within the elastic regime. The transverse strain increment predicted by LS-DYNA during elastic deformation is less than $-0.5\varepsilon_{RD}$, as is the through-thickness strain increment due to the inherent isotropy of elasticity. At the onset of plasticity, LS-DYNA will predict the same value of $\varepsilon_{TD}$ based on the preceding elastic stress tensor, whereas $\varepsilon_{ND}$ will be calculated within the umat based on the principle of conservation of volume. The resulting $\beta_L$ will therefore be less than 1.0, since $\varepsilon_{TD} < -0.5\varepsilon_{RD}$ while $\varepsilon_{ND} > -0.5\varepsilon_{RD}$. To circumvent this anomaly, alterations to the predicted elastic stress tensor are made to promote a transverse strain increment of $-0.5\varepsilon_{RD}$ during elastic deformation (refer to Appendix A). The resulting plastic deformation is truly isotropic given a CE texture component, and both $\beta_{L,t}$ and $\beta_{L,i}$ remain near 1.

Figure 3.7 plots the anisotropic deformation of the CF texture component, where no transverse strain is expected. The evolution of $\beta_{L,t}$ accurately predicts this condition. To produce this strain behaviour, two alternate sets of slip systems activate between each time step. The first set of systems will produce a global stress tensor where $\sigma_{TD}$ is positive, thereby producing a negative transverse strain increment the following timestep. To counteract this effect, a second set of slip systems activates that produces a negative $\sigma_{TD}$, and the subsequent transverse strain increment is positive. The oscillatory nature of the transverse strain increment is an accurate phenomeno-
logical representation, where active slip systems alternate to maintain stability during deformation; should the timestep be reduced to an infinitely small amount, simultaneous activation of these slip systems would be observed as they are necessary to satisfy the desired deformation within the given geometric constraints.

Oscillatory strain increments are also observed for CC deformation (Figure 3.8), though without the short-range (alternating) order previously observed. Increments producing higher values of $\beta_{L,i}$ are countered in subsequent timesteps by lower transverse strain increments. The subsequent value of $\beta_{L,i}$ drops steadily towards zero, then jumps to a value higher than expected; as a result, the overall plastic strain ratio remains below 1.0 throughout the deformation history. Although this outcome deviates from theoretical $R$-values for CC orientations, it is expected since high values of $\beta_{L,t}$ imply that little through-thickness strain is accrued, whereas the plane-stress assumption in these simulations completely eliminates this possibility.

One final inconsistency observed during testing of the umat was the $\beta_{L}$-evolution with variation of the nodal velocity within LS-DYNA. This issue is discussed in Appendix A. Unless otherwise noted, it is assumed that the velocity profile chosen produces an accurate solution in all documented analyses.

**Plane-Stress Deformation, Rotation**

Activating the orientation update subroutine within the umat produces grain rotation paths for bcc structures assuming plane-stress conditions and a dynamic incremental strain tensor. Figure 3.9 compares the results of dynamic plane-stress behaviour having $\{110\}<111>$ and $\{112\}<111>$ slip systems available, with axisymmetric deformation having the same available systems, and a dynamic plane-stress solution including $\{110\}<111>$, $\{112\}<111>$, and $\{123\}<111>$ slip. The comparison highlights qualitative
similarities in grain rotation (towards \langle 100 \rangle and \langle 111 \rangle in compression), and an area of divergence within the rotation field. The location of this divergence path in the dynamic plane-stress condition is shifted relative to axisymmetric deformation, however, due to the anisotropic strain introduced via the texture components.

The rotation paths of the dynamic plane-stress solution are found to be more erratic than in the axisymmetric case. It is postulated that the erratic response is due to an insufficient number of slip systems, as shown in Figure 3.4 for axisymmetric deformation; however, comparison of dynamic plane-stress deformation with and without \{123\}⟨111⟩ slip shows that the stability of grain rotation and location of path divergence is unaffected by the addition of available systems. This observation further supports the theory that mixed \{110\}⟨111⟩ and \{112\}⟨111⟩ slip is sufficient for multiple-element solutions using the dynamic plane-stress approach. The nature of this erratic behaviour therefore lies in the variability of the strain increment; whereas the axisymmetric condition provided a consistent strain increment that produces a smooth rotation if a stable set of slip systems is found, the dynamic strain increment may alter the optimal set of systems active at a given time, causing a lack of consistency.

### 3.3.2 Multiple-Element Analyses

To examine the behaviour of polycrystalline material under deformation while ensuring that no more than one grain is represented per element, multi-element analyses must be performed. Validation of these models is examined by considering texture-based anisotropy during deformation. While it would be advantageous to also perform validation of texture evolution in a multi-element model, no literature currently
exists that provides experimental data outlining discrete orientations pre- and post-deformation with the level of detail required. Instead, validation of this nature is carried out by comparing texture evolution observed in Mo foil studies with numerical analysis, presented in Chapter 4.

During these and all subsequent multi-element simulations, modifications have been made to the parameters initially outlined in Section 3.3, primarily due to element interaction incurred during the elastic deformation regime, as well as confounding inertial problems with larger FE mesh sizes. Appendix B explains these issues in greater detail. The modified parameters are as follows:

- initial elasticity is predetermined – all elements are given an initial stress state and von Mises strain equivalent to the theoretical yield properties of the material to be tested (where none are specified, the properties of Mo are used as placeholders);
- a constant timestep is used to ensure stability in strain increment evolution; and
- constant velocity curves are entered to eliminate strain localization along elements whose nodes are subjected to boundary conditions.

**Texture-Based Anisotropy**

To examine texture-based anisotropy, the work of Chao is once again referenced [3]. As previously discussed, Chao theorized that colonies of grains with specific texture components produced variations in plastic flow. The contrast in Lankford coefficient between cube-on-edge, cube-on-face, and cube-on-corner orientations highlighted the
potential cause of ridging in ferritic stainless steels. This theory forms the basis of validation for polycrystalline, texture-based anisotropy within the current CP model.

Texture bands comprised of similarly-oriented polycrystalline material aligned parallel to the tensile axis are replicated in a FE model, such that a variation in Lankford coefficient between each band should be realized. While mesh size has some effect on the numerical analyses (elucidated in Appendix B), the effect is negligible for the solutions presented herein. A 225-element square mesh is implemented; five alternating texture bands are used, such that each band comprises a 15x3-element section of the mesh. Orientations for the elements in each texture band alternate between CF and CE. Figure 3.10 displays the banded texture model and the simulated through-thickness strain distribution after an applied strain of 20%. The variation in plastic anisotropy is clearly related to the initial texture; that is, preferred thinning of the CF-oriented elements/grains is observed in contrast to the absence of thinning in the CE-oriented regions. The typically isotropic CE texture has been influenced by the highly anisotropic CF regions, such that increased transverse strain in the former is the result of high levels of transverse stress developed in the latter. This interpretation exacerbates the variation in through-thickness strain across the material. The ridging behaviour observed is in good qualitative agreement with the theoretical results presented by Chao [3], and shows how the texture distribution in a polycrystalline material can have a profound impact on the surface topography upon deformation.
3.4 Summary

A multi-scale model that incorporates a Taylor-based crystal-plasticity formulation and a dynamic, explicit finite-element model within LS-DYNA has been developed. The model uses discrete orientation data for no more than one grain per element, allowing an accurate representation of texture effects in a polycrystalline material subject to large plastic deformation. It uses a first-order Renouard-Wintenberger solution to address problems with Taylor ambiguity, and has been calibrated to minimize the effects of timestep, inertia, strain rate, and mesh scale. Validation of the model has been carried out in both single- and multi-element conditions via comparison of numerical solutions with published work (theoretical and experimental). Single-element studies verify the ability of the model to predict both texture-based anisotropy and crystallographic orientation evolution of a grain embedded within a polycrystalline material, while multi-element studies highlight the ability to predict macroscopic effects (e.g. surface roughening) due to local texture distribution. In both cases, numerical results are in good agreement with published findings.
Table 3.1: List of \{111\}\langle110\rangle slip systems for fcc crystal structures [42].

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Table 3.2: List of \{110\}(111) slip systems for bcc crystal structures [44].

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Table 3.3: List of \{112\}(111) slip systems for bcc crystal structures [44].

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Table 3.4: List of $\{123\}(111)$ slip systems for bcc crystal structures [44].

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Table 3.5: Test matrix implemented for model validation (bcc structure).

<table>
<thead>
<tr>
<th>Element Quantity</th>
<th>Deformation Type</th>
<th>Rotation</th>
<th>Available Slip Systems</th>
<th>Number of Tests</th>
</tr>
</thead>
<tbody>
<tr>
<td>Single</td>
<td>Multiple</td>
<td>Axisymmetric</td>
<td>Plane Stress</td>
<td>No</td>
</tr>
<tr>
<td></td>
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</tbody>
</table>
Table 3.6: Active slip systems for \{110\}\{111\} slip, compared to the results of Chin and Mammel [44]. Taylor factors $M$ calculated by the model for specific orientations in each region (shown below) are given.

<table>
<thead>
<tr>
<th>Region/Orientation</th>
<th>Slip Systems$^a$</th>
<th>$M$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Always Active</td>
<td>Sometimes Active$^b$</td>
</tr>
<tr>
<td>1/I</td>
<td>2, 4, 7, -11, -12</td>
<td>–</td>
</tr>
<tr>
<td>2/II</td>
<td>2, 4, 5, 7, 9</td>
<td>–</td>
</tr>
<tr>
<td>3/III</td>
<td>2, 4, 9</td>
<td>3, 6, 7, -12</td>
</tr>
<tr>
<td>4/IV</td>
<td>4, 5, 7, 9</td>
<td>11, 12</td>
</tr>
<tr>
<td>5/V</td>
<td>2, 4, 5, 9</td>
<td>1, 11</td>
</tr>
</tbody>
</table>

$^a$Minus sign indicates slip opposite the direction indicated in Table 3.2

$^b$Indicates slip systems that produce very similar internal work and $\frac{\partial W_T}{\partial \epsilon_{VM}}$, such that the model selects from these possibilities at random, provided sets remain linearly independent

$^c$All potential slip systems are listed. Any systems not shown in the model imply that $\frac{\partial W_T}{\partial \epsilon_{VM}}$ is not minimized with these systems for the orientation tested.
Table 3.7: Active slip systems for \{112\}⟨111⟩ slip, compared to the results of Chin and Mammel [44]. Taylor factors $M$ calculated by the model for specific orientations in each region (shown below) are given.

<table>
<thead>
<tr>
<th>Region/Orientation</th>
<th>Always Active</th>
<th>Sometimes Active$^b$</th>
<th>Chin and Mammel$^c$</th>
<th>$M$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1/I</td>
<td>-3, 4, 6, -8, 10</td>
<td>–</td>
<td>1, -3, 4, 6, -7, -8, 10, -12</td>
<td>2.10</td>
</tr>
<tr>
<td>2/II</td>
<td>-3, 4, 6, 10, 11</td>
<td>–</td>
<td>-3, 4, 6, 10, 11</td>
<td>2.42</td>
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<tr>
<td>3/III</td>
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<td>–</td>
<td>-3, 5, 6, 10, 11</td>
<td>2.79</td>
</tr>
<tr>
<td>4/IV</td>
<td>4, 6, 11</td>
<td>1, -3, 7, 12</td>
<td>1, -3, 4, 6, -9, 11, 12</td>
<td>3.22</td>
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<tr>
<td>5/V</td>
<td>4, 5, 8, 11, 12</td>
<td>–</td>
<td>4, 5, 8, 11, 12</td>
<td>3.18</td>
</tr>
<tr>
<td>6/VI</td>
<td>4, 7, 8, 11, 12</td>
<td>–</td>
<td>4, 7, 8, 11, 12</td>
<td>3.15</td>
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</tbody>
</table>

$^a$Minus sign indicates slip opposite the direction indicated in Table 3.3

$^b$Indicates slip systems that produce very similar internal work and $\frac{\partial W}{\partial \varepsilon_{VM}}$, such that the model selects from these possibilities at random, provided sets remain linearly independent

$^c$All potential slip systems are listed. Any systems not shown in the model imply that $\frac{\partial W}{\partial \varepsilon_{VM}}$ is not minimized with these systems for the orientation tested
Table 3.8: Active slip systems for mixed \{110\}<111> and \{112\}<111> slip. Taylor factors $M$ calculated by the model are compared to the results of Chin and Mammel [44].

<table>
<thead>
<tr>
<th>Axial Orientation</th>
<th>Slip Systems$^{a,b}$</th>
<th>$M$</th>
<th>Model</th>
<th>Chin and Mammel$^c$</th>
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</thead>
<tbody>
<tr>
<td>[100]</td>
<td>-3, 6, -8, 10</td>
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<tr>
<td>[110]</td>
<td>1, 4, 7, 12</td>
<td>–</td>
<td>3.182</td>
<td>3.182</td>
</tr>
<tr>
<td>[111]</td>
<td>3, 4, 7, 8, 11</td>
<td>–</td>
<td>3.182</td>
<td>3.182</td>
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</table>

$^a$Minus sign indicates slip opposite the direction indicated in Tables 3.2 and 3.3

$^b$values in *italics* indicate \{110\}<111> slip systems; *boldface* values represent \{112\}<111> slip systems

$^c$for mixed \{110\}<111>, \{112\}<111> and \{123\}<111> slip, shown below; the latter systems fail to activate at the orientations analysed
CHAPTER 3. DEVELOPMENT OF A MULTI-SCALE MODEL

Material data:
\( E, b, \nu, \tau_{crss}, \text{etc.} \)

Crystal data:
\( \sigma_0, (\gamma_1, \Phi, \gamma_2), \text{etc.} \)

\[
\begin{align*}
\left\{ \begin{array}{l}
t = 0 \\
i = 0
\end{array} \right.
\end{align*}
\]

\( t = 0 \)
\( i = 0 \)

Figure 3.1: Flow diagram illustrating the integration of the crystal plasticity umat and LS-DYNA.
CHAPTER 3. DEVELOPMENT OF A MULTI-SCALE MODEL

1. select five slip systems
2. Save bases in matrix \( \mathbf{U} \)

\[
\det \mathbf{U} = 0？
\]

YES

find \( W_T \)

\[
W_T < (W_T)_{\text{min}}？
\]

YES

1. find \( \frac{dW_T}{dv_{\text{ext}}} \)
2. save slip system ID, \( W_T \), and \( \frac{dW_T}{dv_{\text{ext}}} \) as temporarily active

YES

other sets to choose?

NO

active set selected

\[
\frac{dW_T}{dv_{\text{ext}}} < (\frac{dW_T}{dv_{\text{ext}}})_{\text{min}}？
\]

YES

NO

other sets to choose?

NO

YES

NO

YES

Figure 3.2: Conditional statements governing the selection of active slip systems.
Figure 3.3: Contours of $M$ obtained from Chin and Mammel [44]. Dashed boundaries delineate regions within which a specific set of slip systems are active. (a) Case of \{110\} \langle 111 \rangle slip. (b) Case of \{112\} \langle 111 \rangle slip. (c) Case of \{123\} \langle 111 \rangle slip. (d) Case of mixed slip on \{110\} \langle 111 \rangle, \{112\} \langle 111 \rangle, and \{123\} \langle 111 \rangle.
Figure 3.4: Grain rotation paths of orientations in a standard stereographic triangle. (a) Tensile behaviour of fcc material under axisymmetric deformation, superimposed by X-ray goniometer measurement of polycrystalline copper subjected to wire drawing [49]. (b) Tensile behaviour of fcc material predicted by the umat. (c-g) Compressive behaviour of bcc material predicted by the umat: (c) \{110\}\{111\} slip; (d) \{112\}\{111\} slip; (e) \{123\}\{111\} slip; (f) combined \{110\}\{111\} and \{112\}\{111\} slip; and (g) combined \{110\}\{111\}, \{112\}\{111\}, and \{123\}\{111\} slip.
Figure 3.5: Grain rotation paths for a bcc structure. (a) Solutions for axisymmetric compression produced by LS-DYNA, mixed \{110\}\{111\} and \{112\}\{111\} slip. (b) Solutions for axisymmetric tension produced by LS-DYNA, mixed \{110\}\{111\} and \{112\}\{111\} slip. (c) Rotation field predicted by Calnan and Clews for axisymmetric compression under \{112\}\{111\} slip [51].
Figure 3.6: Evolution of $\beta_{L,i}$ and $\beta_{L,t}$ for a single-element CE-oriented grain under uniaxial tension.
Figure 3.7: Evolution of $\beta_{L,i}$ and $\beta_{L,t}$ for a single-element CF-oriented grain under uniaxial tension.
Figure 3.8: Evolution of $\beta_{L,i}$ and $\beta_{L,t}$ for a single-element CC-oriented grain under uniaxial tension.
Figure 3.9: Grain rotation paths for a bcc structure under uniaxial compression: (a) assuming axisymmetric deformation, combined \{110\}<111> and \{112\}<111> slip; (b) assuming plane-stress, combined \{110\}<111> and \{112\}<111> slip; and (c) assuming plane-stress, combined \{110\}<111>, \{112\}<111>, and \{123\}<111> slip.
Figure 3.10: Banded texture model results: (a) mesh construction, highlighting 15x3-element regions of polycrystalline material with similar orientation and direction of loading (plot of Euler angle $\Phi$ shown – CF = blue, CE = red); and (b) plot of through-thickness strain after an applied strain of 20% along the x-axis.
Chapter 4

Molybdenum Foil Tensile Testing and Simulation

This chapter outlines the deformation behaviour of molybdenum (Mo) foil under uniaxial tension, both numerically and experimentally. Numerical analyses were performed using the multi-scale model outlined in Chapter 3, with the incorporation of an isotropic work-hardening model, used since only monotonic loading is applied. This simplified work-hardening model allows for evaluation of both the finite-element and crystal-plasticity models relative to experimental results, without the possibility of compounding errors from a complex, multi-parametric hardening model\(^1\). Numerical solutions are compared to experimental data via bulk work-hardening behaviour and the evolution of local surface roughening.

\(^1\)Integration of a more detailed work-hardening model is covered in Chapter 5.
4.1 Material Selection

Early studies of ridging in ferritic stainless steels have shown that through-thickness texture variation has an effect on surface topography during deformation [8, 53]. Given that the roughening analyses presented herein rely solely upon surface texture, the thickness of the material was reduced to minimise any subsurface effects. Sample thickness was selected to ensure no more than two grains exist along the normal direction (ND). A high-purity material was also desirable to exclude solute-defect interactions during work hardening; the work-hardening model employed in this thesis does not accurately account for such behaviour [7].

Upon review of high-purity metals available in foil form, Mo was selected. The added benefit of working with Mo is the high melting temperature of this material (2896 K), such that tests performed at room temperature (a homologous temperature of 0.1 \( T_m \)) limit the ductility of the material through the reduction of potentially active slip systems [54, 55]. Here, \{110\}<111> and \{112\}<111> systems are potentially active, while \{123\}<111> systems are reported to remain dormant [55]. This situation increases the accuracy of the numerical analyses performed, as only these two systems are considered for multi-element solutions due to computational expense (see Section 3.3.1).

The material selected for this study was a 100-\( \mu \)m thick Mo foil with a purity of 99.95 %, obtained from Alfa Aesar. The material was cold rolled and subjected to a stress-relieving heat treatment by the manufacturer, performed without an inert atmosphere; such conditions require this initial annealing temperature to be sufficiently below the melting temperature of the material in order to avoid impurity segregation that can lead to intergranular embrittlement [56, 57] – no recrystallization of the
material was observed due to this heat treatment. The textural and microstructural properties of this material in the as-received condition are presented in the following sections.

4.2 Sample Preparation

Strips of Mo foil (5 x 60 mm\(^2\)) for uniaxial tensile specimens were sectioned from the parent material using electrical discharge machining (EDM). The as-received rolling direction (RD) was aligned with the tensile axis. Specimens were then annealed a second time at 1873 K for 1 h in a turbomolecular vacuum furnace (ambient pressure < \(10^{-6}\) torr), to increase the grain size in the material. Each gauge section was then electropolished using a solution of 600 mL ethyl alcohol, 360 mL ethylene glycol monobutyl ether, and 60 mL perchloric acid [58] at 25 V for 30 s. Dry ice was used to keep both the solution and the specimen at 278 K during the polish. Electron channeling contrast (ECC) images taken before and after annealing reveal a recovery of the deformed substructure, and significant grain growth (Figure 4.1). The grains, elongated parallel to the RD, grew from roughly 5 \(\mu\)m to 25 \(\mu\)m in the transverse direction, further reducing the number of grains along the normal direction of the foil strips.

In addition to uniaxial tensile samples, two 15 x 20 mm\(^2\) Mo foil samples were extracted for bulk texture measurements. One was measured prior to annealing and the second was measured post-anneal. Sample preparation was identical to that used for the tensile specimens. Bulk texture measurements via X-ray diffraction (XRD) were acquired at room temperature using an apparatus comprising an Euler cradle with gap and V-filtered Cr radiation obtained from a rotating anode operating at
9.5 kW. Crystallographic orientation distributions (COD’s) were determined from incomplete \{110\}, \{200\}, and \{112\} pole figures (Figure 4.2).

4.3 Experimental Testing and Characterization

Two Mo foil strips (designated A and B) were tested using a servo-hydraulic Instron 8502 with a 100-lbf load cell. Figure 4.3 shows the true stress-strain response of both foils under uniaxial tension at a constant crosshead velocity, providing an initial strain rate of $10^{-4}$ s$^{-1}$. The total applied true strain was approximately 0.10 for foil A and 0.15 for foil B. Plastic strains were calculated by subtracting the amount of purely elastic strain recovered upon load removal from the total strain at the point of yielding. The resultant plastic strain curves do not begin at zero, highlighting a slight warp in the material prior to deformation. This offset is accounted for in experimental calculations and during model calibration.

Material characterization was carried out prior to and following uniaxial tension. Empirical data was collected in two forms: (1) local texture measurements; and (2) surface roughness profiles. To ensure measurements were taken from the same location on each foil strip before and after deformation required some sort of marker. A system was devised in which a portion of each electropolished surface was masked with a 200-$\mu$m mesh from a Cu TEM grid and sputter coated with a fine layer of gold. The marker grid is identifiable via optical means (required for surface scans), and the high atomic number of gold also allows it to be observed via SEM (required for texture scans). Figure 4.4 highlights the visibility of the marker; texture and surface roughness measurements were taken a set distance away from this location to avoid any influence of the gold layer.
4.3.1 Local Texture Measurements

Texture measurements were carried out using a JEOL JSM-840 scanning electron microscope operating at 20 kV with a working distance of 25 mm. Electron backscatter diffraction (EBSD) was used to characterize grain orientation in the form of Euler angles ($\phi_1, \Phi, \phi_2$) using orientation mapping (OM). A $500 \times 500 \mu m^2$ section of each surface was scanned using a $5-\mu m$ step size. Examination of surface grain structure (Figure 4.1(b)) reveals the majority of the grains to be larger than $5 \mu m$, such that grains smaller than this size are deemed to have little influence on texture-based anisotropy during deformation.

OM data is subsequently plotted as texture maps. Figure 4.5 presents these maps for foils A and B. It is clear that the indexing rate\(^2\) for the polished Mo is quite high. The average indexing rate is 92.62 $\%$, which implies the differences between unrefined and refined data is negligible (the concept of refinement is explained further in Section 4.4). Figure 4.6 presents texture maps for the foils after deformation. Slightly larger scan areas are used\(^3\) to account for elongation of the original scan area during deformation. While coincidence in scan areas before and after deformation was maintained, the indexing rate was reduced due to surface roughening post deformation. Nevertheless, hit rates are still high (73.37 $\%$), allowing for confidence in the accuracy of refined texture maps used for comparison with numerical analyses.

To test if the microtexture scan area was sufficient to represent the bulk texture of the foil, pole figures created using the data collected from OM were compared to bulk measures determined from XRD. Figure 4.7 compares these plots; the strong

\(^2\)The indexing rate refers to the total percentage of orientations acquired during OM. Clear orientations may not be present due to grain boundaries or significant substructure development.

\(^3\)500 x 550 $\mu m^2$ for foil A, 500 x 600 $\mu m^2$ for foil B.
cube texture of the bulk material is adequately represented in each local texture scan. Recent studies by Wright et al. [59] indicate as many as 10,000 grain orientations are required to accurately reproduce a bulk orientation distribution function via EBSD for a moderate texture strength. Larger scans could be performed to increase the phenomenological accuracy of these texture plots, but acquiring this larger data set in any deformation simulation would increase the FE computational time significantly, and were therefore not obtained.

4.3.2 Surface Profilometry

Surface profilometry was performed on both Mo foil specimens prior to and after deformation using a WYKO NT3300 non-contact optical profiler. Scan areas were slightly larger than that used for EBSD measurements to ensure coincidence. Optical resolution allowed for surface data to be collected every 1.62 µm, with sub-nanometer precision. Figures 4.8 and 4.9 present undeformed surface profiles for foils A and B, respectively, while Figures 4.10 and 4.11 present surface profiles after deformation. Presentation of the data is done using two colour tables; the larger colour table allows fine details such as grain boundaries, and after deformation, slip lines to be observed. The profile maps are useful to correlate to texture maps. The employment of a smaller colour table focuses attention on the general surface profile across the scan area, and is more advantageous to compare experimental data with numerical results.

4.4 Numerical Analyses

Simulations of uniaxial tension on Mo foil strips were carried out using the multi-scale model outlined in Chapter 3. Several input parameters are required for these
analyses, including:

(i) material properties (e.g. Young’s modulus, Poisson’s ratio);

(ii) crystallographic texture data (grain location/orientation); and

(iii) work-hardening behaviour (e.g. dislocation immobilization and recovery coefficients).

Material properties were collected from published Mo data, in conjunction with the uniaxial tensile data presented in Figure 4.3; these properties are outlined in Table 4.1. Crystallographic texture data is supplied via texture maps obtained using OM. The unrefined texture maps introduced in Section 4.3.1 for the undeformed Mo samples are refined using CHANNEL 5 software from HKL Technology [60], which uses the crystallographic orientation of neighbouring pixels to eliminate zero solutions. The data refinement was necessary to construct a continuous finite-element mesh comprising 5 x 5-µm² elements containing the orientation data of coincident data points from the experimental texture map. The number of elements in the mesh is equivalent to the number of data points in the OM – in all cases where a mesh is generated using OM data within this thesis, ten thousand elements are used. Grain geometry and location is preserved in this process, and the resultant mesh ensures each grain measured via OM in a given sample is represented by a minimum of one element during numerical analyses. Figure 4.12 presents the construction of a finite-element mesh comprising texture coincident with OM-produced maps. Euler angles recorded at each point in the refined OM (Figure 4.12(b)) are input into the variable array $\text{hisv}(\star)$ for each element using the appropriate LS-DYNA input file [47] to replicate the spatial distribution of the local texture in the finite-element model (Figure 4.12(c)).
To account for work-hardening behaviour, the isotropic hardening parameters associated with the mesoscopic work-hardening model developed by Peeters [7] were activated. All variables associated with transient work-hardening effects and kinematic hardening were not considered because monotonic loading was applied and texture evolution was not severe. As outlined in Equation 2.5, the rate of change of the randomly distributed dislocation density, $\dot{\rho}$, is a function of the immobilization coefficient $I$ and the recovery coefficient $R$. These parameters were determined through model calibration; values of $I$ and $R$ are adjusted until the true stress-strain behaviour of the model agrees with the empirical data given in Figure 4.3. Values for these coefficients are included with the physical properties given in Table 4.1\(^4\).

### 4.5 Analysis of Numerical and Empirical Data

Uniaxial tension in both Mo foil samples was simulated using the multi-scale model. Congruency in the work-hardening behaviour observed in both tests allowed for model calibration based on one set of data. Figure 4.13 highlights the behaviour predicted numerically upon calibration with the plastic deformation observed for Mo foil B. While good agreement exists throughout, slight deviation is observed at lower values of $\epsilon_p$; this can be attributed to the weak presence of a yield point in the material. The degree of pronunciation of this yield point varies between the two samples (as evidenced in Figure 4.3), which are attributed to variations in the amount of post-anneal impurities present. While the yield behaviour cannot be effectively factored into the present treatment, such deviation lies within acceptable limits.

\(^4\)The sensitivity of the predicted constitutive response to the values of these coefficients confirms the uniqueness of the determined parameters.
Surface Roughening

The principal test to compare numerical analyses with experimental data is through the texture-based inhomogeneous plastic strains that develop locally with applied deformation, which is manifested as surface roughness. Figure 4.14 presents the roughness profile observed for foil A via optical interferometry, compared with a coincident section of the corresponding finite-element (FE) analysis. Figure 4.15 presents the same comparison for foil B. The amount of through-thickness strain, $\epsilon_{ND}$, is a direct indicator of the extent of roughening in the system; large negative values of $\epsilon_{ND}$ are indicative of thinning, and would therefore be represented as lower points on a surface relief map relative to regions with low (absolute) $\epsilon_{ND}$ values. Figure 4.16 illustrates the correlation between through-thickness strain (via $\beta_L$) and surface roughness. Due to the variation in colour table used in displaying the results of each study, several points have been identified ($\alpha, \beta, \gamma$) to better facilitate comparison. Careful examination of Figures 4.14 and 4.15 confirms strong correlations between texture-based inhomogeneous plastic strains observed experimentally and predicted numerically.

While most simulated features show direct similarity with interferometric data, some dissimilar regions exist, which are labeled $\chi$ and $\xi$ in the aforementioned figures. Regions labelled $\xi$ exhibit excessive thinning, due solely to conditions imposed along the transverse boundaries of the FE mesh. This boundary effect, illustrated in Figure 4.15, leads to inaccurate values of $\epsilon_{ND}$ in these regions and must be ignored in the analyses. In regions labelled $\chi$, grains amenable to thinning are surrounded by material that prefers transverse contraction when tensile strain is applied in the longitudinal direction. While the model suggests the former regions have a lower
surface elevation relative to the latter, interferometric data reveals the opposite to be true. The most promising explanation for this discrepancy was put forth by Wright [4], who suggests that when such a variation in plastic anisotropy exists, the material susceptible to thinning (and therefore averse to deformation along the TD) experiences bending around the RD axis as the surrounding material contracts transversely. Figure 4.17 illustrates this phenomenon. The resultant deformation would result in a thinned region of material that has been forced to bend outwards due to the contraction of the surrounding material. Because the model uses two-dimensional (2D) elements, such out-of-plane bending cannot be predicted.

Quantitative assessment of roughening also shows good agreement. The variation in through-thickness strain, $\Delta \varepsilon_{ND}$, determined numerically is 0.168 for foil A. Since any texture variation along the ND is assumed negligible, no variation in $\Delta \varepsilon_{ND}$ exists through the thickness of the sample, and the degree of roughness on one surface of the foil, $R_t$, can be calculated via:

$$R_t = \frac{1}{2} t (e^{\Delta \varepsilon_{ND}} - 1),$$

(4.1)

where $t$ is the total thickness of the foil. At a measured thickness of 108 $\mu$m, $R_t$ for foil A is 9.88 $\mu$m. This is below the measured $R_t$ of 10.11 $\mu$m; however, the highest elevations on the interferometric surface map are coincident with locations of plastic bending. A significant contribution to the overall surface roughness due to this phenomenon is conceivable. Further support for this claim is evident in the results for foil B. Model results predict a value for $R_t$ of 8.63 $\mu$m, compared to a measured $R_t$ of 15.88 $\mu$m. Elevated surfaces are again associated with regions of plastic bending, and since the level of strain applied to this foil is higher, the contribution of plastic bending
to $R_t$ is expected to be greater as a result. Regardless, producing quantitative results within an order of magnitude of the experimental data in this work is encouraging.

**Texture Evolution**

Texture evolution of both foil samples, presented in Figure 4.18 as refined texture maps and in Figure 4.19 as discretized pole figures, is minimal at both 10 % (foil A) and 15 % (foil B) plastic deformation. Both figures suggest that the primary contribution to texture evolution is not total grain rotation, but rather sub-grain development. Figure 4.18 highlights the formation of low-angle grain boundaries within previously undivided material. This phenomenon is presented in Figure 4.19 as a dissolution of the local texture into a large number of orientations slightly rotated from their original positions. Deformation of this type is difficult to predict numerically for two reasons:

(i) inertial effects, as outlined in Appendix B, prohibit the interior elements of multi-element grains from experiencing strain increments accurate enough to predict sub-grain development; and

(ii) sub-grain development is dependent upon mesh size. Since optimal conditions (regarding inertial effects and computational efficiency) require a coarse mesh with grains comprised of few elements, extensive subdivision of such grains is not feasible.

Figures 4.20 and 4.21 compare experimental and numerically determined discrete-point pole figures for foils A and B, respectively. In both cases, little variation in texture is observed as grain division has produced a slight dispersion of the original
orientations; however, the extent that sub-grain development is overestimated (due to inertial effects) or underestimated (due to mesh refinement) is not known. Deformation to higher values of $\epsilon_p$ would be required to examine this behaviour further.

### 4.6 Summary

Uniaxial tensile tests of 100-µm thick Mo foil strips were performed, and the experimental results compared to numerical solutions acquired using the multi-scale model outlined in Chapter 3, employing an isotropic work-hardening model. The model used local OM texture data to generate a FE mesh with identical grain size, location, and orientation to scanned regions of the foil samples. Work-hardening parameters were calibrated based on true stress-strain curves acquired during sample deformation.

Texture-based inhomogeneous plastic strains were compared by examining the development of surface roughness in the material after applied strains of 0.10 and 0.15. The spatial variation of plastic strains predicted by the numerical model generally correspond to the surface roughness that developed in the tensile samples. Underestimations of the amplitude of roughening were attributed to out-of-plane plastic bending in the material, which cannot be modelled using quasi-2D elements but is clearly identifiable in both numerical and experimental analyses. The influence of this bending phenomenon is believed to increase with the level of applied strain, as variations in the two foil studies suggest. Texture evolution was found to be modest, primarily in the form of grain subdivision. Subgrain development was replicated in the numerical simulations, but mesh size and inertial effects limit the accuracy of these predictions.
Table 4.1: Parameters used as input for Mo foil simulations.

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>E</td>
<td>$315.0 \times 10^9$ Pa</td>
</tr>
<tr>
<td>$\nu$</td>
<td>0.29</td>
</tr>
<tr>
<td>b</td>
<td>$3.147 \times 10^{-10}$ m</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>0.2</td>
</tr>
<tr>
<td>$\tau_0$</td>
<td>$1.250 \times 10^8$ Pa</td>
</tr>
<tr>
<td>I</td>
<td>$7.500 \times 10^{-2}$</td>
</tr>
<tr>
<td>R</td>
<td>$6.100 \times 10^{-9}$</td>
</tr>
<tr>
<td>$\rho_o$</td>
<td>$2.800 \times 10^{12}$</td>
</tr>
</tbody>
</table>
Figure 4.1: ECC images of Mo foil (a) before and (b) after vacuum annealing at 1873 K for 1 h. Of note, the difference in magnification from (a) to (b) is roughly 10 x.
Figure 4.2: Incomplete pole figures of Mo foil (a) before and (b) after 1873-K anneal for 1 h.
Figure 4.3: True stress-strain behaviour of Mo foils A and B under uniaxial tension. Values are given in terms of both total strain and plastic strain ($\epsilon_p$).
Figure 4.4: Gold location marker viewed under a SEM at (a) 50x, and (b) 100x magnification (locations not coincident). Carbon burns resulting from texture scans are visible to the left of the marker at higher magnification.
Figure 4.5: Texture maps acquired using OM of undeformed Mo foil specimens: (a) Foil A, and (b) Foil B. Green areas represent non-indexed regions.
Figure 4.6: Texture maps acquired using OM of deformed Mo foil specimens: (a) Foil A, and (b) Foil B. Green areas represent non-indexed regions.
Figure 4.7: Comparison of pole figures determined from (a) bulk texture measurements using XRD with local texture data acquired using EBSD for (b) foil A and (c) foil B. The tensile direction is aligned with the vertical axis of each plot.
Figure 4.8: Surface profile of Mo foil A prior to deformation: (a) using a large colour table; and (b) using a small colour table.
CHAPTER 4. MOLYBDENUM FOIL TENSILE TESTING ... 96

Figure 4.9: Surface profile of Mo foil B prior to deformation: (a) using a large colour table; and (b) using a small colour table.
Figure 4.10: Surface profile of Mo foil A after deformation: (a) using a large colour table, showing loading direction; and (b) using a small colour table.
Figure 4.11: Surface profile of Mo foil B after deformation: (a) using a large colour table, showing loading direction; and (b) using a small colour table.
Figure 4.12: Example of crystallographic input for the multi-scale model, illustrated using the Eulerian angle Φ: (a) unrefined OM data of foil B prior to deformation; (b) refined OM data using CHANNEL 5 software; and (c) finite-element mesh containing the refined orientation data in (b).
Figure 4.13: Plastic work-hardening behaviour for Mo foil B, compared with results from the multi-scale model. Fluctuations in the experimental curve are due in this case to time-dependent noise in the source hydraulics.
Figure 4.14: Surface roughness of foil A after deformation: (a) the experimental roughness profile; and (b) the simulated through-thickness strain.
Figure 4.15: Surface roughness of foil B after deformation: (a) the experimental roughness profile; and (b) the simulated through-thickness strain. Terminal values of the colour table in (b) have been reduced to decrease the influence of inertial/boundary effects on the overall contour plot.
Figure 4.16: Correlation between $\beta_L$ and surface profile.
Figure 4.17: Plastic bending phenomenon suggested by Wright [4].
Figure 4.18: Refined texture maps of Mo foil A (a) prior to and (b) after 10 % deformation, and Mo foil B (c) prior to and (d) after 15 % deformation. Low-angle grain boundaries (< 10°) are black, while all higher-angle boundaries are green.
Figure 4.19: Experimental (110) and (200) discretized pole figures of Mo foil A (a) prior to and (b) after 10% deformation, and Mo foil B (c) prior to and (d) after 15% deformation.
Figure 4.20: Comparison of discrete-point pole figures for foil A (a) via EBSD prior to deformation, (b) via EBSD after deformation, and (c) simulated using the multi-scale model after deformation.
Figure 4.21: Comparison of discrete-point pole figures for foil B (a) via EBSD prior to deformation, (b) via EBSD after deformation, and (c) simulated using the multi-scale model after deformation.
Chapter 5

Two-Stage Strain Path Analyses in BCC Sheet Material

Previous analyses in this thesis have focused on the development of a three-tier multi-scale model, and how this model is able to predict both local and bulk material response to monotonic loading. This chapter details the response of Mo and IF steel sheet product to more complex applied strain paths, via experimental analysis and simulation of material behaviour using the three-tier multi-scale model. The discussion is segmented into three key areas: experimental data related to model calibration, supplementary experiments concentrating on more conventional orthogonal strain paths, and implementation of the multi-scale model.

5.1 Experimental Data for Model Calibration

As discussed in Section 2.2.1, macroscopic work-hardening behaviour due to complex strain paths has been predicted using a mesoscopic model developed by Peeters et
al. for IF steel sheet [61]. The model employs several parameters to characterise the evolution of dislocation density within a grain that is set in a polycrystalline aggregate. The simulated formation of dislocation sheets within these grains accounts for the transient hardening/softening effects (e.g. cross and Bauschinger effects) due to a change in strain path [62]. To calibrate the parameters in this model, a series of experiments are performed that elucidate the extreme cases of strain-path change. Tests comprising an orthogonal change in strain path produce cross effects, resulting (for the bcc materials tested) in a high transient yield point with a concurrently reduced hardening rate. In contrast, tests comprising a reversal of strain path result in Bauschinger effects that reveal less initial resistance to yielding and temporarily increased hardening rates upon strain-path change. Both phenomena are illustrated in Figure 5.1 for IF steel sheet, and are compared to monotonic tests.

Replicating measurable cross and Bauschinger effects in a laboratory environment remains a challenging task, particularly when attempting to apply a reversal in strain path to sheet material without invoking plastic instability. To circumvent this issue, in-plane shear tests are performed; this allows for the application of complex strain paths to sheet material with a simplified sample geometry. In-plane shear tests are also advantageous in that samples can be deformed to high values of strain before failure ($\varepsilon_{VM} > 0.5$), and materials that are inherently brittle experience greater ductility. The work of Rauch [63] illustrates the utility of simple shear tests for examining the plastic response of sheet materials.

Table 5.1 outlines the experimental test matrix used for the acquisition of model calibration data. The 99.98 % pure, 1.50-mm thick Mo sheet used was obtained from ESPI. It was cold-rolled and subjected to a similar stress-relief heat treatment and high-temperature vacuum anneal as the Mo foil (outlined in Section 4.2). The
IF steel was supplied by Stelco Inc. in 1.75-mm thick, cold-rolled and galvannealed condition. Table 5.2 lists the chemical composition of the material. An elaborate review of the processing and properties of IF steels is given by Hoile [64]. All tests were performed using the large-scale tensile and simple shear test facilities located at the Laboratoire des Propriétés Mécaniques et Thermodynamiques des Matériaux (LPMTM) at the Université Paris 13. The following sections outline the methodology employed for each test.

5.1.1 Monotonic Shear Tests

Specimens of IF steel and Mo sheet material were tested under simple shear using a small-scale planar shear device at LPMTM. The device (shown in Figure 5.2) is designed to be mounted onto a common tensile apparatus; the fixed part of the device holds one half of the sample in place, while the hydraulic ram of the tensile apparatus causes the mobile part of the device to displace vertically, resulting in the desired shear strain path. Specimen dimensions are 30 mm x 18 mm with the longer dimension running parallel to the shearing direction (SD). A sheared gauge region of approximately 30 mm x 2 mm is produced.

To capture the constitutive response of each specimen to loading, a combination of industrial and in-house data acquisition software was used. Stress data was derived from the 10-tonne load cell on the tensile apparatus, a MTS 20/M machine, using TestWorks version 3.09 supplied by MTS. Shear strain was determined by measuring the angular displacement of the material within the gauge region. Each specimen was coated with a white acrylic paint, and a black line applied with permanent marker perpendicular to the SD (Figure 5.3). A camera was mounted to record the relative
displacement of line segments on either side of the gauge region during deformation; this information was sent to in-house image analysis software for assessment of angular displacement and subsequently the overall shear strain applied. This technique assumes a uniform shear in the gauge region, which is confirmed via inspection of the marker. Strain data was then sent to the TestWorks software in real time to monitor the constitutive response of the material during testing. Figure 5.3 shows an undeformed Mo small-scale shear specimen, and one that has been deformed to 40%.

Figure 5.4 outlines the constitutive response of both IF steel and Mo sheet material to in-plane simple shear. In all cases, a strain rate on the order of $10^{-3} \text{s}^{-1}$ was maintained, as was an ambient temperature of approximately 22 °C. The SD was aligned parallel to the RD for each specimen, with the shear plane normal (SPN) parallel to the TD. Samples were bolted into the apparatus using a dynametric wrench set to 22 N·m for IF steel and 23 N·m for Mo specimens; a low applied torque will allow for slippage of the material within the device during tests, while a high applied torque can result in premature failure in the clamped material. An optimal torque level was found through inspection of the clamped material after tests employing a range of applied torques for each material.

### 5.1.2 Orthogonal Strain-Path (Cross) Tests

Large-scale tensile specimens were required to produce the primary deformation stage for the cross tests. The samples had a total length of 250 mm, aligned with the RD, and a gauge region of 180 mm x 40 mm. Figure 5.5 presents a schematic of the specimen geometry. The samples were mounted in the same apparatus used for
small-scale planar simple shear tests (MTS 20/M), with the shear device removed and a wide-grip tensile setup employed, as shown in Figure 5.6. A 10-mm MTS extensometer was used to record strain data, which was viewed in real-time using TestWorks version 3.09. Strain rate and ambient temperature conditions were held at $10^{-3} \text{ s}^{-1}$ and 22 °C, respectively.

Once a specific prestrain was imposed, tensile specimens were unloaded and simple shear specimens were machined from the gauge region. Figure 5.7 shows a tensile specimen that has had three shear specimens removed from it via an off-site computer numerical control (CNC) milling apparatus. The large size of the tensile specimen allows for several smaller shear samples to be removed, which permits better reproducibility of results considering a constant level of primary strain has been imposed to each extracted specimen (this assumes homogeneity in the strain distribution throughout the gauge region; provided that local necking is not observed in the material this is a reasonable assumption). Fewer tensile tests are required, as evidenced in Table 5.1, since multiple shear tests may be performed from a single tensile test.

In-plane simple shear samples were extracted such that the SD was aligned parallel to the tensile axis (TA) of the large-scale specimen. Uniaxial tensile tests were performed with the TA parallel to the RD to allow for a sufficient level of primary strain; the Mo sheet material is comprised of elongated grains along the RD, causing failure at a lower applied tensile strain along the TD due to the possible effect of grain boundary segregation and intergranular fracture [65]. These effects have less impact when the material is subjected to simple shear, as previously mentioned.

The subsequent cross tests were performed using the same methodology as for monotonic simple shear tests. The results of these tests are shown in Figure 5.8 for IF steel and Figure 5.9 for Mo. The constitutive response of each material during
second-stage shear deformation is compared to the response due to monotonic loading. Fewer successful tests were achieved using the Mo sheet due to the inherent brittle nature of the material; at levels of primary tensile strain greater than 0.10, subsequent shear tests caused premature failure of the specimens within the grip region, despite the level of clamping torque used.

In all cross tests, an increase in the yield strength upon strain-path change is observed, with subsequent reduction in the work-hardening rate compared to monotonic tests. The degree of softening after the change in strain path is dependent upon the amount of primary strain that has been imposed; more deformation during the first strain path results in greater softening after a strain-path change once yielding has been achieved. This behaviour remains consistent until the ultimate failure of the material.

5.1.3 Reverse Strain-Path (Bauschinger) Tests

Reversed shear strain paths were applied to the IF steel and Mo sheet material to observe the Bauschinger effect. Two methods were attempted to accomplish the reverse test: imposing both strain paths on 30-mm x 18-mm specimens using the small-scale planar shear device; and extracting 30-mm x 18-mm specimens from a larger sample after a primary shear strain was imposed, in a manner similar to the cross tests described in Section 5.1.2. Although the Bauschinger tests performed using the former method required less preparation, stress concentrations formed within the grip region during primary loading, leading to premature failure upon reversal of strain path in many of the tests. Primary loading on a large-scale shear specimen was therefore utilized in a majority of the reverse tests performed.
Figure 5.10 illustrates the large-scale planar shear apparatus used for application of the primary strain path. The apparatus, developed at LPMTM, consists of a fixed outer region surrounding a central chamber, wherein a mobile grip may translate vertically. Both the mobile grip and the outer fixed grips hold the sample in place through a combination of friction-based grip regions and a series of bolts running along the device. Figure 5.11 illustrates the function of the apparatus. Once assembled, the device was placed on an Instron 1195 tensile apparatus with a 10-tonne load cell, attaching the hydraulic ram to the mobile grip.

A schematic of the large-scale specimens used is given in Figure 5.12; the dimensions are smaller than earlier tests performed by Peeters for IF steel sheet [7] due to the greater strength of the Mo and the larger thickness of the IF steel used. Using 150-mm x 230-mm samples resulted in two 150-mm x 40-mm gauge zones on either side of the mobile ram, between the central chamber and the outer fixed grips. Because the gauge region is considerably larger than that of the small-scale planar shear tests, the material is much more susceptible to buckling during deformation; this is remedied by using thin aluminum wedges between the gaps in the gauge zones within the device. The wedges and sample gauge zones were coated with a boron nitride lubricant. In these tests, both the thickness of the wedges used and the torque applied to the connecting bolts were based on the hardness and thickness of the material being tested. For IF steel specimens, 0.2-mm thick wedges were used and a binding torque of 100 N·m was applied; for Mo specimens, 0.6-mm wedges were used and a binding torque of 120 N·m was applied.

Data acquisition during primary loading was taken using in-house software developed in LabVIEW. Shear stress was calculated from load cell data, while strain in the gauge zones was determined using a linear variable differential transformer (LVDT),
mounted on the tensile apparatus to measure the movement of the shear device. All tests were performed with constant crosshead velocity, resulting in a strain rate on the order of $10^{-3}$ s$^{-1}$. An ambient temperature of 22 $^{\circ}$C was also maintained.

Due to the large areas under simple shear, measurements were performed to ensure homogeneous deformation after each test. Prior to the experiment, specimens were sent to a screenprinter where a 1-mm x 1-mm square grid was applied. After testing, images of the deformed grid were taken using a flatbed scanner and optimized for brightness and contrast using Photoshop LE. The images were then sent to Aphelion, an in-house program developed by LPMTM to identify nodal coordinates on the deformed grid and determine the shear imparted over the gauge region. Isoshear curves were constructed using Tecplot Focus and examined for homogeneity. Figure 5.13 presents the shear distribution over a deformed gauge region in IF steel, after $\gamma = 0.1$ and $\gamma = 0.3$ was applied. For each sample, areas with the most homogeneous shear distribution were identified and small-scale shear specimens were extracted from these locations.

Once extracted, the 30-mm x 18-mm specimens were subjected to simple shear using the small-scale planar shear device as outlined in Section 5.1.1. Due to the nature of the test, both primary and secondary (reverse) loading of the specimens were performed with the SD along the RD and the SPN aligned with the TD. The constitutive response of IF steel and Mo sheet during a reversal in strain path is presented in Figure 5.14 and Figure 5.15, respectively. In both materials, a reduction in the yield strength is observed upon reversal of the strain path. The work-hardening rate appears to be greater than that observed for monotonic deformation, but eventually resumes characteristics similar to monotonic behaviour after a transient period. As with the cross tests, several reverse tests involving Mo sheet specimens failed
prematurely\textsuperscript{1}, limiting the amount of applied primary shear to $\gamma = 0.1$.

\section*{5.2 Conventional Cross-Test Studies}

Cross tests were performed on both IF steel and Mo sheet specimens via a two-stage process whereby the material is subjected to a strain path approximating in-plane plane strain along the RD, followed by uniaxial tension along the TD. This type of complex strain path is more applicable to an industrial setting than a planar shear test; for example, tube bending and hydroforming operations found in automotive manufacturing comprise a nearly orthogonal applied strain path, deformation that leads to reduced formability \cite{6}. The following tests examine the macroscopic constitutive response of both the relatively ductile IF steel sheet and the less-ductile Mo material, and are compared to the planar shear cross-test data used in model calibration. The results are also discussed in terms of the phenomenological accuracy of the model.

\subsection*{5.2.1 Data Acquisition}

To impose a strain path close to plane strain in a flat sheet sample, a notched geometry was developed by Valletta \cite{66} such that the central region of the gauge zone experiences in-plane plane strain. Figure 5.16 provides the design of the primary specimen geometry. A 3-mm x 3-mm array of points was applied to the surface of the gauge region using an in-house deposition tool developed by Kilfoil \cite{67}, with software developed in Image-Pro Plus. The array is used to capture the heterogeneous

\textsuperscript{1}Additional reverse tests were performed with an applied primary shear of $\gamma = 0.2$; application of the secondary (reverse) shear resulted in immediate specimen failure.
deformation within the gauge region, as significant variation in local strain path will be present from the outer notch area to the inner material during the primary tensile deformation [66].

Figure 5.17 presents the experimental setup used for the primary strain path test. All tests were performed using an Instron 8521 hydraulic tensile apparatus, equipped with a 100-kN load cell and 4-inch-wide grips. Images of the gauge zone were recorded during deformation using a digital camera to examine the constitutive response of the material. Initial tests were performed to failure, and a data-bifurcation study was performed to determine the load at which strain localization occurs [67]. Upper limits to the amount of applied primary strain were then determined, and a test matrix for the study was established; Table 5.3 outlines the experimental test matrix.

Once the primary deformation was applied and the amount of imposed plastic strain was confirmed via image analysis, small-scale tensile specimens were extracted from the deformed samples. Figure 5.18 provides a schematic of the tensile specimen used, and illustrates the extraction location within the primary specimen. IF steel specimens were extracted using an abrasive water jet cutter, while the Mo specimens were extracted using a CNC milling machine. All tensile tests were performed using an Instron 8521 hydraulic tensile apparatus with Instron Bluehill data acquisition software to record and display the macroscopic constitutive response of the material during deformation. Load data was supplied via a 100-kN load cell, while strain data was captured using an Instron extensometer with 10-mm gauge length.

Results of the secondary uniaxial tensile tests are presented in Figure 5.19. It is clear that in nearly all cases for both materials, strain localization is achieved immediately after the transition in strain path. In Mo, the failure is brittle in nature (though microyielding is observed), while a more ductile failure is observed in the
IF steel. Work hardening was only observed in the IF steel with the least amount of primary strain ($\epsilon_{RD} = 0.097$). The reason for this immediate failure can be attributed to sufficient thinning of the material during primary deformation – a direct result of plane-strain deformation – coupled with the dramatic increase in transient yield strength during an orthogonal change in strain path. Unfortunately, such immediate failure in the material limits the suitability of this data for comparison with simulated results, as the multi-scale model presented is concerned with material behaviour prior to failure. The data is nevertheless useful in highlighting the limited formability of materials when subjected to such a severe change in strain path, which is of importance in industrial processes [68].

5.3 Assessment of the Three-Tier Model under Strain-Path Change

The parameters necessary for prediction of transient work-hardening behaviour within the multi-scale model were activated, and numerical solutions from the model were compared to results from the calibration tests conducted at LPMTM. Emphasis was placed on the cross-test data, as this is the most complex two-stage test performed. Bauschinger effects arise from a reversal in strain path and have little to do with the formation of new cell-block boundaries (CBB’s) in the material, whereas cross effects involve new CBB formation and microband cut-through; a full discussion of these phenomena is presented in Chapter 2.

Model input in the form of local texture distribution was obtained using electron backscatter diffraction (EBSD) techniques similar to those outlined in Section 4.3.1.
The large sample size required for the two-stage tests and the relatively small specimen chamber within the SEM prohibits the use of texture and roughness evolution techniques previously employed; therefore, only an initial baseline scan of the texture was taken using 12-mm x 20-mm samples for each material (no marking of the scan area was required). Figures 5.20 and 5.21 present the local texture maps for samples of IF steel and Mo, respectively. Figure 5.20 includes pole figure comparisons of the local and bulk textures acquired for the IF steel sheet; given the qualitative agreement between these textures, the local texture data was employed in FE simulations to predict macroscopic plasticity during two-stage strain-path tests.

In the case of the Mo sheet, a 50.1% index rate using a step size of 4 µm meant that a local texture distribution capable of representing the bulk texture could not be obtained. Examination of the material at a higher magnification (Figure 5.21(b)) reveals a bimodal structure where some larger grains are subdivided by low-angle grain boundaries; this mosaic structure limits successful EBSD indexing due to the small size of the defect-free regions relative to the beam step size. Comparison between the bulk Mo sheet texture (Figure 5.21(c)) and the annealed Mo foil (Figure 5.21(d)) reveals qualitative agreement in texture components. Since these materials were annealed concurrently\(^2\), and the Mo foil contains no bimodal structure, interstitial impurities segregated at grain boundaries within the Mo sheet are assumed to be the likely cause of suppressed grain growth during the anneal [69]. Interstitials are also assumed to be responsible for the yield point observed during monotonic and two-stage strain-path experiments using the Mo sheet, effectively pinning dislocation sources. Due to the inability to accurately relate bulk material properties with local

\(^2\)Some difference in the stored work between pre-annealed foil and sheet product will exist, but was concluded to have a minimal impact on the observed differences in grain morphology due to annealing.
texture scans in annealed Mo sheet product, numerical solutions were only carried out for IF steel sheet data.

The first step in model calibration was the activation of parameters \( I \) and \( R \), responsible for the immobilization and recovery of the randomly distributed dislocations responsible for isotropic hardening\(^3\). Table 5.4 presents the calibrated parameters for IF steel, compared with those determined by Peeters for a similar material [7], while Figure 5.22 compares the experimental data from calibration tests with simulated results. When calibrating these parameters, the values determined by Peeters were used as a starting point and adjusted until the numerical solution best reproduced the experimental results (these parameters are sensitive enough to ensure optimal settings without the need for complex error analyses). As with the Mo foil results presented in Section 4.5, some initial variation in the work-hardening behaviour exists, which becomes negligible after \( \gamma = 0.03 \). Once \( I \) and \( R \) have been determined, parameters \( I^{\text{wd}} \) and \( R^{\text{wd}} \) are activated. These parameters are associated with the immobilization and recovery, respectively, of the dislocations forming cell-block boundaries (CBB’s) within the material. While CBB’s are formed during monotonic loading, their most pronounced contribution to the work-hardening behaviour exists during the strain-path transition in a cross test.

Figure 5.22 illustrates how the calibrated model accurately predicts the sharp increase in yield stress as the material is subjected to a secondary orthogonal strain path; deviation in these curves is due mainly to the point where plastic deformation is defined in the experimental data, but conservative estimates place the numerically predicted yield stress immediately after strain-path change to within 10 MPa of the experimental data. Also of note is the contribution of \( I^{\text{wd}} \) and \( R^{\text{wd}} \) to monotonic

\(^3\)Refer to Section 2.3.1 for pertinent equations.
hardening behaviour; the rapid immobilization of dislocations that eventually form CBB’s in the material results in a more accurate hardening rate during the initial stage of deformation, reducing the initial variation in predicted work-hardening behaviour when only $I$ and $R$ are active.

The final set of parameters associated with cross effects in the hardening model simulate effects concerning non-currently generated (NCG) CBB’s. Parameter $R_{ncg}$ captures dislocation recovery on the older dislocation sheets, while $\beta_1$ and $\beta_2$ simulate the formation of microbands that cut through these sheets. Figure 5.23 illustrates how the activation of $R_{ncg}$, $\beta_1$ and $\beta_2$ affects the transient work-hardening behaviour using the original Peeters model [7]. In contrast, increasing the value of $R_{ncg}$ from zero to values equal to and above that presented by Peeters does not produce a similar response in the current three-tier model, as shown in Figure 5.24.

Examination of elements within the FE mesh reveal grains whose CBB slip systems are constantly changing. In some cases this state of flux is necessary to predict the plastic strain ratio for a given orientation (outlined in Chapter 2). Instances arise, however, where this dynamic behaviour is a result of the preferential hardening along CBB’s. Specifically, the subsequent global stress tensor calculated by the crystal plasticity subroutine includes a slight out-of-plane shear, which causes a change in the strain increment at the next time step, resulting in the activation of a new set of slip systems. Once the shear has been corrected, the original set of systems is selected and the cycle is repeated. Regardless of the cause, this constant change of CBB’s suppresses recovery events on the dynamically activated dislocation sheets, to the point where dramatic increases of $R_{ncg}$, $\beta_1$ and $\beta_2$ will have little impact on the accuracy of the transient response during cross tests.

Figure 5.24 reinforces the above statement; that is, increasing the value of $R_{ncg}$
results in a full recovery of CBB’s developed during primary deformation, followed by increased hardening due to the development of multiple sets of CBB’s. Analysis of dislocation density evolution on NCG CBB's in grains where dynamic CBB selection exists supports this hypothesis. In grains where no dynamic CBB selection exists, no spurious hardening is observed.

The dynamic behaviour exhibited by the Peeters hardening model in the present implementation was not accounted for in its original form, due to the use of a static prescribed strain increment in previous analyses [7]. The presence of a dynamic strain increment introduces irrecoverable errors into numerical analyses, which are most pronounced when the recovery of NCG CBB’s are required for a reduction in the work-hardening rate. Solutions to this problem require a thorough investigation of the factors that promote dynamic CBB selection, the phenomenological accuracy of the theory presented in the mesoscopic hardening model, and experimental observation to support or refute the model behaviour. Such work is considered outside the scope of this thesis.
Table 5.1: Experimental test matrix for calibration of the mesoscopic hardening model.

<table>
<thead>
<tr>
<th>Test Performed</th>
<th>Number of Tests</th>
</tr>
</thead>
<tbody>
<tr>
<td>Primary Strain Path</td>
<td>Secondary Strain Path</td>
</tr>
<tr>
<td>Monotonic simple shear</td>
<td>Orthogonal simple shear</td>
</tr>
<tr>
<td>Uniaxial tension, $\epsilon_{RD} = 0.01$</td>
<td>Orthogonal simple shear</td>
</tr>
<tr>
<td>Uniaxial tension, $\epsilon_{RD} = 0.02$</td>
<td>Orthogonal simple shear</td>
</tr>
<tr>
<td>Large-scale shear, $\gamma = 0.10$</td>
<td>Reverse simple shear</td>
</tr>
<tr>
<td>Large-scale shear, $\gamma = 0.20$</td>
<td>Reverse simple shear</td>
</tr>
<tr>
<td>Large-scale shear, $\gamma = 0.30$</td>
<td>Reverse simple shear</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Table 5.2: Chemical composition (wt %) of the investigated IF steel.

<table>
<thead>
<tr>
<th>C</th>
<th>Mn</th>
<th>P</th>
<th>S</th>
<th>Si</th>
<th>Cu</th>
<th>Ni</th>
<th>Cr</th>
<th>Mo</th>
<th>V</th>
<th>Nb</th>
<th>B</th>
<th>Ti</th>
<th>Sn</th>
<th>ASA</th>
<th>N</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.004</td>
<td>0.12</td>
<td>0.003</td>
<td>0.008</td>
<td>0.019</td>
<td>0.014</td>
<td>0.011</td>
<td>0.005</td>
<td>0.02</td>
<td>0.005</td>
<td>0.003</td>
<td>0.063</td>
<td>0.002</td>
<td>0.027</td>
<td>0.004</td>
<td></td>
</tr>
</tbody>
</table>
**Table 5.3: Experimental test matrix for conventional cross-test analyses.**

<table>
<thead>
<tr>
<th>Test Performed</th>
<th>Number of Tests</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Primary Strain Path</strong> (In-Plane Plane Strain)</td>
<td><strong>Secondary Strain Path</strong> (Orthogonal Uniaxial Tension)</td>
</tr>
<tr>
<td>to failure</td>
<td></td>
</tr>
<tr>
<td>$\varepsilon_{RD} = 0.05$</td>
<td>to failure</td>
</tr>
<tr>
<td>$\varepsilon_{RD} = 0.10$</td>
<td>to failure</td>
</tr>
<tr>
<td>$\varepsilon_{RD} = 0.20$</td>
<td>to failure</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Table 5.4: Material parameters for IF steel used in the three-tier model, compared to those of Peeters [7].

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Peeters Model</th>
<th>Three-Tier Model</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>2.2 $10^{-2}$</td>
<td>2.60 $10^{-2}$</td>
</tr>
<tr>
<td>R</td>
<td>8.5 $10^{-10}$</td>
<td>8.5 $10^{-10}$</td>
</tr>
<tr>
<td>$R_{wd}$</td>
<td>9.4 $10^{-1}$</td>
<td>6.00 $10^{-1}$</td>
</tr>
<tr>
<td>$R_{wd}$</td>
<td>2.6 $10^{-8}$</td>
<td>2.6 $10^{-8}$</td>
</tr>
<tr>
<td>$\tau_0$</td>
<td>42.0 MPa</td>
<td>60.5 MPa</td>
</tr>
</tbody>
</table>
Figure 5.1: A typical constitutive response for IF steel sheet under extreme cases of strain path change [61]. Above: cross tests after 10 and 20 % tensile prestrain, compared to monotonic loading behaviour. Below: Bauschinger tests after preshear values of $\gamma = 0.1$ and $\gamma = 0.3$. 
Figure 5.2: Planar simple shear device. *Clockwise from top-left:* mounting of the rig in a hydraulic tensile apparatus; detail of the rig highlighting mobile (left in the figure) and immobile (right in the figure) parts; and mounted camera for image acquisition during analyses.
Figure 5.3: Small-scale Mo specimens subjected to simple shear (units shown are cm). From left to right: an unprepared sample, a sample after the application of a white latex paint and black line along the SPN to monitor the total applied shear strain, and a sample after 40% shear strain is imparted.
Figure 5.4: Constitutive response of IF steel and Mo to in-plane simple shear, with SD parallel to the RD and the SPN parallel to the TD.
Figure 5.5: Schematic detailing the large-scale tensile specimen geometry (dimensions in inches).
CHAPTER 5. TWO-STAGE STRAIN PATH ANALYSES ...

Figure 5.6: Large-scale tensile apparatus used for primary deformation of cross tests.
Figure 5.7: Extraction of secondary simple shear specimens from a deformed large tensile sample.
Figure 5.8: Constitutive response of IF steel sheet under a two-stage cross test, compared to monotonic simple shear (upper and lower bounds represent standard deviations from the average data).
Figure 5.9: Constitutive response of Mo sheet under a two-stage cross test, compared to monotonic simple shear (upper and lower bounds represent standard deviations from the average data).
Figure 5.10: Large-scale planar shear device, mounted within a hydraulic tensile apparatus. *Left:* mounting of the rig. *Right:* detail of the rig with mounted LVDT (top-left in figure).
Figure 5.11: Exploded view of the large-scale shear device, presenting the outer fixed grips (top-left, top-right) which clamp the ends of the sample, while the mobile grip (bottom center) clamps the center of the sample (from [7]). A specimen deformed using the device is shown still clamped to the mobile grip. Arrows indicate the direction of relative displacement during deformation.
Figure 5.12: Schematic detailing the large-scale shear specimen geometry (dimensions in inches).
Figure 5.13: Shear strain distribution over the gauge zone in an IF steel sheet sample: (a) $\gamma = 0.1$; and (b) $\gamma = 0.3$. 
Figure 5.14: Constitutive response of IF steel sheet under a two-stage reverse test (upper and lower bounds represent standard deviations from the average data).
Figure 5.15: Constitutive response of Mo sheet under a two-stage reverse test (upper and lower bounds represent standard deviations from the average data).
Figure 5.16: Schematic of the specimens used for primary strain-path tests in conventional cross-test studies (dimensions in inches).
Figure 5.17: Setup used for the primary strain-path tests in conventional cross-test studies. 

A: data acquisition system. 
B: high-intensity lights for image capture. 
C: image capture via digital camera or video. 
D: wide-grip mounts.
Figure 5.18: Small-scale tensile specimens used for secondary strain-path tests in conventional cross-test studies: (a) extraction scheme using the predeformed specimen; and (b) schematic of the extracted tensile sample (dimensions in inches).
Figure 5.19: Constitutive response of (a) IF steel and (b) Mo sheet during application of the secondary strain path in conventional cross-test analyses.
Figure 5.20: EBSD scan of a representative IF steel sample used for two-stage strain-path tests. A comparison of pole figures for the local (complete, bottom left) and bulk (incomplete, bottom right) textures is provided.
Figure 5.21: Mo sheet texture scans: (a) unrefined local texture scan using a 4-\(\mu\)m step size; (b) local texture scan using a smaller 0.3-\(\mu\)m step size, refined using CHANNEL 5 software to predict non-indexed orientations (low-angle grain boundaries in light blue, boundaries with misorientations > 10° in black); (c) incomplete bulk texture pole figures for the Mo sheet; and (d) incomplete bulk texture pole figures for the Mo foil.
Figure 5.22: Comparison of experimental calibration data for IF steel with numerical results, upon activation of $I$, $R$, $I_{wd}$, and $R_{wd}$. 

- Monotonic loading simulation, $I_{wd} = R_{wd} = 0$, $\tau_0 = 47.5$ MPa
- Cross test simulation, $I_{wd} = 6.00E^{-1}$, $R_{wd} = 2.60E^{-8}$, $\tau_0 = 60.5$ MPa
- Experiment (monotonic and cross tests)
Figure 5.23: Simulated behaviour of cross tests using the original Peeters model, with (a) no activation of recovery effects associated with non-currently generated CBB's, (b) activation of $R_{ncg}$, and (c) activation of $R_{ncg}$, $\beta_1$ and $\beta_2$ [7].
Figure 5.24: Simulated behaviour of the three-tier model, with increasing values of $R_{ncg}$ ($\beta_1 = \beta_2 = 0$).
Chapter 6

Discussion

A detailed review of the three-tier model developed in Chapter 3 and validated in Chapters 4 and 5 is presented herein. The suitability of the model for predicting the constitutive response, surface roughening, and texture evolution of bcc materials under monotonic and complex strain paths is discussed. In addition, the implication of experimental results with respect to the validity of the underlying theory used in this thesis is explored, which leads to suggestions for improving the current understanding of plasticity in bcc materials.

6.1 Qualification of LS-DYNA within the Three-Tier Model

The use of a dynamic explicit finite-element (FE) model to simulate microscopic constitutive behaviour is a novel approach. While most FE models make use of continuum mechanics for deformation analyses, the capturing of local phenomena is inherently difficult with this approach. In the case of heterogeneous work-hardening
CHAPTER 6. DISCUSSION

behaviour due to crystallographic texture, such models are ill-suited and crystal-plasticity theory must be employed. The incorporation of such theory into a subroutine within LS-DYNA facilitates the goals of this thesis, while introducing several unique challenges due to the dynamic explicit nature of the FE code. Two key properties are directly influenced by the use of LS-DYNA: the simulation of texture-based anisotropy; and localization artifacts due to inertial effects.

6.1.1 The Development of Texture-Based Anisotropy

The representation of a single grain within the FE model by a minimum of one element allows for a variation in local work-hardening behaviour that is dependent on the crystallographic orientation of the material. Under normal conditions, the constraint of representing a grain with one element results in an overestimation of the predicted stiffness during deformation that would be relieved by mesh refinement; however, due to the restrictions imposed by inertial effects in the model, mesh refinement would localize the variation in strain across grains to the grain boundaries and further degrade the accuracy of the solution. While the crystal plasticity subroutine is responsible for determining active slip systems at a given orientation, it is the dynamic nature of the incremental strain tensor, $\Delta \epsilon_{ij}$, that allows for accurate representation of the orientation-dependent plastic strain ratio, $\beta_L$. Figure 6.1 illustrates the development of the incremental ($\beta_{L,i}$) and total ($\beta_{L,t}$) plastic strain ratio for two ideal orientations: cube-on-edge (CE) and cube-on-face (CF). As outlined in Section 3.3.1, $\beta_{L,t}$ for a CE texture is 1, while $\beta_{L,t}$ for a CF texture is 0. Although the total plastic strain ratio for both orientations is accurately represented by the model, the instantaneous ratio for the CF texture is oscillatory in nature. It is the dynamic
nature of the incremental strain tensor that causes a change in the set of active slip systems over successive time steps, stabilizing the net transverse strain of the element at 0. Had a static strain tensor been employed, the active set of slip systems would remain constant and a nonzero transverse strain would be inaccurately predicted. For this reason, the three-tier model developed within LS-DYNA can accurately simulate orientation-dependent anisotropy during deformation, which is a unique contribution to current numerical methodology since other static FE models cannot reproduce these variations in $\beta_L$.

Challenges with LS-DYNA arise when initializing $d\varepsilon_{ij}$. Due to the explicit nature of the FE formulation, the prescribed strain increment for an element is based on the global stress tensor from the preceding timestep. Since no such timestep exists at the start of a simulation, the strain increment is derived from the prescribed nodal velocities within the model input files. Problems with this derivation occur when $\beta_L$ determined from the prescribed strain increment differs greatly with the expected $\beta_L$ of a given orientation. Considering a CE orientation under uniaxial tension, an initial $d\varepsilon_{ij}$ contains no transverse strain component; since the active set of slip systems for this orientation produce no global transverse stress, there will be no dynamic evolution of $d\varepsilon_{TD}$ for subsequent timesteps, resulting in $\beta_{L,t} = 0$ instead of $\beta_{L,t} = 1$. The problem is further compounded in multi-element models where nodal velocities are traditionally applied as boundary conditions, resulting in a lack of prescribed deformation to interior elements. Inertial effects in larger models prevent an appreciable level of strain from reaching interior elements for the first few timesteps; however, due to the nature of the crystal plasticity subroutine, active slip systems will be chosen that may produce an inaccurate representation of the stress state within these elements. In many cases, these events lead to model instability.
Solutions to such issues may be found by using an implicit scheme, where the initial $\beta_L,i$ may be optimized for a given crystallographic orientation. Problems resulting from insufficient nodal velocities for interior elements could also be addressed by setting a threshold for the incremental von Mises strain increment $\Delta \varepsilon_{VM}$, below which no stress tensor would be calculated. It has been found, however, that the most efficient solution is to prescribe nodal velocities for each element within the input file, including an inferred transverse strain where necessary. The approach nullifies inertial effects that would result from the application of prescribed nodal velocities at only the model boundaries, and allows for accurate development of $\beta_L$ while benefiting from the computational efficiency of explicit FE models versus their implicit counterparts.

One additional modification to the existing model is the consideration of elastic anisotropy, which would improve predicted surface profiles by capturing not only anisotropic deformation at the onset of deformation, but during the elastic unloading of the material. Studies have also shown elastic anisotropy to have an impact on dislocation interactions during plasticity [70]. The potential benefits of modelling material-specific anisotropic behaviour during both elastic and plastic deformation warrants further consideration.

6.1.2 Inertial Effects and the Courant Condition

While setting initial nodal velocities in an LS-DYNA input file circumvents inertial effects at the onset of the numerical solution, issues associated with the designated element mass persist during simulation. This phenomenon is evident in discrete-point pole figures of Mo foil tests, outlined in Chapter 4. Figures 4.20 and 4.21 provide experimental pole figure data for two samples, compared to numerical analyses subjected
to the same deformation path and using an identical initial texture. The extent of simulated crystallographic rotation in these cases is either overestimated in elements possessing a high level of contrast in crystallographic orientation across adjacent elements, or underestimated in elements with little contrast. In physical terms, this effect causes elements near high-angle grain boundaries to experience significantly higher deformation relative to elements located within a grain interior. While some variation in the extent of deformation is expected to occur across a grain, the disparity between these two groups of elements is the direct result of a heightened level of prescribed inertia in the model.

The need for an increase in element mass arises as a requirement for satisfying the Courant condition within LS-DYNA, which stipulates that the timestep $\Delta t_e$ must conform to the equation:

$$\Delta t_e = \frac{L_s}{c}, \quad (6.1)$$

to ensure there are no errors introduced due to the interference of propagating stress waves during analyses of high-speed deformation [71]. In Equation 6.1, $L_s$ is the characteristic element length of the element, and $c$ is the speed of sound, defined as:

$$c = \sqrt{\frac{E}{\rho(1-\nu)}}, \quad (6.2)$$

The characteristic element length for square shell elements is equivalent to the specified element length in the model input file, which is less than 10 $\mu$m for all analyses in this thesis. Given the average physical properties (Young’s modulus $E$, mass density $\rho$, and Poisson’s ratio $\nu$) for the materials tested, a Courant timestep on the order of $10^{-12}$ s is typical. The simulated time needed to complete the desired deformation
ranged from 20-60 s, depending on the complexity of the strain path, resulting in over $10^{13}$ timesteps. Such a model would require many years to run to completion for even single-element studies, making the ideal model settings unrealistic. To remedy this time issue, a user-defined timestep size can be added to the LS-DYNA input file; the model then conforms to this timestep while satisfying the Courant condition via mass scaling. This approach is an acceptable compromise provided high-strain-rate tests (e.g. impact tests) are avoided, since modifications to the inertia of the material will typically have little effect on deformation carried out at lower strain rates; however, the level of mass scaling utilized in the current simulations is significant due to the microscopic element lengths required, which results in some influence of model inertia on strain localization near high-angle grain boundaries.

The extent of the influence arising from mass scaling can be estimated from comparisons of the simulated roughening of Mo foil to experimental results (Figures 4.14 and 4.15). Qualitative agreement in these cases suggests the inertial effects are not severe at modest levels of imposed strain, but should be recognized as a source of error in quantitative analyses. Whether this error is due to a nominal degree of influence by mass scaling or by the interaction of grains with contrasting texture-based anisotropy has not been determined, but may be assessed with further simulation and experimental testing to higher strain levels where this interaction is more pronounced.

Similar crystal-plasticity FE models have been successfully developed (e.g. the models of Dawson et al. [1] and Inal et al. [72]) using static FE programs, which suggests that implementing the multi-scale model presented in this thesis may be achieved in an environment that is not concerned with stress-wave propagation and the consequent imposition of a Courant condition. Although a loss of quantitative accuracy could result from implementing a multi-scale model in an implicit scheme
with rate-dependence, it has been shown that inhomogeneous plastic deformation could still be qualitatively assessed; for instance, Wu et al. [13] have developed a multi-scale model capable of determining the texture components responsible for roping in aluminum sheet AA6111, incorporating local texture data captured via EBSD into a FE program and predicting the surface roughness during deformation with various texture components removed.

It was also shown by Wu et al. [13] that an increased step size during EBSD measurements, while not capturing every grain in the area of interest, was still capable of predicting the general trends in surface roughening when used as model input. Therefore, it is possible that using a larger EBSD step size (and therefore, a larger element length) would relax the constraint imposed by the Courant condition and reduce the inertial effects observed in the three-tier model; the tradeoff with this approach, however, is the lack of a true representation of neighbouring grains in the material. The influence of surrounding grains must be addressed before changes to the texture scan resolution are implemented.

6.2 Qualification of an Integrated Taylor-Based Crystal Plasticity Model in LS-DYNA

Crystal plasticity models based on the Taylor theory [16] are utilized in a modest portion of modern deformation studies due primarily to the phenomenological accuracy of the deformation mechanism presented and the computational efficiency of the analysis. Traditional Taylor-based models have suffered from the lack of maintaining force equilibrium across grains (i.e. iso-strain assumption), and from ambiguity
in selecting active slip systems in the event of an equivalence in calculated internal work. While a great deal of effort has been spent on the development of more sophisticated models to circumvent these issues, a loss of phenomenological accuracy and computational efficiency invariably results.

The integration of established Taylor-based crystal plasticity theory within a FE model allows for the maintenance of both strain compatibility and force equilibrium, with no loss of accuracy and efficiency. In this thesis, the issue of Taylor ambiguity is addressed passively via the work-hardening model of Peeters, since the non-uniform hardening that occurs over the set of potentially active slip system prevents equivalence in internal work calculations [48]. One time at which ambiguity may occur is at the initial timestep, prior to the evolution of the critically resolved shear stress on each potentially active slip system. By including a Renouard-Wintenberger formulation that examines the rate of change of work due to strain \( \frac{dW_T}{de_M} \) in the event of work equivalence, proper system selection leading to correct grain rotation can be realized [21].

Proof of model effectiveness lies in the grain rotation fields presented in Figures 3.4 and 3.5. The fields are theoretically accurate, and the slip systems selected for a given orientation and strain path have been confirmed in benchmark studies of data reported by Chin and Mammel [44]. It is clear from these studies that certain systems are dominant depending on the orientation of the crystal, and are therefore necessary to include when considering deformation in a bcc system. While \{110\}\langle111\rangle systems are dominant for orientations centered in the stereographic triangle (particularly along the divergent grain rotation path), \{112\}\langle111\rangle systems are predominantly active at orientations near \langle100\rangle when subjected to uniaxial tension/compression. The combination of both sets of systems provides an accurate prediction of grain
rotation paths across the range of crystallographic orientations, although inclusion of \{123\}\langle111\rangle systems would improve upon this accuracy, particularly for orientations near \langle110\rangle under uniaxial compression (Figure 3.4(e)). Theoretically, the accuracy of the crystal-plasticity model would continue to improve if a greater number of potentially active slip systems were considered, ultimately leading to the inclusion of pencil glide in the model [44]; currently, the advantages of greater accuracy must be offset by the loss of computational efficiency resulting from the evaluation of a significantly larger number of linearly independent slip systems. The simulation of monotonic tests in Chapters 4 and 5 supports the hypothesis that accurate bcc deformation may be modelled using \{110\}\langle111\rangle and \{112\}\langle111\rangle as potentially active slip systems for the integrated three-tier model employed. These assumptions have also been confirmed experimentally by Rauch [73] and Christian [55] for other bcc materials.

**Single-Grain-per-Element Representation in FE Models**

The ability to accurately simulate texture-based anisotropy is advantageous when each element of the FE model is limited to predicting the deformation behaviour of a single grain and the spatial topography of the texture represented is consistent with the original material. Correlation between the local surface texture distribution of the material and the derivative texture of the FE model was successfully achieved using electron backscatter diffraction (EBSD) techniques, but limitations with the accuracy of the simulated texture exist. As presented in Figure 4.7, agreement between the local texture captured and the bulk texture of the material must be maintained to ensure accuracy in the predicted macroscopic work-hardening behaviour. In most cases, the grain size is sufficiently large to allow for element lengths between 2.5 and 5.0 \(\mu m\); while elements this size will introduce inertia-based artifacts into the numer-
ical solution (Section 6.1.2), the quantitative error has been shown to be acceptable (Section 4.5).

When the crystallographic orientation of a grain is not clearly identifiable using EBSD scans at these settings, problems arise, as was the case for the analysis of Mo sheet subject to complex strain-path tests (Section 5.3). Texture scans of material containing a bimodal structure or grains with significant substructure present cannot be successfully captured at an acceptable magnification. For the Mo sheet, a beam step size for the EBSD raster scan (and consequently, the element length of the FE model) of 0.3 $\mu$m is required to properly index the majority of the scan area. Since the structure is bimodal, a disproportionately large area of the scanned region is comprised of texture data for larger grains. The scan area necessary to produce an accurate representation of the bulk texture would require thousands of additional scan points, corresponding to a fine FE mesh that is unable to reach a solution in a realistic time frame. It is clear that a consistent undeformed grain structure is ideal for the current type of texture data acquired for model input.

**Plane-Stress Assumptions in Quasi-Two-Dimensional Analyses**

The use of Taylor-based crystal plasticity theory infers that the resultant stress tensor calculated within the LS-DYNA subroutine will be deviatoric in nature [16]; to produce an incremental strain tensor, however, the FE model requires a global stress tensor with both hydrostatic and deviatoric stress components. As mentioned in Section 3.2.1, the hydrostatic stress is assumed to be equal to $-\sigma_{ND}^{g}$ such that the global through-thickness stress is reduced to zero and a plane-stress assumption is maintained. The assumption is reasonable for the foil and thin sheet product used in this thesis, and has been used for several numerical studies of sheet material using
crystal-plasticity theory [13, 33, 34], but would not be suitable for plate or parts with complex geometries.

Quantitative analyses of roughening in Mo foil validate the use of a plane-stress assumption, and confirms the negligible influence of texture along the normal direction of these specimens. The assumption that the evolution of through-thickness strain on surface grains is indicative of the underlying grain behaviour leads to the derivation of Equation 4.1 and the calculation of the surface roughness $R_t$, which exhibits good agreement with experimental results. Moreover, the roughening of the surface opposite the one studied is assumed to be identical; whether or not this is the case cannot be confirmed using the current methodology. Furthermore, such assumptions may not be valid for thin sheet product whose grain size is notably smaller than the sheet thickness, given the potential for extensive through-thickness texture variation.

6.3 Qualification of Mesoscopic Hardening Theory in a Multi-Scale Model

The accuracy of the model developed by Peeters et al. [7] for both simple and complex strain paths has been addressed in the literature [39, 61, 62]. The dislocation-based development of substructure within the bcc materials tested was confirmed using transmission electron microscopy, and the simulated evolution of bulk texture during deformation was found to be correct. While the evolution equations and the corresponding crystal plasticity framework are similar to previous work, the use of the Peeters model in this treatment has evolved in two ways:

(i) rather than a prescribed static strain tensor, a dynamic incremental strain tensor
is provided for each timestep via the main LS-DYNA FE program; and

(ii) the spatial representation of a local texture map in the FE mesh allows for the influence of neighbouring grains in work-hardening calculations.

The influence of the FE model to the perceived work-hardening behaviour ranges from negligible to significant, depending on the level of complexity in the strain path chosen, and subsequently, the interaction of predominantly active slip systems.

6.3.1 Isotropic Hardening under Monotonic Strain Paths

The observed constitutive response of both IF steel and Mo foil and sheet under monotonic loading can be correctly reproduced using the three-tier model. The parameters associated with isotropic hardening of the material – the immobilization coefficient ($I$) and the recovery coefficient ($R$) of the randomly distributed dislocations in a grain – closely resemble the fitting parameters used in the original Peeters work [7], as outlined in Table 5.4. The work-hardening data is underestimated during the onset of plasticity (when plastic shear $\gamma < 0.03$); Figure 6.2 compares the predicted response of an IF steel material using the three-tier model with the earlier Peeters treatment of a similar material. The accuracy of the three-tier model is further improved when the parameters associated with the formation of cell-block boundaries (CBB’s) are activated, resulting in an increase in the predicted yield response during the initial plastic deformation (Figure 6.2(b)).

Inclusion of CBB formation in numerical analyses of monotonic loading highlights the advance in accuracy (both numerical and phenomenological) such a model possesses under isotropic hardening conditions. The heterogeneous distribution of dislocation substructure within a grain allows for a loss of ambiguity in slip system
selection, and the rapid saturation of dislocations within CBB’s accounts for the contribution of $I^{wd}$ and $R^{wd}$ to initial plasticity calculations. It is postulated that further increases in model accuracy would be realized if solute-defect interactions were better accounted for in the model, such as a term dependent on the level of solute responsible for Cottrell pinning [74, 75] incorporated into the dislocation density evolution formulae (Equations 2.5 to 2.13).

Examination of Table 5.4 shows that while the transition from the original Peeters model to the three-tier model results in little change to $I$ and $R$ values, there is a noticeable change to $I^{wd}$ despite a consistent constitutive response in the IF steel tested. The primary reason for this change in $I^{wd}$ is the presence of dynamic slip system selection as outlined in Section 5.3, producing non-currently generated CBB’s during monotonic loading that result in elevated global stress calculations. An additional modification to these parameters may arise due to the influence of neighbouring grains on the internal strain of the material, since it will not be the same as the prescribed strain of the Peeters treatment. The modification would affect both the density of dislocations within CBB’s and randomly oriented dislocation densities, such that a slight adjustment to $I$ results. Whether these effects are artifacts of the integrated three-tier FEM model or phenomenologically accurate modifications to previous work remains to be confirmed; however, these effects allow for a greater level of numerical accuracy in the representation of plastic behaviour under monotonic loading.

6.3.2 Analyses of Complex Two-Stage Strain-Path Behaviour

The influence of non-currently generated (NCG) CBB’s becomes significant when a severe change in strain path exists. Representation of the transient work-hardening
behaviour is consistent with empirical data, further validating the parameters set in the monotonic tests. A lack of recovery on inactive CBB’s upon strain-path transition – represented by the parameters $R_{ncg}$, $\beta_1$, and $\beta_2$ – has been identified as the result of dynamic CBB selection in a modest number of grains after the change in strain path, leading to a suppression of NCG CBB recovery and a significant over-prediction of the work-hardening rate.

The dynamic nature of the CBB selection is caused by the crystallographic orientation of the grain, the influence of neighbouring grains, the value of the recovery parameters chosen, or a combination of these effects. It is clear that modification of the LS-DYNA subroutine containing the crystal-plasticity and work-hardening code is required; whether this modification involves threshold settings to address truncation errors, averaging techniques to stabilize orientation-independent dynamic behaviour, or evolution of the underlying theoretical assumptions remains to be investigated. Current research suggests that each approach must be implemented to advance the accuracy and range of application for the three-tier model.

A notable source of error in the Peeters model has been observed via the empirical data collected for IF steel in this thesis; experimental research performed at the Laboratoire des Propriétés Mécaniques et Thermodynamiques des Matériaux (LPMTM) presents plastic behaviour that conflicts with key assumptions made in the Peeters theory related to substructure evolution following a change in strain path. Figure 6.3 compares the constitutive response of similar IF steel sheet specimens during a cross test. Data presented by Peeters [7] intimates the eventual annihilation of NCG CBB’s upon a change in strain path, leading ultimately to the reproduction of monotonic work-hardening behaviour once transient effects have resolved. Data from cross tests similar to those outlined in Section 5.1.2 appear to support this hypothesis, as
the constitutive response of the material after sufficient strain is imposed along the secondary strain path is seen to become asymptotic with the data from monotonic tests. The fallacy of these assumptions is noted when these tests are carried out to higher levels of applied strain. The data presented in Figure 6.3(b) proves the constitutive response of cross tests do not actually become asymptotic to monotonic data; rather, the work-hardening rate upon a change in strain path diminishes with increasing levels of applied strain along the primary path. Furthermore, this reduced rate is not transient in nature, persisting until material failure.

The erroneous nature of assumptions made in the Peeters theory lead to a loss of model accuracy, through the use of Equations 2.8 and 2.9. The lack of phenomenological accuracy in substructure development may have introduced numerical imprecision into the multi-scale model presented. It appears that the use of \( R_{\text{neg}}, \beta_1, \) and \( \beta_2 \) in the present treatment is unrealistic, and that an additional mechanism is required to explain the loss of work hardening observed.

Unfortunately, other models capable of predicting transient work-hardening behaviour during the application of a complex strain path are equally incompatible with the three-tier model proposed in this thesis. A recent model by Holmedal et al. [34], which uses an evolved form of the original Peeters [7] hardening model, captures cross and Bauschinger effects using seven fitting parameters (reduced from the eleven used in the Peeters model) for fcc aluminum sheet. As with the Peeters model, softening of the dislocation sheets on inactive slip systems is responsible for the predicted macroscopic constitutive response, such that dynamic slip system activation in the three-tier model would inhibit CBB recovery on these systems. A model developed by Teodosiu and Hu [76], later modified by Wang et al. [77], has been proven successful in capturing transient effects in ferritic steels using a physically-based continuum
approach with four material parameters. As discussed in Section 2.2, use of continuum mechanics implies homogeneity in the material response, which is necessary for the orientation-dependent phenomena studied in Chapters 3 and 4. For specific focus on the macroscopic constitutive response of a material due to complex loading, this continuum model may be the most computationally efficient, while the model developed by Peeters [7] may be the most phenomenologically accurate.

6.4 Contributions to the Field

The incorporation of Taylor-based crystal-plasticity theory and a mesoscopic work-hardening formulation into a dynamic FE code represents a novel approach to the examination of local and macroscopic constitutive response of bcc materials. Previous work has focused on either the former (through the representation of a limited number of grains in a crystal plasticity code) or the latter (using continuum mechanics or other homogenization schemes, typically within FEM programs), with a deficiency in research examining the constitutive response of materials at both length scales simultaneously. A multi-length-scale approach is vital to establishing a direct link between microscopic phenomena and bulk deformation.

In this thesis, a three-tier model has been developed that captures texture-based anisotropy and grain interaction while simulating bulk material response to applied deformation. The predicted heterogeneity in work hardening is both numerically and phenomenologically accurate, and is carried out with computational efficiency using modest resources. The analytical procedure offered is well-suited to examine most common industrial formability concerns related to the deformation of bcc foil and sheet material.
The three-tier model presented in this thesis represents a significant advancement of the seminal work of Peeters et al. in the areas of local work hardening, texture morphology, and surface roughness evolution during plastic deformation. The methodology behind the identification and recording of micron-scale texture fields using scanning electron microscopy in conjunction with optical interferometry has allowed for confirmation of the theory that plastic bending due to texture-induced heterogenous deformation is a contributing factor to surface roughening [4]. The qualitative and quantitative agreement between experimental test data and numerical predictions highlights the importance of considering the spatial topography of the local texture distribution when determining inhomogeneous macroscopic characteristics such as surface roughness.

Experimental research performed in this thesis has also been valuable in identifying the plastic response of bcc material under complex loading scenarios. In particular, the revelation of material softening during cross tests based on the amount of primary strain warrants a revisitation of mesoscopic work-hardening theory. Studies presented for Mo foil and sheet products deformed under a variety of strain paths is beneficial, as data of this kind is scarce in literature, due mainly to the difficulties in preparing and deforming such inherently brittle material.
Figure 6.1: Comparison of $\beta_L$ for (a) CE-oriented grains and (b) CF-oriented grains under uniaxial tension, using constant nodal velocity $v_n$ and nodal acceleration $a_n$ profiles (see Appendix A).
Figure 6.2: Comparison of (a) a solution of the original Peeters model for an IF steel under monotonic loading with (b) a solution of the three-tier model with and without active $I^{wd}$ and $R^{wd}$ parameters.
Figure 6.3: Comparison of (a) cross-test data of IF steel sheet presented by Peeters [7] with (b) data acquired from tests at LPMTM of a similar material.
Chapter 7

Conclusions and Recommendations

7.1 Conclusions

In this thesis, the importance of microscopic and mesoscopic characteristics in the study of macroscopic plastic deformation was examined for bcc materials under simple and complex strain paths. Integral to this work was the development and validation of a multi-scale model capable of efficient simulation of material deformation with a high degree of quantitative and phenomenological accuracy; as such, a series of experimental and numerical analyses were performed. The following conclusions were realised from this study.

- The integration of Taylor-based crystal-plasticity theory and a dynamic explicit finite-element scheme allows for numerical analyses of bcc material deformation wherein both force equilibrium and strain compatibility is maintained. The issue of Taylor ambiguity is resolved passively through the disparate work-hardening rates across potentially active slip systems in the simulated grains, and via application of a first-order Renouard-Winterberger solution in rare cases of
internal work equivalence.

- The three-tier model was found to not only capture proper slip system activation and subsequent grain rotation in benchmark studies for bcc materials, but the dynamic nature of LS-DYNA allowed for strong agreement in predicted texture-based anisotropy with theoretical Lankford coefficients. Solutions for crystallographic orientations believed to have a high plastic strain ratio are noticeably reduced due to the plane-stress conditions imposed.

- Inertial effects attributed to the microscopic element lengths within the model and the desire to satisfy the Courant condition were experienced. The issue was resolved by initialising uniform isotropic deformation across all nodes within the mesh on the first timestep, and via the prescription of a constant nodal velocity for all simulations. Experimental data acquisition was also carried out at a constant rate of deformation for comparison.

- A procedure whereby deposition of a 200 x 200-µm² marker grid via gold sputter-coating was developed to ensure coincidence between optical measurements of the local surface profile using interferometry techniques, and local texture measurements via electron backscatter diffraction. The technique allowed for the study of surface roughness and texture evolution using Mo foil samples under tension, examining the contribution of localised texture to macroscopic characteristics such as surface roughening.

- Simulation of Mo material subject to uniaxial tension showed regions of material adverse to thinning surrounding material with a high resistance to contraction in the direction transverse to the tensile axis. These incidents corresponded
to the highest amplitudes of surface topography under experimental observation, confirming the existence of a texture-induced plastic bending that is a notable contribution to the overall surface roughening of thin material during deformation.

- Predicted surface profiles of Mo foil material subjected to a simple strain path were found to be both qualitatively and quantitatively accurate. Some degree of disparity exists in the predicted evolution of texture, due primarily to inertial effects across grains with a large variation in anisotropy. This disparity is consequently mesh-sensitive, such that element size should be restricted to the smallest microscopic feature desired in the model.

- Numerical solutions for complex strain-path tests become inaccurate when a significant change in the prescribed strain path occurs. The underestimation of recovery on non-currently-generated cell-block boundaries exists due to the dynamic nature of the predominantly active slip systems, inhibiting recovery of the dislocation densities along these systems. While such events are observed in monotonic simulations, the effects are not notable until after a significant increase in the yield stress of the material (such as in the transient region of a cross test).

- High-strain cross tests of IF steel sheet have identified an inconsistency with assumptions used in the integrated mesoscopic work-hardening model. The transient constitutive response of materials subjected to a change in strain path is assumed to be defined by the dislocation density evolution related to cell-block boundaries, while equations defining recovery on non-currently-generated cell-block boundaries infer that after a sufficient degree of transient strain, full
recovery is observed. This leads to the premise that the material will eventually revert to a rate of work hardening similar to that seen in monotonic tests. Experiments carried out in this work have shown such assumptions to be unfounded, and that the rate of work hardening following a change in strain path is dependent on the amount of primary strain imposed.

- Orthogonal tests incorporating in-plane plane-strain paths highlight a dramatic reduction in the formability of the materials tested when subjected to certain complex strain paths. IF steel sheet, capable of considerable plastic deformation ($\epsilon_p > 0.30$) under monotonic loads, experiences failure when subjected to an orthogonal strain path after a primary applied plastic strain of 0.10.

### 7.2 Recommendations for Future Work

In reviewing the research performed in this work and the conclusions made herein, several proposals for further study merit consideration. The recommendations that follow are considered to have the greatest impact on the development of the research presented.

- The use of a plane-stress assumption has been validated for foil and thin sheet studies, but this premise is ill-suited for thicker material. A study on the effects of varying hydrostatic stress and the subsequent global stress tensor is necessary to establish model sensitivity for a range of sheet thicknesses.

- A modification of the quasi-two-dimensional model developed herein is recommended to further study the effects of plastic bending due to variations in texture-based anisotropy. The validation of a fully three-dimensional model
would allow for analyses of the out-of-plane deformation inferred by this work. A thorough investigation of element formulations – both solid and shell – is required.

- Use of a dynamic explicit finite-element code has led to issues primarily related to inertial effects, but also to potential instability when elastic-plastic transition is considered. These issues may be rectified by adapting the present subroutine to an implicit scheme, such that more reasonable strain increments may be realized upon yielding and during subsequent plastic deformation.

- The variation of through-thickness texture has a negligible effect on the surface roughening observed in the Mo foil samples tested, but confirmation of this phenomena for sheet product has not yet been pursued. A similar modelling approach may be possible using a three-dimensional model with the inclusion of numerous elements along the sample normal direction. The use of a neutron or synchotron x-ray source would be instrumental in acquiring local sub-surface texture measurements, using the marker deposition technique developed in this thesis.

- Previous work by Peeters et al. [62] confirmed the presence of dislocation sheets in IF steels after deformation. Due to the dynamic selection of slip systems, a focused experimental analysis of grains that present inhibited cell-block boundary recovery in the three-tier model is warranted. Observation via transmission electron microscopy of CBB’s along slip systems that should have recovered would validate the simulated dynamic behaviour.

- Further investigation of complex strain-path effects should be carried out to
determine the sensitivity of the dynamic model to deviations from monotonic loading conditions. A series of two-stage tensile tests with varying degrees of severity in path change would provide an efficient means of producing empirical data for analyses, and may highlight phenomenological behaviour unforseen in the current theoretical treatment.

• Expand the number of candidate bcc materials for analysis. While the use of Mo ensured computational efficiency due to a reduced number of potentially active slip systems at room temperature, the present work has confirmed that texture evolution for more commonly used materials such as IF steel can be adequately modelled using \( \{110\}\langle111\rangle \) and \( \{112\}\langle111\rangle \) slip systems.
References


REFERENCES


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REFERENCES


[77] J. Wang, V. Levkovitch, F. Reusch, B. Svendsen, J. Huetink, and M. van Riel.  
Appendix A

Dependence of Plastic Strain Ratio upon Nodal Velocity within LS-DYNA

The influence of the input nodal velocity profile on the plastic strain ratio $\beta_L$ of various texture components is presented here. Analyses of several crystallographic orientations are necessary as the stress tensor (and hence the incremental strain tensor) produced in each case will create unique dynamic effects within LS-DYNA. Three standard orientations are analysed here: cube-on-edge (CE); cube-on-face (CF); and cube-on-corner (CC).

A.1 Cube-on-Edge Analysis

Theory shows the CE texture component to be isotropic when a tensile load is applied along the rolling (i.e. longitudinal) direction [3]. Initial solutions to a similar loading
scheme using the multi-scale model developed in Section 3 show some agreement; Figure A.1 illustrates the development of strain – and consequently $\beta_L$ – over time. It is clear that while initial $\beta_L$-values correspond to isotropic deformation, anisotropy is observed in later stages. The primary reason for this stems from inertial effects produced by the LS-DYNA source code, which are most visible with this texture component due to the nature of the resultant stress tensor.

The plane-stress tensor determined by the multi-scale model of the LS-DYNA umat comprises the general form:

$$
\begin{bmatrix}
\sigma_{11} & \sigma_{12} & \sigma_{13} \\
\sigma_{21} & 0 & \sigma_{23} \\
\sigma_{31} & \sigma_{32} & 0
\end{bmatrix}^g,
$$

where 1 is the rolling/loading direction, 2 the transverse, and 3 the normal. The lack of through-thickness stress is trivial as subsequent determination of the corresponding strain increment is found assuming a conservation of volume exists (Equation 3.11). More problematic is the lack of transverse stress; this prediction, while phenomenologically accurate, causes the nodal velocity of the element to remain invariable, assuming a constant applied nodal velocity $v_n$. During tensile deformation the incremental strain in the rolling direction will decrease (due to a constant applied $v_n$ coupled with an increasing element length in the rolling direction) while the incremental transverse strain increases (due to a constant transverse $v_n$ coupled with a decreasing transverse element length). Error in $\beta_L$ is further introduced as the incremental through-thickness strain is calculated in Equation 3.11 from an underestimated $d\varepsilon_{RD}$ and an overestimated $d\varepsilon_{TD}$. This sequence of events causes a
degradation of accuracy in the plastic strain ratio.

Figures A.2 and A.3 reveal the sensitivity of total strain and $\beta_L$ to varying magnitudes of constant $v_n$. As expected, increasing values of $v_n$ will result in an increased rate of deviation from isotropy. In each case however, the terminal value of $\beta_L$ — instantaneous and total — remain consistent over the range of velocities used. Observation of Figure A.3 shows some discrepancy in this consistency; this is induced by the variation of $\beta_{L,i}$ at the onset of plasticity, illustrated in Figure A.3(a). It is therefore not only the velocity profile which affects the evolution of the plastic strain ratio, but the initial strain state at the onset of plasticity (i.e. during the first timestep that the plastic model is evoked), particularly in cases where a CE texture component is encountered as the lack of transverse stress denotes an inability to correct any initial discrepancy.

To ensure an isotropic strain increment is applied at the onset of plasticity, alterations must be made to the elastic deformation model provided by LSTC [47]. Specifically, the through-thickness strain increment is set to some proportion of the applied strain increment:

$$d\varepsilon_{33} = md\varepsilon_{11},$$  \hspace{1cm} (A.1)

where $m$ is the constant of proportionality. Table A.1 presents the variation in $\beta_L$ that results from the elastic subroutine. Setting $m$ to 0.21 produces accurate isotropy once the plastic subroutine is enabled.

In addition to variation of $v_n$, analyses of varying the timestep at a constant $v_n$ were performed; these results are shown in Figure A.4. No sensitivity to timestep is observed, although two points of interest must be mentioned:

(i) a smaller timestep was used (where necessary) within the elastic portion of the
APPENDIX A. THE DEPENDENCE OF PLASTIC STRAIN RATIO ...

solution, to ensure the requisite strain ratio was attained before the onset of plasticity; and

(ii) the level of $dt$ selected for plastic deformation must be reached before plasticity, e.g. if the initial timestep is $1.0E-3$ seconds and the desired timestep for plastic deformation is $1.0E-1$ seconds, a smooth transition must be made from the two values during elasticity. Failure to reach this timestep within the elastic region – with the requisite strain ratio – may lead to instabilities upon initiation of the plasticity subroutine.

This latter point is important, as a compromise must be made between using a larger timestep to reduce unnecessary runtime, and keeping $dt$ small enough to prevent instability. Calibration of each velocity and timestep profile within the LS-DYNA input file must be made for any variation to the applied strain, runtime, or element size.

Nodal Acceleration Curves

To overcome the inertial limitations of the model, increasing-velocity profiles were implemented. These may be separated into two types: constant-strain-rate profiles and constant-acceleration profiles. The results of the constant-strain-rate profiles will be examined first.

Production of a constant-strain-rate velocity profile was performed by specifying the nodal velocity required at a given timestep to propagate a constant increment of true strain. Figures A.5 and A.6 present the results of several strain-rates on the evolution of $\beta_L$; these show that with higher strain rates, there appears to be an improvement in accuracy, i.e. there is less deviation from isotropy. These results may
be misleading however, since the $\beta_L$ for each case at the onset of plasticity may be a significant source of this apparent behaviour. Despite this trend, it is clear that an increasing velocity profile via constant-strain-rate assumptions does improve upon the solutions given using a constant-velocity profile; a deviation from isotropy still remains, however. A further point of interest is that the velocity profiles implemented should result in a total applied strain of 0.30, while that observed was 0.275. Reasons for this may include losses during elastic deformation (as the velocity curve is modified within the first 0.5 seconds to allow for a stable transition to plasticity), and the inertial effects within LS-DYNA that may inhibit the specified element deformation.

In addition to varying the strain rate, tests were performed to observe the sensitivity of these profiles to timestep. The results, shown in Figure A.7, imply little to no sensitivity is experienced due to changes in $dt$. Again, it is believed that any variations are the result of digressions in the initial $\beta_L$ at plasticity.

Use of a constant-acceleration profile produces the results illustrated in Figures A.8 and A.9. Improvement to the accuracy of the model is notable, particularly when examining the consistency of an isotropic, instantaneous $\beta_L$ at a nodal acceleration ($a_n$) of 4.0E-10 m/s$^2$. Accelerations above and below this $a_n$ produce plastic strain ratios below and above 1.0, respectively. It is apparent that the evolution of $\beta_{L,i}$ is non-linear, such that the velocity profile should be equally so; this is supported by Figures A.10 and A.11, where a reduction in the applied strain and runtime is used to simulate the preliminary stages of the first test. In this shortened test, a nodal acceleration of 6.0E-10 m/s$^2$ is more accurate, implying a variation in the ideal value of $a_n$ over time. The degree of non-linearity in these tests is small however, and due to the amount of customization that must be performed with each change in applied strain, runtime, and element size, a simpler linear acceleration is opted. Comparison
of model accuracy using original and optimized velocity profiles is offered in Figure A.12.

**A.2 Cube-on-Face and Cube-on-Corner Analyses**

Analyses of CF and CC texture components are simplified due to the presence of a transverse stress component. Examination of Figures A.13 and A.14 illustrate the $\beta_{L,i}$-evolution for each orientation, with original ($v_n = 2.44E-8$ m/s) and optimized ($a_n = 4.0E-10$ m/s$^2$) velocity profiles. The CF texture (Figure A.13) reveals that while the original velocity profile produced an accurate strain evolution, a divergent $\beta_{L,i}$ exists; this may lead to instabilities in the solution. Use of the optimized profile results in a slight increase in strain-evolution accuracy, with a stable, convergent $\beta_{L,i}$. This highlights the importance of an optimized velocity profile in orientations other than the isotropic CE. Investigation of the CC orientation shows little change in solution.
Table A.1: Variation of strain ratio from elasticity ($\beta_{L,el}$) to the onset of plasticity ($\beta_L$) due to changes in the proportionality constant $m$.

<table>
<thead>
<tr>
<th>$m$</th>
<th>$\beta_{L,el}$</th>
<th>$\beta_L$</th>
</tr>
</thead>
<tbody>
<tr>
<td>-0.41</td>
<td>0.595</td>
<td>0.324</td>
</tr>
<tr>
<td>-0.21</td>
<td>1.56</td>
<td>0.478</td>
</tr>
<tr>
<td>0.01</td>
<td>-42.0</td>
<td>0.700</td>
</tr>
<tr>
<td>0.21</td>
<td>-2.40</td>
<td>1.02</td>
</tr>
<tr>
<td>0.41</td>
<td>-1.43</td>
<td>1.46</td>
</tr>
<tr>
<td>code$^a$</td>
<td>1.00</td>
<td>0.429</td>
</tr>
</tbody>
</table>

$^a$Refers to the original elasticity code provided by LSTC [47], where $\epsilon_{33} = \epsilon_{22} = -\nu \epsilon_{11}$, and $\nu$ is Poisson’s ratio for the material (here, 0.29)
Figure A.1: Evolution of (a) total strain and (b) $\beta_L$ for a single-element, CE-oriented grain under uniaxial tension with a constant nodal velocity $v_n$. 
Figure A.2: Evolution of (a) applied strain, and (b) transverse and through-thickness strains for a single-element, CE-oriented grain under uniaxial tension, with varying levels of constant $v_n$. 
Figure A.3: Evolution of (a) incremental $\beta_{L,i}$ and (b) total $\beta_L$ for a single-element, CE-oriented grain under uniaxial tension, with varying levels of constant $v_n$: $\varepsilon_{RD} = 0.275$. 
Figure A.4: Evolution of (a) applied strain, and (b) transverse and through-thickness strains for a single-element, CE-oriented grain under uniaxial tension, with varying timestep (dt): $v_n = 2.44E-8$ m/s.
Figure A.5: Evolution of (a) applied strain, and (b) transverse and through-thickness strains for a single-element, CE-oriented grain under uniaxial tension, with varying levels of constant $\dot{\varepsilon}$.
Figure A.6: Evolution of (a) incremental $\beta_{L,i}$ and (b) total $\beta_{L,t}$ for a single-element, CE-oriented grain under uniaxial tension, with varying levels of constant $\dot{\varepsilon}$: $\varepsilon_{RD} = 0.275$. 
Figure A.7: Evolution of (a) applied strain, and (b) transverse and through-thickness strains for a single-element, CE-oriented grain under uniaxial tension, with varying timestep (dt): $\dot{\varepsilon} = 3.0E-2 \text{ s}^{-1}$. 

\begin{figure}
\centering
\includegraphics[width=\textwidth]{figA7}
\caption{Evolution of (a) applied strain, and (b) transverse and through-thickness strains for a single-element, CE-oriented grain under uniaxial tension, with varying timestep (dt): $\dot{\varepsilon} = 3.0E-2 \text{ s}^{-1}$.}
\end{figure}
APPENDIX A. THE DEPENDENCE OF PLASTIC STRAIN RATIO ...

Figure A.8: Evolution of (a) applied strain, and (b) transverse and through-thickness strains for a single-element, CE-oriented grain under uniaxial tension, with varying levels of constant $a_n$. 
Figure A.9: Evolution of (a) incremental $\beta_L$ and (b) total $\beta_L$ for a single-element, CE-oriented grain under uniaxial tension, with varying levels of constant $a_n$: $\epsilon_{RD} = 0.275$. 
Figure A.10: Comparison of (a) applied strain, and (b) transverse and through-thickness strains for a single-element, CE-oriented grain under uniaxial tension, using initial conditions as shown in Figure A.8, and under a shortened test run.
Figure A.11: Comparison of (a) incremental $\beta_L$ and (b) total $\beta_L$ for a single-element, CE-oriented grain under uniaxial tension, using initial conditions as shown in Figure A.8, and under a shortened test run.
Figure A.12: Comparison of (a) strain evolution, and (b) $\beta_L$ for a single-element, CE-oriented grain under uniaxial tension, using original and optimized velocity profiles.
Figure A.13: Comparison of (a) strain evolution, and (b) $\beta_L$ for a single-element, CF-oriented grain under uniaxial tension, using original and optimized velocity profiles.
Figure A.14: Comparison of (a) strain evolution, and (b) $\beta_L$ for a single-element, CC-oriented grain under uniaxial tension, using original and optimized velocity profiles.
Appendix B

Issues in Multi-Element FE Analyses

In moving from single-element test cases to multi-element analyses, additional challenges are introduced. The influence that adjacent elements pose on each other is an advantageous quality of finite-element modelling; however, in some cases this interference can have an adverse effect on results. In addition, the scale of a finite-element mesh can affect model accuracy – particularly when inertial effects are a concern. Model sensitivity to both issues is presented here.

B.1 Adverse Effects of Neighbouring Elements

Section 3.3.2 presents a banded-texture multi-element analysis. In this study, the impact of anisotropic CF texture on isotropic CE material is observed; however, the accuracy of CE-oriented element deformation is dependant upon an isotropic strain increment at the onset of plasticity. To observe the initial plastic strain ratio, a
simplified three-element mesh of alternating CF and CE orientations is constructed (Figure B.1). Deformation was provided via an idealized velocity profile along the x axis, with a variable timestep curve that allows for smaller time increments during the relatively short period of elastic deformation. This was found in single-element cases to produce a stable, controllable strain increment prior to plasticity; unfortunately, this trend was not reproduced in multi-element tests. Since the modified strain ratio in the elastic subroutine is not isotropic, the stress tensors produced influence subsequent strain increments of neighbouring elements—a non-issue in single element analyses. This effect produces an unpredictable strain ratio, such that isotropic plasticity cannot be initialized across all elements using this elastic subroutine. Adverse effects were further compounded in the use of a variable timestep, which served to increase the instability of the incremental strain across the mesh.

To remedy these effects, the FE model is modified to account for elastic deformation in the material; because the amount of elastic deformation is relatively small, and no anisotropy or texture evolution is observed in this regime, it is acceptable to remove this analysis from the subroutine provided the yield conditions are represented in the model. Constitutive behaviour upon yield is accounted for in two ways:

(i) the von Mises strain upon yield is hard-coded into \( \text{hisv}(\ast) \), where the total strain data is kept; and

(ii) a stress tensor (in this case, one representing uniaxial tension) equivalent to the yield stress of the material is initialized for each element in the model input file.

Empirical data is used for these yield conditions. The resultant solution assumes elastic deformation to have already occurred, and is therefore entirely plastic. To ensure \( \beta_L \) is 1.0 during the first time increment, initial nodal velocities for each element
are specified in the input file. Deformation in subsequent timesteps occurs solely via the input velocity curve specified in boundary conditions.

B.2 Inertial Effects

Due to the specification of a relatively large timestep in the model input files, inertia has become a subject that requires attention. Compulsary mass scaling within LS-DYNA has produced a scenario where the influence of neighbouring elements cannot propagate into the surrounding mesh as accurately and effectively as would be realized with no scaling present. Two studies are performed to investigate the severity of these effects: banded-texture studies that look at mesh scale effects; and models with multiple elements along the tensile axis to examine the effects of a nonlinear velocity profile.

Mesh Scale Effects

To examine mesh scale effects, the 1x3-element banded-texture model displayed in Figure B.1 is refined to produce 1x9- and 1x15-element models. Texture bands remain identical, except each region of similar orientation is now represented by three and five elements, respectively. In all simulations, the material is subjected to 20% strain along the x axis. Solutions for each model are presented in Figure B.2, using the transverse strain as a basis of comparison. It is clear from this study that mesh refinement leads to an overestimation of the influence of crystallographic texture. Transverse strain in the CE region increases with the number of elements used to represent it. Furthermore, strain localization in fine-mesh models is observed in the elements closest to changes in orientation. This suggests a grain represented by several
elements will experience some variation in strain due solely to the mesh used; inertial effects are at fault, as elements are unable to fully distribute the changes in strain brought about by neighbouring elements.

To minimize these effects, a coarse-mesh model is used to carry out all simulations. Strain localization at grain boundaries due to inertial effects are reduced, as are overestimations of grain interactions. The degree of refinement is based on the smallest desired grain size. In most of the studies presented in this work, grains less than 5 \( \mu \text{m} \) in diameter are considered too small to have an effect on surrounding material, thus the element size is fixed at this dimension.

**Effects Regarding Applied Nodal Velocity**

Single-element studies illustrated the benefits of using a constant-acceleration nodal velocity profile to produce the most accurate simulation of texture-based anisotropy during deformation (Appendix A). This assumption is now validated for multi-element simulations by comparing the effects of multiple elements of similar orientation along the tensile axis, using both constant-velocity and constant-acceleration profiles as input. Figure B.3 illustrates multi-element CE solutions using constant-acceleration profiles to produce a total strain of 25% along the x axis. It is apparent that by increasing the number of elements along the tensile axis, the amount of strain localization intensifies at the nodes where this boundary condition is applied. This is once again due to inertial effects; since the bounding nodes are subjected to an acceleration, the elements to which they belong experience large amounts of strain – excessive mass inertia prevents this acceleration from propagating through the mesh.

This effect is further supported by running the model using alternate time steps.
APPENDIX B. ISSUES IN MULTI-ELEMENT FE ANALYSES

As outlined in Table B.1, larger time steps increase the amount of localization since the mass scaling required for this larger dt results in a higher inertia. Ideally, the solution to this would be to reduce dt until strain localization fell under acceptable limits; however, there are two reasons why this is not feasible. First, with the larger mesh sizes used in full solutions, the timestep size required to allow for sufficient strain dispersion using an accelerated velocity profile would take months to complete given current computing availability. Also, in reproducing these timestep studies using CF- and CC-oriented elements, numerical precision became insufficient at smaller time steps (shown in Table B.1).

In contrast, solutions using a constant-velocity profile produce negligible variation in strain along the mesh, and are thus insensitive to time step insofar as localization is concerned. While single-element studies have shown that such profiles are not as accurate in predicting texture-based anisotropy when compared to constant-acceleration profiles, the only case where this is significant is with the isotropic CE orientation, and even in this case the effects of localization in a multi-element solution are far worse than inaccuracies that may be encountered using a constant-velocity profile. It is therefore deemed necessary to use constant-velocity profiles for multi-element analyses, while constant-acceleration profiles are encouraged for single-element studies.
Table B.1: Ratio $\kappa$ of the longitudinal strain of the outermost element to that of the innermost element along the tensile axis, under a total applied strain of 25%.

<table>
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<th>$dt$ (s)</th>
<th>Orientation/Mesh Size</th>
<th>CE/3x1</th>
<th>CE/5x1</th>
<th>CE/7x1</th>
<th>CE/9x1</th>
<th>CF/3x1</th>
<th>CC/3x1</th>
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<td>1.04</td>
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<td>unstable</td>
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</tbody>
</table>
Figure B.1: 1x3-element mesh used to analyze $\beta_L$ at the onset of plasticity (plot of Euler angle $\Phi$ shown – CF = blue, CE = red).
Figure B.2: Mesh scale effects: contour plots of transverse strain after an applied strain of 20% along the x axis (interpolation suppressed to discretize solution). Results are given for models under varying refinement: (a) 1x3-element mesh; (b) 1x9-element mesh; and (c) 1x15-element mesh sizes.
Figure B.3: Effects of constant-acceleration velocity profiles in multi-element solutions. Contour plots of the longitudinal strain in (a) a 3x1-element CE mesh, (b) a 5x1-element CE mesh, (c) a 7x1-element CE mesh, and (d) a 9x1-element CE mesh, subjected to a total strain of 25% along the x axis.