Multiscale Modeling of Heterogeneous Material Systems

by

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Doctor of Philosophy

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ABSTRACT

Damage detection in heterogeneous material systems is a complex problem and requires an in-depth understanding of the material characteristics and response under varying load and environmental conditions. A significant amount of research has been conducted in this field to enhance the fidelity of damage assessment methodologies, using a wide range of sensors and detection techniques, for both metallic materials and composites. However, detecting damage at the microscale is not possible with commercially available sensors. A probable way to approach this problem is through accurate and efficient multiscale modeling techniques, which are capable of tracking damage initiation at the microscale and propagation across the length scales. The output from these models will provide an improved understanding of damage initiation; the knowledge can be used in conjunction with information from physical sensors to improve the size of detectable damage. In this research, effort has been dedicated to develop multiscale modeling approaches and associated damage criteria for the estimation of damage evolution across the relevant length scales. Important issues such as length and time scales, anisotropy and variability in material properties at the microscale, and response under mechanical and thermal loading are addressed. Two different material systems have been studied: metallic material and a novel stress-sensitive epoxy polymer.

For metallic material (Al 2024-T351), the methodology initiates at the microscale where extensive material characterization is conducted to capture the microstructural variability. A statistical volume element (SVE) model is constructed to represent the
material properties. Geometric and crystallographic features including grain orientation, misorientation, size, shape, principal axis direction and aspect ratio are captured. This SVE model provides a computationally efficient alternative to traditional techniques using representative volume element (RVE) models while maintaining statistical accuracy. A physics based multiscale damage criterion is developed to simulate the fatigue crack initiation. The crack growth rate and probable directions are estimated simultaneously.

Mechanically sensitive materials that exhibit specific chemical reactions upon external loading are currently being investigated for self-sensing applications. The “smart” polymer modeled in this research consists of epoxy resin, hardener, and a stress-sensitive material called mechanophore. The mechanophore activation is based on covalent bond-breaking induced by external stimuli; this feature can be used for material-level damage detections. In this work Tris-(Cinnamoyl oxymethyl)-Ethane (TCE) is used as the cyclobutane-based mechanophore (stress-sensitive) material in the polymer matrix. The TCE embedded polymers have shown promising results in early damage detection through mechanically induced fluorescence. A spring-bead based network model, which bridges nanoscale information to higher length scales, has been developed to model this material system. The material is partitioned into discrete mass beads which are linked using linear springs at the microscale. A series of MD simulations were performed to define the spring stiffness in the statistical network model. By integrating multiple spring-bead models a network model has been developed to represent the material properties at the mesoscale. The model captures the statistical distribution of crosslinking
degree of the polymer to represent the heterogeneous material properties at the microscale. The developed multiscale methodology is computationally efficient and provides a possible means to bridge multiple length scales (from 10 nm in MD simulation to 10 mm in FE model) without significant loss of accuracy. Parametric studies have been conducted to investigate the influence of the crosslinking degree on the material behavior. The developed methodology has been used to evaluate damage evolution in the self-sensing polymer.
To my parents.

For supporting me in pursuing my doctoral degree

and helping me to make this dissertation a reality
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Nickerson, and all the advisory board members for their useful feedback which keeps our research in the right direction.
# TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>LIST OF TABLES</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>v</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>LIST OF FIGURES</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>vii</td>
</tr>
</tbody>
</table>

## CHAPTER

1. **INTRODUCTION**

1.1. Motivation ........................................ 1

1.2. Background of Multiscale Modeling for Metallic Material ............. 2

1.3. Background of Multiscale Modeling for Self-Sensing Polymer Material .. 10

1.4. Objectives ........................................ 15

1.5. Outline of the Dissertation ................................ 17

2. **MATERIAL CHARACTERIZATION AND MULTISCALE MODELING OF ALUMINUM ALLOY 2024-T351**

2.1. Introduction ........................................ 20

2.2. Single Crystal Plasticity Theory .................................. 22

2.3. User Defined Material Subroutine .................................. 25

2.4. Material Characterization ........................................ 29

2.5. Feature Parametric Study ......................................... 33

2.6. Validation of the SVE Model ...................................... 43

2.7. Summary ........................................ 47

3. **PHYSICS BASED DAMAGE EVALUATION & VALIDATION OF ALUMINUM ALLOY 2024-T351**

3.1. Introduction ........................................ 49

3.2. Physical Phenomenon of Fatigue Crack Formation ....................... 51
### CHAPTER 3.3. Damage Criterion for Nucleation of Micro Cracks ........................................ 56
3.4. Damage Criterion for Coalescence of Micro Cracks ........................................ 63
3.5. Damage Criterion for Crack Formation in Thermal Mechanical Fatigue .. 64
3.6. Simulation Result and Experimental Validation ........................................ 73
3.6.1. Case 1: Uniaxial Cyclic Loading on Lug Joint Specimens ...................... 73
3.6.2. Case 2: Biaxial FALSTAFF Loading on Cruciform Specimens ........... 79
3.6.3. Case 3: TMF Loading on Lug Joint Specimens .................................. 89
3.7. Summary ........................................................................................................ 94

### CHAPTER 4. DEVELOPMENT OF SPRING-BEAD BASED NETWORK MODEL TO SIMULATE A SELF-SENSING POLYMERIC MATERIAL RESPONSE .......... 96
4.1. Background ........................................................................................................ 96
4.2. MD Simulation of Bond Clusters at the Microscale ................................... 98
4.2.1 Self-Sensing Behavior of the Smart Material .......................................... 98
4.2.2 Statistical Crosslinking Degree in MD Simulation .................................. 100
4.2.3 Mechanical Properties of Self-Sensing Polymer in MD Simulation .... 104
4.3. Development of Spring-Bead Model to Represent Bond Clusters at The Microscale ........................................................................................................ 108
4.4. Development of Network Model at the Mesoscale .................................... 111
4.5. Optimization of Mechanical Equivalence Between MD Model and Network Model .................................................................................................. 116
4.6. Equivalent Strain and Strain Energy in Network Model ......................... 122
4.7. Summary ........................................................................................................ 125
### CHAPTER 5. MULTISCALE MODELING OF SELF-SENSING POLYMER USING STATISTICAL NETWORK MODEL

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.1. Background</td>
<td>126</td>
</tr>
<tr>
<td>5.2. Parametric Study of Statistical Network Model</td>
<td>127</td>
</tr>
<tr>
<td>5.2.1 Heterogeneous and Homogeneous Distribution of Crosslinking Degree</td>
<td>127</td>
</tr>
<tr>
<td>5.2.2 Homogeneous and Statistical Distribution of Crosslinking Degree</td>
<td>130</td>
</tr>
<tr>
<td>5.2.3 Effect of Spring Length in Network Model</td>
<td>133</td>
</tr>
<tr>
<td>5.3. Multiscale Integration Based on Statistical Network Model</td>
<td>134</td>
</tr>
<tr>
<td>5.3.1 Validation of Statistical Network Model</td>
<td>134</td>
</tr>
<tr>
<td>5.3.2 Local Strain and Crosslinking Degree in the Network Model</td>
<td>138</td>
</tr>
<tr>
<td>5.3.3 Comparison Between Network Model and FE Model</td>
<td>139</td>
</tr>
<tr>
<td>5.4. Damage Estimation Using Statistical Network Model</td>
<td>141</td>
</tr>
<tr>
<td>5.4.1 Evaluation of Self-Sensing Intensity of Smart Polymer</td>
<td>141</td>
</tr>
<tr>
<td>5.4.2 Strain Based Damage Evaluation to Predict Failure</td>
<td>147</td>
</tr>
<tr>
<td>5.5. Summary</td>
<td>150</td>
</tr>
</tbody>
</table>

### CHAPTER 6. SUMMARY AND FUTURE DIRECTIONS

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.1. Metallic Material</td>
<td>152</td>
</tr>
<tr>
<td>6.1.1 Innovative Nature of This Research</td>
<td>152</td>
</tr>
<tr>
<td>6.1.2 Important Observations</td>
<td>154</td>
</tr>
<tr>
<td>6.1.3 Future Directions</td>
<td>155</td>
</tr>
<tr>
<td>6.2. Self-Sensing Polymer Part</td>
<td>155</td>
</tr>
<tr>
<td>6.2.1 Innovative Nature Of This Research</td>
<td>155</td>
</tr>
<tr>
<td>6.2.2 Important Observations</td>
<td>157</td>
</tr>
<tr>
<td>Table</td>
<td>Page</td>
</tr>
<tr>
<td>-------</td>
<td>------</td>
</tr>
<tr>
<td>2.1 Specified Composition for 2024-T351 (Wt%) (Bussu, 2003)</td>
<td>29</td>
</tr>
<tr>
<td>2.2 Mechanical and Physical Properties of 2024-T351 at Room Temperature (Rodopoulos, 2004)</td>
<td>31</td>
</tr>
<tr>
<td>2.3 Summarized SVE Feature Values</td>
<td>42</td>
</tr>
<tr>
<td>3.1 Material Parameters for Al 2024-T351 (Luo, 2009; Needs, 1987)</td>
<td>57</td>
</tr>
<tr>
<td>3.2 Creep Dependent Parameters for Al 2024</td>
<td>70</td>
</tr>
<tr>
<td>3.3 Thermal Expansion Factor of Al 2024-T351 (Fridman, 1975)</td>
<td>72</td>
</tr>
<tr>
<td>3.4 Experimental Results of Fatigue Life and Crack Direction</td>
<td>76</td>
</tr>
<tr>
<td>3.5 Simulation Results of Fatigue Cycles and Crack Direction</td>
<td>78</td>
</tr>
<tr>
<td>3.6 Experimental Results of Fatigue Life and Crack Direction (Mohanty, 2010)</td>
<td>86</td>
</tr>
<tr>
<td>3.7 Fatigue Cycles Prediction to Reach a 3 mm Crack and Corresponding Direction</td>
<td>88</td>
</tr>
<tr>
<td>3.8 Young’s Modulus, Yield Strength, and CRSS of Al 2024-T351 at Different Temperatures</td>
<td>92</td>
</tr>
<tr>
<td>3.9 Fatigue Crack Growth Rate Estimation of TMF Simulation</td>
<td>93</td>
</tr>
<tr>
<td>4.1 Components in the Self-Sensing Polymer</td>
<td>101</td>
</tr>
<tr>
<td>4.2 Configuration and Evaluation of Network Models with Different Combination Methods</td>
<td>116</td>
</tr>
<tr>
<td>5.1 Crosslinking Degree and Degree of Heterogeneity in the Four Network Models</td>
<td>128</td>
</tr>
<tr>
<td>5.2 Equivalent Strain in Network Models to Study Degree of Heterogeneity Effect</td>
<td>129</td>
</tr>
<tr>
<td>5.3 Equivalent Strain In Statistical and Homogeneous Network Models</td>
<td>132</td>
</tr>
</tbody>
</table>
Table

5.4 Mechanical Properties in Network Models of Different Spring Lengths. ............... 134
5.5 Simulation and Experimental Results of Young’s Modulus............................ 137
<table>
<thead>
<tr>
<th>Figure</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.1 Comparison Between: A) Actual Microstructure Scans; B) Constructed SVE. Colors Represent Different Grain Orientations</td>
<td>21</td>
</tr>
<tr>
<td>2.2 Multiplicative Decomposition of Deformation Gradient (Luo, 2009)</td>
<td>22</td>
</tr>
<tr>
<td>2.3 Flowchart of Subroutines and Subprograms in UMAT</td>
<td>28</td>
</tr>
<tr>
<td>2.4 EBSD Scan of Al 2024-T351: (A) Rolling Direction and Position of Scans (B) Statistical Information of Grains in EBSD Scans</td>
<td>32</td>
</tr>
<tr>
<td>2.5 OOF2 Used to Mesh the Mesoscale EBSD Scans</td>
<td>32</td>
</tr>
<tr>
<td>2.6 Mesoscale RVE Model of Al 2024-T351</td>
<td>33</td>
</tr>
<tr>
<td>2.7 Flattened 3d Polar Plots of Crystal Orientation: A) {1,0,0}; B) {1,1,0}; C) {1,1,1}</td>
<td>34</td>
</tr>
<tr>
<td>2.8 Distribution of Misorientation in Nine SVE Models</td>
<td>35</td>
</tr>
<tr>
<td>2.9 Statistical Distribution Used for Misorientation Feature Identification: A) Actual Data; B) Generated SVE (Model 7)</td>
<td>36</td>
</tr>
<tr>
<td>2.10 Comparison of the SVE Models with Reference SVE: A) Difference vs. Orientation; B) Average Errors</td>
<td>37</td>
</tr>
<tr>
<td>2.11 SVEs Constructed For Feature Study: A) Baseline; B) Misorientation; C) Principal Axis Direction; D) Grain Size; E) Aspect Ratio; F) Grain Shape. Feature Effects Could be Studied Through Comparison of Results with Respect to the Baseline</td>
<td>39</td>
</tr>
<tr>
<td>2.12 Variation In Average Plastic Strain Energy Density vs. Time</td>
<td>41</td>
</tr>
<tr>
<td>Figure</td>
<td>Page</td>
</tr>
<tr>
<td>-------------</td>
<td>------</td>
</tr>
<tr>
<td>2.13 Plastic Strain Energy Density Distributions Within SVEs: A) Baseline; B) Misorientation; C) Principal Axis Direction; D) Grain Size; E) Aspect Ratio; F) Grain Shape</td>
<td>42</td>
</tr>
<tr>
<td>2.14 FEA Model with RVE and SVE at the Same Hot Spot</td>
<td>44</td>
</tr>
<tr>
<td>2.15 Distribution of Strain Energy Density in RVE Model</td>
<td>45</td>
</tr>
<tr>
<td>2.16 Distribution of Strain Energy Density in an SVE Model</td>
<td>45</td>
</tr>
<tr>
<td>2.17 Comparison Between RVE and SVE</td>
<td>46</td>
</tr>
<tr>
<td>2.18 Local Von Mises Stress Field Distribution Within Lug Joint A) with SVE; B) Without SVE</td>
<td>47</td>
</tr>
<tr>
<td>3.2 Element Analysis of Damaged Al 2024-T351 Sample Using EDAX Technique: A) Micro Crack Incubation in Intermetallic Particles Results in Major Crack Growth; B) Element Mapping of Aluminum; C) Element Mapping of Copper; D) Element Mapping of Iron; E) Element Mapping of Magnesium</td>
<td>54</td>
</tr>
<tr>
<td>3.3 EDAX Analysis to Identify Element Composition for Intermetallic Particles</td>
<td>55</td>
</tr>
<tr>
<td>3.4 Intermetallic Points Represented in SVE Model</td>
<td>56</td>
</tr>
</tbody>
</table>
3.5 A) Slip Planes In FCC Unit Cell; B) Two Perpendicular Material Planes Which are Totally Independent; C) Two Parallel Material Planes Which are Totally Dependent; D) Two Material Planes With an Arbitrary Degree Which are Partly Dependent

3.6 Plastic Zone Around the Micro Crack

3.7 Micro Crack Length Increase Cycle by Cycle in Slip Directions

3.8 Schematic Procedure of Projection of Micro Cracks to Major Crack

3.9 Variable Temperature Condition for Thermal Mechanical Fatigue Tests

3.10 Variable Mechanical Load Condition for Thermal Mechanical Fatigue Tests

3.11 Distribution of Damage Accumulation in Slip System \{1 1 1\} \langle1 1 0\rangle at (A) Room Temperature and (B) 200°C

3.12 Lug Joint Specimen for Fatigue Test: A) Crack Initiates in the Shoulder of Lug Joint and B) Geometric Dimension

3.13 Experimental Test Frame for Fatigue Loading (MTS Bionix 370.02)

3.14 Boundary Conditions and Implementation of a Two-Scale Mesh at the Structural Hot Spot of an Aluminum Lug Joint

3.15 Simulation Results of Probable Crack Direction

3.16 FALSTAFF Loading (79 Cycles)

3.17 Cruciform Specimen: A) A Round Hole in Center for Test; B) A 45° Notch at the Center Hole for Fatigue Test; C) Geometric Dimension of Cruciform; D) Geometric Dimension of the Center

3.18 RMS Model Based Loading (79 Cycles)
3.19 Distribution of Plastic Strain Energy Density in A) RMS Model After 79 Cycles; B) FALSTAFF Model After 79 Cycles .............................................................................................................. 84
3.20 Average Plastic Strain Energy Density in SVE Model for FALSTAFF & RMS Loading Conditions with a Frequency of 20HZ. ................................................................. 85
3.21 MTS Biaxial Tension-Torsion Test System .............................................................................................................. 86
3.22 Cracks in Experimental Specimens .............................................................................................................. 87
3.23 Loading Conditions and Implementation of SVE Model at the Structural Notch Tip of an Al 2024-T351 Cruciform ..................................................................................................................... 88
3.24 Dog Bone Specimen for Tensile Test at Different Temperatures: A) Geometric Dimension and B) Crack Takes Place in the Middle of Dog Bone Specimen. ............... 90
3.25 Instron Material Test Frame 985 with Thermal Chamber. ................................................................. 91
3.26 Stress-Strain Relation of Al 2024-T351 at Different Temperatures ........................................ 92
3.27 Crack Initiation Takes Place in Shoulders of Lug Joint Specimen in TMF Test. ... 94
4.1 Modeling of Self-Sensing Polymer Materials at the Microscale, Mesoscale, and Macroscale. .............................................................................................................. 98
4.2 Schematic of UV-Initiated Cyclobutane Generation and Damage-Induced Cinnamoly Group Generation......................................................................................................................... 99
4.3 Fluorescence Observation in Self-Sensing Polymer with Increasing Load: A) No Crack and No Fluorescence Observed; B) Micro Crack and Slight Florescence Intensity; C) Major Crack And Higher Florescence Intensity. ................................................. 100
<table>
<thead>
<tr>
<th>Figure</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.4 Components of Self-Sensing Polymer: A) Epoxy Resin, B) Hardener, C) Smart Material to Form, and D) RVE Model.</td>
<td>101</td>
</tr>
<tr>
<td>4.5 Schematic of Crosslinked Structure of Epoxy Resin and Hardener: A) Molecular Structure of Epoxy Resin with Two Active Sites; B) Hardener With Five Active Sites; C) Epoxy Resin and Hardener are Crosslinked to Generate Polymer Structure. Black Solid Lines Represent Covalent Bonds.</td>
<td>102</td>
</tr>
<tr>
<td>4.6 Statistical Distribution of Crossing-Linking Degrees Based on MD Simulations (N = 500).</td>
<td>103</td>
</tr>
<tr>
<td>4.7 Uniaxial Deformation Test in MD Simulation: A) Tensile Load and B) Compressive Load of Self-Sensing Polymer.</td>
<td>106</td>
</tr>
<tr>
<td>4.8 Relationship Between Crosslinking Degrees and A) Tensile Modulus, B) Compressive Modulus and C) Shear Modulus.</td>
<td>107</td>
</tr>
<tr>
<td>4.9 A) Spring-Bead Model; B) Simplified Spring-Bead Model; C) Mechanical Response of Spring-Bead Models with Different Crosslinking Degrees.</td>
<td>110</td>
</tr>
<tr>
<td>4.10 Different Arrangements of Spring-Bead Models to Form a: A) 3 Neighbor Based; B) 4 Neighbor Based; C) 6 Neighbor Based; D) 8 Neighbor Based; E) 12 Neighbor Based Network Model.</td>
<td>112</td>
</tr>
<tr>
<td>4.11 The 6, 8, And 12 Neighbor Based Network Models.</td>
<td>113</td>
</tr>
<tr>
<td>4.12 Isotropic Representation of A) 8 Neighbor Based, and B) 12 Neighbor Based Network Models Corresponding to Stiffness Ratio of Long Spring to Short Spring.</td>
<td>115</td>
</tr>
<tr>
<td>Figure</td>
<td>Page</td>
</tr>
<tr>
<td>--------</td>
<td>------</td>
</tr>
<tr>
<td>4.13 Fitting Curves of Modulus as a Function of Spring Stiffness: A) Tensile Modulus; B) Compressive Modulus; C) Shear Modulus</td>
<td>120</td>
</tr>
<tr>
<td>4.14 Comparison Between MD Simulation and Optimization Results</td>
<td>121</td>
</tr>
<tr>
<td>4.15 Linear Fitting Curve of Spring Stiffness Based on Optimization Results</td>
<td>122</td>
</tr>
<tr>
<td>4.16 Beads, Springs, and Subzone in 8 Neighbor Based Network Model</td>
<td>124</td>
</tr>
<tr>
<td>5.1 A) Specific Network Model to Study Effect of Degree of Heterogeneity and B) Spring Stiffness in Subzone A and B of the Network Model 1, 2, 3 and 4</td>
<td>128</td>
</tr>
<tr>
<td>5.2 The Difference in Neighbor Crosslinking Degree Influences the Difference Between Maximum and Minimum Equivalent Strain in the Network Model</td>
<td>129</td>
</tr>
<tr>
<td>5.3 Crosslinking Degree Distribution in A) Statistical Network Model and B) Homogeneous Network Model (Unit: %)</td>
<td>131</td>
</tr>
<tr>
<td>5.4 Equivalent Strain Distribution in A) Statistical Network Model and B) Homogeneous Network Model</td>
<td>132</td>
</tr>
<tr>
<td>5.5 A) The Probability Distribution of Crosslinking Degree in the Statistical Network Model, B) Network Model 1, C) Network Model 2, and D) Network Model 3</td>
<td>136</td>
</tr>
<tr>
<td>5.6 Average Equivalent Strain In Three Statistical Network Models v.s. Loading Strain</td>
<td>137</td>
</tr>
<tr>
<td>5.7 Simulation of Statistical Network Model Under Biaxial Tensile Load: A) Crosslinking Degree Distribution in Network Model and B) Distribution of Equivalent Strain in Network Model</td>
<td>138</td>
</tr>
<tr>
<td>5.8 Dimensional Drawing of Dog Bone Specimen for Simulation</td>
<td>139</td>
</tr>
<tr>
<td>Figure</td>
<td>Page</td>
</tr>
<tr>
<td>--------</td>
<td>------</td>
</tr>
<tr>
<td>5.9. Strain Distribution in the Hot Spot Using A) Network Model and B) FE Model.</td>
<td>140</td>
</tr>
<tr>
<td>5.10 Strain Distribution Within Notched Specimen A) with Network Model and B) Without Network Model</td>
<td>141</td>
</tr>
<tr>
<td>5.11 Fluorescence Observation of Self-Sensing Polymer. A) Integrated Intensity Density v.s. Loading Strain in Fluorescence Observation, B) Microscopic Images and Detected Fluorescence of Specimen at 4% Strain, and C) Microscopic Images and Detected Fluorescence of Specimen at 6% Strain</td>
<td>143</td>
</tr>
<tr>
<td>5.12 Network Model Based Simulation Results: A) Average Equivalent Strain in Network Model; and Equivalent Strain Distribution at Different Global Strain at B) 3%, C) 5%, D) 8%, and E) 10%</td>
<td>147</td>
</tr>
<tr>
<td>5.13 Tensile Mechanical Responses of Self-Sensing Polymer at Variable Crosslinking Degrees Based on the MD Simulation</td>
<td>148</td>
</tr>
<tr>
<td>5.14 Equivalent Strain Distribution in Statistical Network Model 1 at Different Loading Strain: A) 5%, B) 8%, C) 10%, and D) 11.2%</td>
<td>150</td>
</tr>
<tr>
<td>5.15. Experimental Results of Tensile Tests</td>
<td>150</td>
</tr>
</tbody>
</table>
1. Introduction

1.1. Motivation

Damage detection, accurate material modeling techniques and structural health monitoring (SHM) are emerging technologies critical to both current and future multidisciplinary applications (Carol, 1997; Bond, 2000; Glisic, 2008; Giurgiutiu, 2008; Farrar, 2006; Mohanty, 2010). The goal of an SHM framework is to detect, quantify, and classify the nature of damage in a structure in order to assess the current state and determine the residual useful life (RUL). As a comprehensive technology, SHM integrates sensors and sensing techniques, damage detection algorithms, and prognosis for accurate estimation of RUL. A significant amount of research has been conducted in this field to enhance the fidelity of damage assessment models in metallic materials and composites (Clayton et al., 2004; Fan et al., 2001; Bakis, 2002; Kadi, 2006; Hochhalter et al., 2010; Horstemeyer and McDowell, 1998; Sundararaghavan and Zabaras, 2008; Chattopadhyay et al., 2009). An integrated framework of damage detection that includes material characterization, multiscale modeling, sensing, prognosis, experimental validation and information management has been developed by Chattopadhyay et al. (Chattopadhyay, 2009). However, a general sensing methodology that can be used for every conceivable damage state in a structure is currently not available. Also, there is a considerable limitation on the size of detectable damage using off-the-shelf sensors. Therefore, there is a need for multiscale modeling techniques to understand damage initiation and track its evolution across the length scales. Information on damage initiation at the microscale and its manifestation at the macroscale, obtained from the
multiscale models, can be combined with physical sensor data to construct a hybrid data base for damage estimation and detection. The output of this effort can be used in diagnostics as well as prognostics. Most importantly, multiscale modeling is the key to understanding precursors to damage.

In this thesis, effort has been dedicated to develop multiscale modeling approaches and associated damage criteria for the estimation of damage evolution which is essential to damage detection. Two different materials, aluminum alloy and smart particle embedded epoxy polymer (which will be discussed in more details in the following sections) are studied. Important issues, such as length and time scales, variability in material properties and mechanical behavior at the microscale due to crystallography and geometry of grains for metal and crosslinked microstructure for polymer, are addressed in this research. A background of the relevant research is discussed in the following sections.

1.2. Background of multiscale modeling for metallic material

A broad range of multiscale modeling techniques have been reported in recent literature using the meso representative volume element (RVE) approach to merge the length scales (Balzani, 2009; Kanit, 2003; Trias, 2006). Nakamachi (2007) developed a two-scale homogenization theory to assess the sheet metal formability. A realistic RVE model was employed for the micro polycrystal structure, which was determined by the scanning electron microscopy and the electron backscattering diffraction (SEM-EBSD) measurement. Using this technique, the morphological and crystallographic textures of the microstructure can be obtained with an accurate spatial resolution. St.-Pierre et al.
(2008) developed a new methodology based on Voronoi tessellation to create realistic 3D microstructures of polycrystalline materials. Experimental inputs from SEM-EBSD measurements were used to reproduce the grain morphology, including grain boundaries and the anisotropy of the grain shape. Luo (2009) directly obtained a meso RVE through microstructure scans of actual material samples containing various differently oriented grains. The material behavior in hot spots or areas of high stress concentrations was explicitly modeled using an RVE containing microstructure in order to capture grain size and orientation effects, while homogenous material properties were used outside the hot spots. This multiscale model captures anisotropic behavior at the microscale due to crystalline orientations while maintaining the isotropic material behavior at larger scales in accordance with the isotropic macroscale material behavior obtained from experiments. Experiments were implemented using lug joint specimen under uniaxial fatigue loading and cruciform specimen under biaxial fatigue loading. While this methodology provides both crack length and direction of crack growth with sufficient accuracy when compared to experiments, it requires large amounts of experimental data and associated pre-processing. Also, for accuracy, the material scan has to be acquired from the same exact location where the RVE is positioned at the structural scale. In addition, such an approach is deterministic in nature; therefore for a different sample, the RVE model must be reconstructed based on a new material scan. This is time-consuming, CPU intensive, and more challenging in applications with limited accessibility. The shortcoming of the RVE model has been addressed through the development of the statistical volume element (SVE) model to study polycrystalline microstructures. A
considerable amount of research has been reported on SVE models in the context of stochastic modeling. Groeber (2007, 2008) made significant improvements on characterization of 3D polycrystalline microstructures and 3D SVE modeling by taking into consideration grain features, including orientation, misorientation, and grain size in the generation of an SVE model. SVE models have also been applied in the prediction of crack initiation and fatigue life. Yin et al. (2008) developed an SVE method to analyze, quantify, and calibrate microstructure-constitutive property relations using statistical means. Voids (defects) were randomly generated in their SVE model prior to studying the material’s constitutive response. However, the crack incubation and nucleation stages were not studied in their work. Hochhalter (2010) focused on a comprehensive study of crack nucleation prediction and growth in grain boundaries. Grain features, including grain orientation, misorientation, and boundary shape were considered in their model, and based on their results, it was seen that grain orientation had a significant effect on the nucleation metrics. Although the focus of their study was on small fatigue cracks (length in the order of 10 µm), their work could be used in further construction of SVE models and mesoscale crack prediction (up to 1 mm length). Guilleminot et al. (2011) generated an SVE model using strain energy density criteria. This SVE model showed a more accurate response because the construction of the SVE is based on mechanical properties. However, the geometric features of the material are neglected in their SVE model to improve simulation efficiency. Therefore, an SVE model based multiscale modeling approach is required in which both the geometric features and crystallographic features are taken into account. In addition to capturing statistical effects, the use of SVEs may
also reduce preprocessing time and computational effort. The methodology outlined in this work results in a significant increase in computational efficiency through a reasonable reduction of elements in the analysis, which is essential for the use of multiscale models in sensing applications.

Fatigue crack prediction for metallic materials is an important consideration in the design and maintenance planning of many structural components in aerospace vehicles (Clayton, 2004; Fan, 2001; Hochhalter, 2010; Horstemeyer, 1998; Sundararaghavan, 2008; James, 1997; Newman, 1999). Extensive research has been conducted over the past several decades; however, accurate prediction of the fatigue crack remains a challenging problem. Fatigue crack growth has been characterized to be both multiscale and stochastic in nature (McDowell, 2011). Experimental studies of material fatigue have been performed over the last 100 years, including several observations on the multiple stages of fatigue. To investigate fatigue phenomenon in different stages, Schijve (1967) divided fatigue life into four stages: micro crack nucleation, micro crack growth, macro crack growth, and failure. Forsyth (1969) first noted that fatigue cracks usually start at the surface of a structural component. He argued that major cracks typically start from micro cracks on crystallographic slip planes in intermetallic particles and gradually grow in a direction perpendicular to the external applied load. Pearson (1975) compared the initiation of fatigue cracks and the subsequent growth of very short cracks (0.006mm-0.5mm) using two types of aluminum alloys, and observed that short tensile cracks first initiated at the interface between a surface inclusion and the matrix or within an inclusion. Once formed, the cracks grew into the matrix in directions approximately
perpendicular to the applied tensile stress. Chaussumie (2010) states that the phenomenon of fatigue involves multiple length scales including micro crack nucleation at the microscale, coalescence of micro cracks at the meso scale, and major crack propagation at the macro scale. Hochhalter (2010) presented a comprehensive study of micro crack nucleation and growth in grain boundaries and found that grain orientation had a significant effect on the nucleation metrics. It should be mentioned that for aluminum alloy 2024, only large iron bearing particles, Al$_7$Cu$_2$Fe ($\beta$-phase) contributed to the crack nucleation process (Merati, 2005). Mo (2008) studied the phenomena of coalescence of neighboring micro cracks, formation of larger micro cracks, and subsequent propagation of a major crack. The cracks in intermetallic particles were considered as micro cracks that coalesced together and provided a weak path for fatigue crack propagation. Final fracture occurred when the percentage of cracked particles increased to a threshold level during the fatigue process. Taylor (2002) studied the behavior of short fatigue cracks at the microstructural level and proposed that the size of short cracks should be of the same order of magnitude as the microstructure, typically less than ten grain diameters.

In general there are two major types of modeling methodologies for fatigue crack prediction: i) a method based on material properties and the damage accumulation rule, and ii) a method based on fracture mechanics and crack growth analysis, using a physical approach to damage tolerance analysis. An important drawback of these methods is that they fail to take into account either the length scale effects or the physical nature of fatigue. Therefore, it is necessary to develop a length scale dependent and physics-based model for accurate simulation in order to understand a material’s performance and
ultimately assess the reliability of current aerospace vehicles. Two critical issues need to be resolved to ensure the viability of such an approach: developing a model that accurately accounts for the material properties and their variability and a damage criterion capable of capturing crack initiation and growth. It is important to note that defects, such as cracks, initiate at the microscale before manifesting at the macroscale and thus can become a critical factor in final structural failure. As such, prediction of damage initiation and crack growth can be simulated and verified by applying physics based multiscale models. To model the nucleation, growth, and coalescence of micro cracks in complex metallic microstructures, multiscale analysis techniques have been proposed. A realistic treatment of length scale effects on damage evolution, for instance, is becoming feasible now when sufficiently sophisticated constitutive laws are used. Tekoglu (2010) modeled the void nucleation by integrating a damage model with a Mori–Tanaka type mean-field homogenization scheme that explicitly accounts for the per-phase behavior. Sun (2008) developed a multiscale continuum model to study the effect of grain size on the macroscopic dissipative response during isothermal thermoelastic phase transition. Groh (2009) proposed a numerical, hierarchical multiscale modeling methodology involving two distinct bridges over nano, micro, and meso scales that predicts the work hardening of face-centered cubic crystals in the absence of physical experiments. In order to study the length scale effects on fatigue crack growth, it is necessary to take into account crystal dislocation mechanics, material microstructure, and macro scale behavior in the continuum description of finite strain plasticity. Crystal dislocation provides an atomistic interpretation of the slip process and strain hardening of
metals. Jiang (2000) developed a three-dimensional fatigue damage criterion under multiaxial, non-proportional loading. The effect of grain orientations in fatigue damage was investigated by Kalnaus (2006). He proposed a damage criterion on a critical slip plane for single crystalline microstructures. Luo (2011) extended Jiang and Kalnaus’s fatigue damage criterion to polycrystalline materials. Aluminum alloy 2024-T351 was studied in his work. A multiscale model was constructed that linked the relationship between the damage criteria at the microscale to the crack initiation at the mesoscale. The multiscale model with fatigue damage criteria initiated at the microscale and the effects of grain orientation, shape and size were included through material characterization and crystal plasticity based constitutive relation. It must be noted that the microstructure in such approaches is generated by using single crystal plasticity theory which neglects defects such as intermetallic particles within and between grains. Thus, a damage estimation approach considering both crystal dislocation mechanics and micro crack nucleation in intermetallic particles is required.

In this dissertation, a multiscale modeling approach is developed for aluminum alloy (Al 2024-T351). The research starts with material characterization to incorporate statistical microstructural features. The effects of grain features including orientation, misorientation and size on the damage evolution are studied in detail and a microstructural database is created. The SVE model is developed based on this microstructural database. Details on material characterization, construction of statistical database, development and parametric study of the SVE model are discussed in the chapter 2. A physics-based multiscale damage criterion is developed to capture the crack
initiation at the microscale and growth at the mesoscale. This criterion is energy based since the damage index is directly related to the plastic strain energy density. The derivation of the multiscale fatigue damage criterion and some applications of this damage model for different structural components and load conditions are presented in the chapter 3.
1.3. **Background of multiscale modeling for self-sensing polymer material**

Interest in stimuli-responsive materials that exhibit specific chemical reactions upon external stimuli such as temperature, pH, ion, light, and electric field has increased significantly in the last twenty years (Suzuki, 1996; Qiu, 2001; Richter, 2008; Bawa, 2009; Tanaka, 2012). Particularly of interest are stress-sensitive materials responsive to mechanical loading (also known as mechanophores), which open novel ways to study post-yield behavior at material level (Chang, 1987; Thostenson, 2006; Wu, 2008). Cho and Chung (Cho, 2010; Chung, 2004) developed a cyclobutane based mechanophore consisting of carbon-carbon covalent bonds. Under mechanical loading, the cyclobutane transforms into cinnamate groups, which emit green fluorescence. Zou et al. (2014) developed a novel self-sensing technique by embedding the Tris-(Cinnamoyl oxymethyl)-Ethane (TCE) as the cyclobutane-based self-sensing material in polymer matrix. They incorporated the cyclobutane-containing crosslinked polymers into an epoxy matrix, studied the effect on mechanical properties and demonstrated early damage detection through mechanically induced fluorescence. The experimental research has shown significant promise in developing mechanophore embedded polymer materials which can be used to detect damage initiation in polymeric composite materials (Zou, 2014). Previous studies have reported the experimental characterization and fabrication of nanoparticle-embedded polymers (Gibson, 2010). However, the determination of mechanical properties through testing is labor intensive and expensive. Modeling techniques are now necessary to simulate the multiscale response of these “smart” polymers.
In epoxy based polymers the crosslinked bond clusters between the resin and the hardener molecules generate a larger scale of network structure. The heterogeneous crosslinked network at the microscale has significant effect on the local mechanical properties (Flory, 1943; Krumova, 2000; Fan, 2007). Therefore to design and synthesize polymers with multifunctional capabilities it is important to develop a fundamental understanding of the effects of microscale variability on material properties and response such as Young’s modulus, heterogeneous stress/strain distribution and damage initiation. Numerous approaches have been developed to model polymeric systems integrated with nanoparticles. These include homogenization techniques, finite element (FE) method, molecular dynamics (MD) simulation, Monte Carlo (MC) simulation, and the Mori-Tanaka approach (Ghosh, 1995; Borodin, 2005; Fermeglia, 2007). Among these techniques the MD model and FE model are two of the most widely used methods to understand the material behavior of epoxy based systems at the nanoscale and microscale. The heterogeneous material properties of polymer, which is influenced significantly by crosslinking degree, can be effectively captured by MD simulation (Flory, 1943; Fan, 2007; Krumova, 2000). Fan et al. (2000) performed MD simulations to characterize the material properties of the crosslinked epoxy resin compound. Linear thermal expansion coefficients and Young's modulus of the material can be captured using their model. Yarovsky and Evans (Yarovsky, 2002) investigated the strength and molecular mechanisms of adhesion between an inorganic substrate and a cured epoxy resin using MD simulation. In their model, the crosslink density and corresponding material properties of the crosslinked system were successfully estimated. However, the
significantly high computational cost associated with large-scale MD simulations is a major hurdle and often limits its application beyond the nanoscale. The FE model is computationally efficient and can capture the material performance of polymers. Onck et al. (2005) developed a two-dimensional model to study the strain stiffening of crosslinked filamentous polymer. In their work the FE method was used to discretize the filament with Euler-Bernoulli beam elements accounting for stretching and bending. Jiang et al. (2007) performed a parametric study using FE analysis to compute the material properties and scratch behavior of crosslinked polymer. Their simulation results correspond well with the mechanical properties obtained from experiment. Chen and Lagoudas (2008) developed a constitutive theory for polymers in which the crosslinking density is considered to influence the mechanical behavior. Their model was implemented and extended using FE method by other researchers to study thermoelasticity, viscoelasticity and nonequilibrium relaxation (Westbrook, 2011; Volk, 2010; Diani, 2012). However, the FE method cannot be used to model heterogeneous microstructure because the definition of discontinuous material properties is often infeasible in FE approach. Therefore, new techniques with improved computational efficiency and high accuracy are desired for investigating the material behavior of polymers at the microscale.

Discrete material techniques, such as the spring-bead model, have been developed to study polymer material (Buxton, 2002; Iwata, 2003; Schwarz, 2006). Underhill and Doyle (2005) developed a new method for generating coarse-grained models of polymers. The spring-bead chains were further crosslinked to generate a network model
to represent the larger scale material behavior of polymer (Indei, 2012). A spring-bead based network model, which bridges nanoscale information to higher length scales, was developed by the authors (Zhang et al., 2014) to model this class of epoxy polymers embedded with TCE monomer. The material was partitioned into discrete mass beads which were linked using linear springs at the microscale. By integrating multiple spring-bead models a network model was constructed to represent the material properties at the mesoscale. A series of MD simulations were performed initially to define the spring stiffness in the statistical network model. Compared with the MD model, only the equivalent mechanical responses which influence the damage initiation significantly was captured in the spring-bead based network model. The other material properties, such as the thermal properties and chemical properties were neglected to improve simulation efficiency. The developed multiscale methodology was computationally efficient and it was able to provide a possible means to bridge various length scales (from 10 nm in MD simulation to 10 mm in FE model) without significant loss of accuracy. In this work, the statistical network model is further investigated to understand the effects of the model parameters on material response and damage in the TCE embedded polymer. The model is also used to develop a relationship between mechanical strain and experimentally observed fluorescence, with damage growth, in the self-sensing polymer under multiaxial loading.

The parameters in the crosslinked network model (such as the crosslinking degree, chain flexibility and chain length) affect the material performance (Espuche, 1995; Chzarulatha, 2003; Park, 2006). These effects were studied by observing their mechanical
properties. Among all variability, the crosslinking degree which represents the degree of microscopic crosslinked covalent bonds was shown to have a more significant effect on the mechanical properties (Zosel, 1993; Espuche, 1995; Halary, 2000; Berger, 2004). Urbaczewski-Espuche et al. (1991) developed a crosslinked network model and studied the influence of the crosslinking degree on the mechanical properties of epoxy. The results showed that the mechanical properties including Young’s modulus, ultrasonic modulus, thermomechanical relaxation, and plastic behaviors are affected by crosslinking degree. Svaneborg et al. (2005) investigated the effect of microscopic disorder on the mechanical response of network models of the same crosslinking degree. They concluded that the heterogeneities in the randomly generated crosslinked network models cause significant differences in the localization of monomers. Parametric study through the developed network model can help to understand the self-sensing polymeric material’s microscopic performance.

In this dissertation, a spring-bead based network model is developed to bridge nanoscale information to higher length scales for modeling epoxy polymers embedded with smart particles. A series of MD simulations are performed to capture the generation of crosslinked bonds in the self-sensing polymer; this information is further used to construct the probability distribution of crosslinking degrees. Mechanical equivalence optimization was implemented to bridge the mechanical properties between the MD system and the network model. The MD simulation results, details of the spring-bead model, network model, and mechanical equivalence optimization are discussed in chapter 4. Parametric study based on the developed statistical network model is performed to
understand the influence of design variables on material behavior. A series of simulations are performed to compare the effects of the crosslinking degree on the strain distribution. The knowledge obtained is important to the enhancement of the material performance by controlling the crosslinking degree during the manufacturing process. Experiments were conducted to validate the network model. The average equivalent strain of network model is used to capture the fluorescence intensity of the self-sensing material. A physics based damage evolution is developed to estimate the damage evolution. The parametric study, validation and damage evolution of the network model are presented in chapter 5.

1.4. Objectives

Multiscale modeling of Al 2024-T351

A multiscale modeling framework is developed, which includes characterization of microstructural features and variability, development of a meso SVE model to represent the material behavior, development of a physics-based damage criterion, and experimental validation to predict the fatigue life of Al 2024-T351. The key objectives of this research are as follows.

1) Characterize microstructural material properties including grain features and intermetallic particle features to construct a statistical data base;

2) Implement parametric studies of grain features including grain orientation, misorientation, grain size, grain shape, aspect ratio and principal axis direction to assess the sensitivity of each parameter;

3) Develop a meso SVE model to represent the material properties and perform validation through RVE based simulation;
4) Develop a physics based multiscale damage criterion to predict fatigue life and crack direction in Al 2024-T351 based complex structural components. Two important stages of the crack initiation are modeled: micro crack nucleation and major crack formation;

5) Modify the physics based multiscale damage criterion to predict crack formation in thermo-mechanical fatigue (TMF) loading;

6) Perform damage analysis using the multiscale model and the damage criterion in lug joints under uniaxial fatigue loading, cruciform specimen under biaxial fatigue loading and lug joints under uniaxial TMF loading.

**Multiscale modeling of a self-sensing polymer material**

A spring-bead based network model is developed to model the mechanical properties of a novel mechanophore crosslinked polymer which is capable of detecting damage precursor. The modeling framework includes mechanical equivalence optimization based on properties obtained from MD simulations, parametric studies of microscopic variability, experimental validation and estimation of damage precursor in polymeric material based on MD simulation and network model. The present multiscale modeling work of the self-sensing polymer material addresses the following objectives.

1) Develop a spring-bead based network model to represent the mechanical properties of self-sensing polymer material; simulate the mechanical response of the crosslinked springs in the network model using statistical material behavior obtained from MD simulation;
2) Conduct configuration analyses and mechanical equivalence optimization to construct the optimal arrangement of the network model;

3) Perform parametric studies of the network model to understand the influence of design variables such as distribution of crosslinking degree and spring length on material behavior;

4) Validate the mechanical properties of the spring-bead based network model through experiments;

5) Capture the self-sensing fluorescence intensity observed in experiment through the network model based simulation;

6) Evaluate the damage evolution using a strain based index based on MD simulation and network model.

1.5. Outline of the dissertation

The dissertation is structured as follows. Six chapters are presented.

Chapter 2 provides an introduction of single crystal plasticity theory which is used to capture the crystallographic and geometric effects of grains at the microscale. A subroutine UMAT is introduced to incorporate the single crystal plasticity in the FEA program. Material characterization procedures from Electron Backscattering Diffraction (EBSD) scans are discussed. Development of an SVE model based on the statistical features of material at the microscale is presented. A parametric study is performed to assess the sensitivity of grain features. The SVE model is validated through comparative simulations using an RVE based model.
Chapter 3 presents studies on material characterization and microstructure investigations. The microstructural features of intermetallic particles are obtained from scanning electron microscope (SEM) and energy dispersive X-ray microanalysis (EDAX). The development of a multiscale physics damage criterion is discussed. The damage criterion is further modified to capture damage initiation under TMF loading. Details of simulation results and experimental validations are discussed.

Chapter 4 presents a multiscale framework to represent a self-sensing polymer material. Self-sensing behavior of the smart material and atomistic scale studies using MD simulation are introduced. Development of a spring-bead based network model, analyses of different combination arrangements of springs and beads in network model and mechanical equivalence optimization are discussed. Definition of equivalent strain and strain energy density in the network model is also introduced at the end of this chapter.

Chapter 5 presents the parametric studies conducted using the network model to understand the influence of microscopic variability on material behavior. The development of a statistical network model is presented. Validation of the network model is performed through experiments and FE simulations. Correlation between fluorescence intensity observed in experiments and average equivalent strain in the network model based simulation is presented. The development of a strain based damage evaluation approach to estimate the damage evolution based on MD simulation and network model is also introduced.
Chapter 6 summarizes the research work reported in this thesis, and emphasizes the important original contributions and findings of this dissertation. Suggestions on future research directions and recommendations are also discussed at the end of this chapter.

2.1. Introduction

A broad range of multiscale modeling techniques have been reported in previous research and within these, the meso representative volume element (RVE) approach is a popular technique. The RVE model is directly obtained through microstructure scans of actual material samples containing various differently oriented grains. While this type of approach has qualified accuracy, it requires large amounts of experimental data and associated pre-processing. Also, for accuracy, the material scan has to be acquired from the same exact location where the RVE is positioned. In addition, such an approach is deterministic in nature; therefore for a different sample, the RVE model must be reconstructed based on a new material scan. This is time consuming, CPU intensive, and more challenging in applications with limited accessibility.

The statistical volume element (SVE) methodology for multiscale analysis and fatigue life prediction is outlined in this section. The primary goal of this research is to improve the computational efficiency and reduce the preprocessing effort associated while maintaining accuracy. Simplified grain shapes are employed because they offer ease of assembly, reduced preprocessing time, and reduced total number of elements used (irregular grain shapes result in small features, thereby requiring a large number of small elements). Using the SVE methodology, grains with features that are statistically sampled from pools of measured experimental characterization data are assembled, as shown in
Figure 2.1(b). This approach provides a computationally efficient alternative to traditional techniques while maintaining statistical accuracy.

![Figure 2.1 Comparison between: a) actual microstructure scans; b) constructed SVE.](image)

Colors represent different grain orientations.

To capture the crystallographic effect of grains at the microscale, single crystal plasticity is introduced. This is then incorporated into the commercial finite element (FE) program ABAQUS (version 6.10.1) with the help of a user material (UMAT) subroutine. Material characterization, including Electron Backscattering Diffraction (EBSD) scans and OOF2 (Object-Oriented Finite) meshing are implemented to capture the geometric and crystallographic features of grains. Representative volume element (RVE) and SVE models are developed to demonstrate material properties and mechanical responses occurring at the mesoscale. Finally, a series of simulation validations is performed. The results show that the SVE model is capable of representing the bulk material and mechanical responses of the polycrystalline material.
2.2. Single crystal plasticity theory

To study the mechanical properties of aluminum alloy 2024-T351, which is face centered cubic (FCC) crystalline structure, the single crystal plasticity theory is introduced to capture the crystallographic orientation effects on polycrystalline material. The kinematic theory for single crystal deformation in this research is based on the pioneering works of Taylor (1938), Hill (1966), Rice (1971), and Asaro (1983). In these works, the deformation gradient, $F = \partial \mathbf{x} / \partial \mathbf{X}$, is decomposed into elastic and plastic components under standard multiplicative decomposition assumption (Figure 2.2 and Equation 2.1) as follows:

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

(2.1)

where $\mathbf{F}^p$ represents plastic deformation of the material in an intermediate configuration in which the lattice orientation and spacing remain the same as in the reference configuration. $\mathbf{F}^e$ represents elastic component of the deformation gradient, which
includes two parts: stretching and rotation of the lattice. The velocity gradient, \( \mathbf{L} = \partial \mathbf{v} / \partial \mathbf{x} \), in the current configuration can be expressed as:

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

(2.2)

where \( \mathbf{L}^e \) and \( \mathbf{L}^p \) represent the elastic and plastic components of the velocity gradient, as shown in Equation 2.3 and 2.4, respectively:

\[
\mathbf{L}^e = \dot{\mathbf{F}}^e (\mathbf{F}^e)^{-1}
\]  

(2.3)

\[
\mathbf{L}^p = \mathbf{F}^e \dot{\mathbf{F}}^p (\mathbf{F}^p)^{-1} (\mathbf{F}^e)^{-1}
\]  

(2.4)

The inelastic deformation of single crystal is assumed to be solely from the crystalline slip. The plastic velocity gradient, \( \mathbf{L}^p \), can then be expressed in terms of the resolved slip rate \( \dot{\gamma}^{(\alpha)} \), the slip direction \( \mathbf{s}^{(\alpha)} \), and the normal direction to the slip plane \( \mathbf{m}^{(\alpha)} \) as follows:

\[
\mathbf{L}^p = \sum_{\alpha} \dot{\gamma}^{(\alpha)} \mathbf{s}^{(\alpha)} \otimes \mathbf{m}^{(\alpha)}
\]  

(2.5)

where \( \alpha \) denotes the \( \alpha \)th slip system of the single crystal. The resolved shear stress, which plays an important role in promoting slip, is derived from the Cauchy stress tensor as:

\[
\tau^{(\alpha)} = \mathbf{\sigma} : (\mathbf{s}^{(\alpha)} \otimes \mathbf{m}^{(\alpha)})
\]  

(2.6)

In Equations 2.5 and 2.6, the slip direction and the vector normal to the slip plane are defined for the deformed configuration, but not for the reference configuration. The relation between deformed and reference configurations of slip direction or normal vector can be expressed as follows:

\[
\mathbf{s}^{(\alpha)} = \mathbf{F}^e \mathbf{s}^{(\alpha)}_0
\]  

(2.7)
\[ m^{(\alpha)} = m_0^{(\alpha)} (F^e)^{-1} \]  

The velocity gradient in the current state can be decomposed into the symmetric rates of stretching tensor \( D \) and anti-symmetric spin tensor \( \Omega \) in Equation 2.9:

\[ L = D + \Omega \]  

The stretching and spin tensor can be further decomposed into lattice and plastic parts, respectively:

\[ D = D^l + D^p \]  
\[ \Omega = \Omega^l + \Omega^p \]

From Equations 2.3 and 2.5, the Equations 2.10 and 2.11 can be further expressed as follows:

\[ D^l + \Omega^l = \dot{F}^e (F^e)^{-1} \]  
\[ D^p + \Omega^p = \sum_{\alpha} \dot{\gamma}^{(\alpha)} s^{(\alpha)} \otimes m^{(\alpha)} \]  

Following the methodology developed by Hill and Rice (Hill, 1966; Rice, 1971; Hill and Rice, 1972), the relation between stretching tensor and the Jaumann rate of Cauchy stress \( \tilde{\sigma} \) is as follows:

\[ \tilde{\sigma} + \dot{\sigma} (1 : D^l) = L : D^l \]  

Based on the work of Horstemeyer and McDowell (1998, 1999), a power law is used in the flow rule to calculate the slip increment in polycrystal elastoplasticity as follows:

\[ \dot{\gamma}^{(\alpha)} = \dot{\gamma}_0^{(\alpha)} \left| \frac{\tau^{(\alpha)} - \chi^{(\alpha)}}{g^{(\alpha)}} \right|^n \text{sign}(\tau^{(\alpha)} - \chi^{(\alpha)}) \]
where $\dot{\gamma}^{(\alpha)}$ and $\tau^{(\alpha)}$ represent the shear strain rate and shear stress on the $\alpha$th slip system, $n$ is the strain rate exponent parameter, and $g^{(\alpha)}$ and $\chi^{(\alpha)}$ represent the isotropic and kinematic hardening, respectively. The hardening law for $g^{(\alpha)}$ and $\chi^{(\alpha)}$ are as follows (Huang, 1991):

$$\dot{g}^{(\alpha)} = \sum_{\beta} h_{\alpha\beta} \dot{\gamma}^{(\beta)}$$

$$\dot{\chi}^{(\alpha)} = b\dot{\gamma}^{(\alpha)} - r\chi^{(\alpha)} |\dot{\gamma}^{(\alpha)}|$$

where $h_{\alpha\beta} = \begin{cases} h(\gamma) = h_0 \text{sech}^2 \left( \frac{h_0\gamma}{\tau_s-\tau_0} \right), & \alpha = \beta \\ q \cdot h(\gamma) & \end{cases}$ are called self and latent hardening moduli, respectively. Here, $b$, $r$, and $q$ are material constants, $h_0$ is initial hardening modulus, $\tau_s$ is the stage I stress, and $\tau_0$ is yield stress. The cumulative shear strain of all slip systems in the polycrystalline materials can be obtained as follows:

$$\gamma = \sum_{\alpha} \int_{0}^{t} |\dot{\gamma}^{(\alpha)}| dt$$

More details of hardening theory for crystalline materials can be found in Asaro and Peirce (Asaro, 1983; Peirce et al, 1982).

### 2.3. User defined material subroutine

In this multiscale modeling approach, a UMAT subroutine based on Huang’s single crystal plasticity theory (Huang, 1992) is used. Luo (2009) and Zhang (2012) modified the UMAT subroutine and add a developed damage criterion to evaluate microscale damage initiation and growth. In their work, the UMAT subroutine was used to incorporate single crystal plasticity in the finite element program ABAQUS. The finite element formulation of elastic-plastic and viscoplastic single crystal deformation was
taken into account, including versions for small deformation theory and for a rigorous
theory of finite strain and finite rotation. Inelastic deformation of a single crystal occurs
as a result of crystalline slip, which is assumed to obey Schmid’s law (Asaro, 1979).
Various self and latent hardening relations between resolved shear stress and shear strain
in slip systems are presented and incorporated as options in the subroutine. An option of
using the linearized solution procedure and evaluating the stress and solution dependent
state variables at the start of the time increment (time t), or using the Newton-Rhapson
iterative method to solve the nonlinear increment and evaluating the stress and solution
dependent state at the end of the time increment \((t + \Delta t)\) is provided.

In this research, the polycrystalline material Al 2024-T351, in which the orientations
of grains change from one grain to another, is approached. To account for the arbitrary
crystal orientations, two coordinate systems, global coordinate system for specimen and
local coordinate system for crystalline are applied in the simulation. The global
coordinate system is fixed to the reference configuration while the local coordinate
system is aligned with the crystal lattice. At the beginning of each time increment, the
global strain increment, the time increment, global stress, and the solution-dependent
state variables are given to the subroutine from the main program in ABAQUS. The
subroutine UMAT is used to transform the global strain increment and stress into the
local system. In the local coordinate system, the incremental stress is computed based on
single crystal plasticity theory (Huang, 1993) and transformed into the global system. At
the end of each incremental step, the stress and state variables are updated for use in the
main program in ABAQUS. Then, the next load increment is applied and a new strain
increment is generated. This loop is repeated until computation at all incremental time steps is completed.

The subroutine UMAT is written for cubic crystals. The subroutine can accept, as input, up to three sets of slip systems for each cubic crystal. There is observation of the activation of slip system \{1 1 0\}<1 1 1>, \{1 2 1\}<1 1 1>, and \{1 2 3\}<1 1 1> in BCC metal crystals, and \{1 1 1\}<1 1 0> in FCC metal crystals. There are seven user supplied function subprograms, F, DFDX, HSELF, HLATNT, GSLP0, DHSELF, and DHLATN in the main subroutine UMAT. These characterize the crystalline slip and hardening of slip systems. The function subprogram F provides the slipping rate \(\dot{\gamma}(\alpha)\), as shown in Equation 2.15 at the start of the increment, while function subprogram DFDX gives its derivative as \(\frac{d\dot{\gamma}(\alpha)}{d(\tau(\alpha)/\theta(\alpha))}\). The function subprograms, HSELF and HLATNT, provide the self and latent hardening moduli defined in the incremental formulation (Equation 2.16). The function subprogram GSLP0 provides the initial value of the current strength \(\theta_0(\alpha)\), and its default is the yield stress \(\tau_0\). The function subprograms, including DHSELF and DHLATN, necessary only when the Newton-Rhapson iterative method is used, provide the derivative of self and latent hardening moduli.

There are eight subroutines, ROTATION, SLIPSYS, STRAINRATE, GSLPINIT, LATENTHARDEN, ITERATION, LUDCMP, and LUBKSB in the main subroutine UMAT. The relation of the first five subroutines with the main subroutine UMAT and function subprograms are shown in figure 2.3. The subroutine ROTATION determines the initial orientation of a cubic crystal in the global system, while SLIPSYS generates all slip systems (slip directions and normal to the slip planes) in the same set for a cubic
crystal in the reference state. The subroutine STRAINRATE, which calls functions subprograms F and DFDX, calculates the slip rates in all slip systems at the start of increment. The function subprogram F is also called by the main subroutine UMAT if the iteration method is used. The subroutine LATENTHARDEN, which calls function subprograms HSELF and HLATNT, generates the hardening matrix, i.e., the self-hardening moduli on the diagonal and the latent hardening moduli on the off diagonal. The subroutine GSLPINIT, which calls the function subroutine GSLP0, calculates the initial value of the current strength in all slip systems at the reference state. The subroutine ITERATION, which calls the function subprograms DHSELF and DHLATN, provides the arrays for the Newton-Rhapson iterative method. The last two subroutines, LUDCMP and LUBKSB, are used together to solve linear equations; LUDCMP performs the LU decomposition, LUBKSB completes the backward substitution. More details of the subroutine UMAT can be found in Huang’s work (Huang, 1992).

Figure 2.3 Flowchart of subroutines and subprograms in UMAT

UMAT: main subroutine

ROTATION: orientation of local cubic system in global system
CROSS: cross product of two vectors
SLIPSYS: generating all slip systems
LINE: [mmm] type of slip systems
LINE1: [0mn] type of slip systems
GSLPINIT: initial values of current strain hardening functions in all slip systems
GSLP0: user supplied functional subroutine for the initial value in each system
STRAINRATE: shear strain rate in all slip systems
F: user supplied functional subroutines for the shear strain rate in each slip system
DFDX: user supplied functional subroutine for the derivative of function F
LATENTHARDEN: hardening matrix
HSELF: user supplied functional subroutine for the self-hardening modulus
HLATNT: user supplied functional subroutine for the latent hardening modulus

2.4. Material characterization

The material used in this research is aluminum alloy 2024-T351. Relevant material compositions and properties are shown in Table 2.1 and Table 2.2. To capture the mechanical response of the polycrystalline material at the mesoscale, a RVE model is required to characterize the geometric and crystallographic properties of the grains. The mesoscale model is constructed based on the microscale scans, which contain 2,127 grains, which is sufficient to construct an RVE model. In the RVE model, each grain has a single crystal structure.

| Table 2.1 Specified Composition for 2024-T351 (wt%) (Bussu, 2003) |
|-----------------|---|---|---|---|---|---|---|---|---|---|
| Element        | Cu | Mg | Mn | Fe | Si | Zr | Cr | Ni | Pb | Sn | Al |
| 2024-T351      | 3.8-| 1.2-| 0.3-| 0.5| 0.5| 0.2| 0.1| 0.05| 0.05| 0.05| Rem |
Table 2.2 Mechanical and Physical Properties of 2024-T351 at Room Temperature  
(Rodopoulous, 2004)

<table>
<thead>
<tr>
<th>Property</th>
<th>Value 1</th>
<th>Value 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Elastic modulus (GPa)</td>
<td>72-74</td>
<td></td>
</tr>
<tr>
<td>Shear modulus (GPa)</td>
<td>27-28</td>
<td></td>
</tr>
<tr>
<td>Poisson's ratio</td>
<td>0.33</td>
<td></td>
</tr>
<tr>
<td>Mon. yield stress (MPa)</td>
<td>325-340</td>
<td></td>
</tr>
<tr>
<td>Cyclic yield stress (MPa)</td>
<td>420-450</td>
<td></td>
</tr>
<tr>
<td>Hardness (HB)</td>
<td>115-120</td>
<td></td>
</tr>
<tr>
<td>Fr. toughness (MPa·m$^{1/2}$)</td>
<td>31-34</td>
<td></td>
</tr>
<tr>
<td>Ult. tensile strength (MPa)</td>
<td>490-520</td>
<td></td>
</tr>
<tr>
<td>Endurance limit (MPa, R=-1)</td>
<td>135-140</td>
<td></td>
</tr>
<tr>
<td>Shear strength (MPa)</td>
<td>285-301</td>
<td></td>
</tr>
</tbody>
</table>

The first step of material characterization is to take a number of EBSD scans (Figure 2.4) from which are obtained the crystal orientation and geometric properties of each grain. In the EBSD scans, in which grains are represented by various colors, it is obvious that the grain features are affected by the rolling direction in the material manufacturing. The principal axis direction of grain, for example, slants towards the rolling direction (as shown in Figure 2.4a).
The software package OOF2 (version 2.1.11) is a finite element analysis tool, which is available from the National Institute of Standards and Technology (NIST) and is used to create and mesh the mesoscale structure from the EBSD scan (Figure 2.5). In the mesh model generated by OOF2, the mesh in the grain boundary can be refined using the snap nodes option and by selecting different threshold values.
Finally, the geometric and crystallographic properties obtained from EBSD are assigned to the grains to generate the meso RVE model using the commercial FEA software ABAQUS and the previously developed UMAT subroutine (Figure 2.6). The RVE model is used to bridge the crystalline grain microstructure at the microscale to the structural response of a component at the macroscale.

Figure 2.6 Mesoscale RVE model of Al 2024-T351

2.5. Feature parametric study

Figure 2.7 shows three pole figures for grain orientations. The distributions do not exhibit any trends, and therefore, are assumed to be normally distributed. It must be noted that when formulating the SVE, the orientations were chosen at random from the pool of available material characterization data. The misorientations between neighbor grains were determined from the arrangement of the grains in the SVE. To accomplish this, nine randomly orientated SVEs were generated (Figure 2.8). A typical histogram of their misorientation is shown in Figure 2.8 (a)-(i). The misorientation was chosen to closely match that of the experimental data (Figure 2.9). The difference, i.e., the error between the randomly generated SVEs and the experimental data, is shown in Figure 2.10. The
seventh generated SVE is the closest match to the experimental data, and therefore, was used in this analysis.

Figure 2.7 Flattened 3D polar plots of crystal orientation: a) \{1,0,0\}; b) \{1,1,0\}; c) \{1,1,1\}.

(a) Model 1
(b) Model 2
Figure 2.8 Distribution of misorientation in nine SVE models.
Figure 2.9 Statistical distribution used for misorientation feature identification: a) actual data; b) generated SVE (model 7).
To understand the effects and sensitivity of each feature used in the SVE formulation, several parametric studies were conducted. The features considered in this study were grain orientation, misorientation (Groeber, 2007; Wang, 2009), principal axis direction, size, aspect ratio, and shape. In order to create an optimal SVE, each feature has to be represented by an appropriate statistical observation. However, this process can be complex and time consuming. In this work, only grain orientation was chosen as a statistical feature because it is a primary factor in single crystal plasticity that results in damage initiation (Asaro, 1977; Hill, 1966; Hochhalter, 2010). Experimental observation has shown that this data is randomly distributed. The remaining features, except misorientation, are geometric features and can be implemented as a constant value based on the average experimental observation. To validate this assumption, a feature study was performed to evaluate the effect of each geometric feature.
The feature data was obtained for a total of 2,127 grains using EBSD scans. To ascertain the effect of each feature, one baseline SVE and five other SVEs, each emphasizing a different feature, were constructed. The baseline SVE (SVE-A), shown in Figure 2.1, was constructed using a representative value for each geometric feature. These values were obtained via random sampling and ordering of grain orientation, resulting in an approximate random misorientation. A change in a single variable from the reference SVE leads to a new SVE. For example, SVE-B was created to investigate the effect of misorientation; therefore, the order of the grains was changed, but their size, shape, aspect ratio, and principal axis direction were held constant. Similarly, the role of SVE-C is to investigate the effect of a change in principal axis direction, while its misorientation is maintained as close as possible to SVE-A. SVE-D considers grain size by increasing the number of grains fourfold while keeping all other factors constant. SVE-E helps to analyze the aspect ratio by increasing the number of columns and reducing the number of rows resulting in a 1:4 aspect ratio. The role of SVE-F is to explore grain shape by modeling a hexagon instead of a square. Figure 2.11 shows the SVE configurations with the numbers indicating particular grain orientations. The grain size shown is not representative of those used in the analysis but instead demonstrates its relative effects. Approximately 100 representative grains of the same size were used, except in SVE-D. The size of the SVE was held constant at 1 mm×1 mm.
Figure 2.11 SVEs constructed for feature study: a) baseline; b) misorientation; c) principal axis direction; d) grain size; e) aspect ratio; f) grain shape. Feature effects could be studied through comparison of results with respect to the baseline.

Each SVE was analyzed by performing a multiscale analysis. A cyclic tensile loading (489 N-4890 N) was used and the local plastic strain energy densities within the SVEs were compared. Figure 2.12 shows the average plastic strain energy density of all six SVEs with respect to time for the first loading cycle. Based on the work by Huang (1992)
and Jiang (2000) it is clear that the damage is influenced greatly by accumulation of plastic strain energy. They have shown that the plastic strain energy increases with loading time and reaches the maximum value at the end of the loading history; therefore, the SVEs were compared at this point. The difference between SVE-A and SVE-C was 2.90% and between SVE-A and SVE-E was 0.01%, shown in Table 2.3. Figure 2.13 shows the local plastic strain energy density fields within each SVE. The distributions of plastic strain energy density in all the SVEs are similar. Additionally, for different SVEs, the maximum local plastic strain energy densities appear at the right edge of the SVE. Some interesting observations can be made from these results. The highest average density appears in SVE-C, but the highest local maximum density appears in SVE-F. The lowest average density appears in SVE-A, but the lowest local maximum density appears in SVE-B. This shows that the plastic strain energy density is variable for different points in the SVE model and that it is a local value. Based on the performed simulations, this implies that the effect of these factors may be a local phenomenon, not a global one. It must be noted that the damage initiation criteria depends on the response of the SVE as a whole and not on the response of a single grain (Horstemeyer and McDowell, 1998; Ghosh, 2011); therefore the overall effect, considering all grains, is more appropriate in life prediction. Based on the results, the average difference in plastic strain energy densities is small when compared to the variability in experimental data, and therefore each feature can be effectively represented by its average value.
Figure 2.12 Variation in average plastic strain energy density vs. time.

a) SVE-A

b) SVE-B

c) SVE-C

d) SVE-D
Figure 2.13 Plastic strain energy density distributions within SVEs: a) baseline; b) misorientation; c) principal axis direction; d) grain size; e) aspect ratio; f) grain shape.

Table 2.3 Summarized SVE Feature Values

<table>
<thead>
<tr>
<th>Features</th>
<th>Misorientation</th>
<th>Principal axis direction</th>
<th>Grain size</th>
<th>Aspect ratio</th>
<th>Grain shape</th>
</tr>
</thead>
<tbody>
<tr>
<td>Average percent difference</td>
<td>1.70%</td>
<td>2.90%</td>
<td>0.30%</td>
<td>0.01%</td>
<td>1.80%</td>
</tr>
</tbody>
</table>

The SVE model is constructed by assembling grains whose features are statistically sampled from pools of measured experimental characterization data. This approach provides a computationally efficient alternative to traditional techniques while maintaining statistical accuracy. The non-statistical parameters, including grain size, shape, aspect ratio, and principal axis direction, were carefully chosen to be representative of the average response of the material. The gain size was chosen to be 0.025 mm$^2$, while the measured average value was 0.0225 mm$^2$. This is to ensure that an exact number of grains fit within a 1 mm by 1 mm square SVE. A rectangular grain shape is used to efficiently assemble the grains within the square SVE. The aspect ratio was chosen to be 0.4, while the average measured value was 0.384, for the same reason as
previously stated. Finally, the principal axis direction was chosen to align with the rolling direction. The final architecture of the SVE can be seen in Figure 2.1(b). As mentioned previously, the orientation was chosen based on the statistical features and as such its distribution was studied.

2.6. Validation of the SVE Model

The RVE model has been applied successfully in similar research work conducted by Luo (2009). Based on Luo’s approach, in this research a comparison is made to validate the SVE model’s capability to represent material properties and mechanical responses with that of an RVE model. In this validation, an RVE model and a SVE model are implemented in the hot spot zone of a lug joint structural model (Figure 2.14). Both two lug joint specimens are cyclically loaded using a sinusoidal waveform with a load range between 489 N and 4890 N (load ratio 0.1) at a rate of 20 Hz. The distributions of strain energy in the hot spot at the maximum loading are shown in Figure 2.15 and Figure 2.16. And the average strain energy density of SVE model and RVE model are compared in Figure 2.17.
a) FEA model with RVE.

b) FEA model with SVE.

Figure 2.14 FEA model with RVE and SVE at the same hot spot
From the results, the distribution of strain energy density in both RVE model and SVE models are similar. The maximum value of strain energy density appears at the same location. Also, the average strain energy density of RVE matches well with that of an SVE model. Thus, it is clear that an SVE model is just as capable of representing material properties and mechanical responses as an RVE model.
Another validation has been implemented to test the effect of SVE on hot spot locations and in far fields. To ensure that SVE is representative of the bulk material and mechanical responses, both measures must remain consistent with or without an SVE implemented in the finite element model. The SVE is expected to have a direct influence on the local fields near the hot spot due to local crystal plasticity effects. Therefore implementation of the SVE model at the hot spot will allow calculation of the damage at the microscale for fatigue life estimation. Figure 2.18 shows comparison of von Mises stress distributions in the lug joint models, with and without an SVE. The overall contours show similar trends, i.e., the implemented SVE has a small effect on the mechanical response outside of the SVE. The hot spot location remains unchanged at the inside corner radius below the loading pins and the magnitude remains approximately the same. The distribution of stress in the far field outside of the hot spot position also remains the same. With the far field value nearly unchanged, the SVE based multiscale modeling technique is proven capable of representing the homogeneous material outside
of the SVE model. Also, the overall mechanical response of the SVE model is almost the same as the bulk material in the same zone. The introduction of SVE model provides the possibility to evaluate damage growth based on statistical material properties at the microscale.

![SVE model](image)

Figure 2.18 Local von Mises stress field distribution within lug joint a) with SVE; b) without SVE.

### 2.7. Summary
Single crystal plasticity was used to capture the crystallographic and geometric effects of grains at the microscale. The results show that the model can capture local anisotropic material behavior at grain level. A subroutine UMAT was introduced to incorporate the single crystal plasticity in the FEA program. Material characterization was implemented to generate an RVE model at the mesoscale. To improve simulation efficiency, a SVE model was developed based on the statistical features of material at the microscale. The SVE captured the statistical distribution of orientation and misorientation while implementing the average response of geometrical features, including grain principal axis direction, size, shape, and aspect ratio. A parametric study was performed to assess the sensitivity of each factor. Principal axis direction and misorientation were determined to be two of the most important features affecting the mechanical response of the constructed SVE. The SVE model was verified through comparative simulations to be capable of representing the bulk material and mechanical responses.
3. Physics Based Damage Evaluation & Validation of Aluminum Alloy 2024-T351

3.1. Introduction

The broad application of metallic materials in many structural components requires a better understanding of metal fatigue mechanisms. An important first step in metal fatigue studies is analyzing the initiation of fatigue cracks, which can be decomposed into two stages: i) nucleation of micro crack and ii) coalescence of micro cracks and formation of a major crack. Previous work has shown that grain orientation significantly influences the slip direction and, as a result, also impacts the nucleation mechanics (Kalnaus, 2006; Groh, 2009; Hochhalter, 2010). Therefore, it can be assumed that fatigue cracks will nucleate in particular slip directions of polycrystalline material at the microscale. To capture this phenomenon, an energy and slip-based damage criterion is developed. It is hypothesized that the micro cracks generated by nucleation grow individually, coalesce together, and result in a serrated major crack, as shown in Figure 3.1 (a). The serrated shape of the major crack also indicates that the major crack consists of a set of micro cracks across its path. By studying growth rates and directions of micro cracks that are governed by slip mechanics and damage accumulations, major crack formation and propagation can be predicted.

In this chapter, a physics based multiscale damage criterion is developed to simulate the initiation of fatigue crack growth, including nucleation of micro cracks and formation of major cracks. The material property and mechanical response of aluminum alloy 2024-
T351 are represented using the developed SVE model. The physics of micro crack nucleation and coalescence is experimentally studied at different length scales and used as the input for the multiscale model. The micro cracks, which are dominated by shear crystallographic slipping, nucleate within intermetallic particles. The coalescence of micro cracks results in the formation of macro crack. The multiscale model and damage criterion are used to predict fatigue crack growth and direction in polycrystalline materials. This damage criterion is developed based on single crystal plasticity, and therefore it only works well in prediction of microstructural small crack growth (Lankford et al., 1984). As overall fatigue life is most influenced by low growth rate behavior, the accelerated and subthreshold extension of small flaws can lead to potentially dangerous over-predictions of life. Relevant lengths of small crack are chosen to take into consideration the crack categories as defined by Ritchie (1986). In Ritchie’s research, it has been shown that crack tip strain fields for large and microstructural small fatigue cracks, driven by nominally equivalent cyclic stress intensities, are qualitatively and quantitatively dissimilar. It is thus observed that small cracks and long cracks at the same nominal driving force can propagate at different growth rates. The microstructural small crack is defined to be less than 10 times of the critical microstructural dimension, which is average grain size for polycrystalline materials (Taylor, 2002). In this research, the average grain area is around 0.0225 mm$^2$ (see Chapter 2). The corresponding grain size (diameter) is 0.1693 mm based on a hypothesis that the grains are considered in circular shape. Therefore the microstructural critical small crack length is taken as 1 mm ~ 2 mm for Al 2024-T351. And the size of the corresponding meso SVE is the same as
the critical major crack size. The developed multiscale fatigue damage criterion is capable of predicting fatigue life and crack direction simultaneously. Three sets of experiments are conducted to validate the multiscale damage criterion: under uniaxial cyclic loading on lug joint specimens, biaxial Fighter Aircraft Loading Standard for Fatigue (FALSTAFF loading on cruciform specimens, and thermal mechanical fatigue (TMF) loading on lug joint specimens.

3.2. **Physical phenomenon of fatigue crack formation**

In this work, aluminum alloy (Al 2024-T351) was chosen as the case study material. From Merati’s study (Merati, 2005), there appeared to be two physically and chemically distinguishable types of intermetallic particles, Al$_7$Cu$_2$Fe ($\beta$-phase) and CuMgAl$_2$ ($S$-phase), in this alloy. Most of the fatigue cracks nucleated at intermetallic particles. And it was concluded that only the iron bearing particles contributed to the crack nucleation process. Microstructure observation using scanning electron microscope (SEM) also verified that micro cracks were incubated from $\beta$-phase particles, shown in Figure 3.1 (b), and grew from intermetallic particles into surrounding grains (see Figure 3.1 (c)). Also, no micro crack nucleation was observed in $S$-phase particles (see Figure 3.1 (d)).

An energy dispersive X-ray microanalysis (EDAX) was conducted to further study the effect of intermetallic particles on micro crack initiation in Al 2024-T351. EDAX is an analytical technique used for the elemental analysis or chemical characterization of materials. It relies on an interaction of some source of X-ray excitation and a sample. The characterization capabilities of EDAX are due in large part to the fundamental principle that each element has a unique atomic structure allowing a unique set of peaks on its X-
ray spectrum (Goldstein, 2003). In this study, a damaged sample of Al 2024-T351 was analyzed using the EDAX technique. A series of intermetallic particles with incubated micro cracks were observed around major cracks, as shown in Figure 3.2 (a). Some of the micro cracks nucleated in intermetallic particles and contributed to the generation of a major crack. Element mappings of Al, Cu, Fe and Mg on the same sample surface are shown in Figure 3.2 (b), (c), (d), and (e), respectively. The highlighted sites in the element mapping represent the elements detected by X-ray. The difference between Al\(_7\)Cu\(_2\)Fe (\(\beta\)-phase) and CuMgAl\(_2\) (S-phase) intermetallic particles are components Fe and Mg. Characterization of intermetallic particles, therefore, can be implemented by a comparison between the element mapping of Fe (Figure 3.2 (d)) and Mg (Figure 3.2 (e)). The same conclusion was verified in element identification using EDAX, namely, that micro cracks were incubated from \(\beta\)-phase (iron-rich) particles.
Figure 3.1 SEM observation of major crack and micro crack nucleation: a) major crack and intermetallic particles in the path; b) micro crack incubation in iron-rich particle; c) micro crack nucleation in iron-rich particles; d) no micro crack nucleation observed in magnesium-rich particles.
Figure 3.2 Element analysis of damaged Al 2024-T351 sample using EDAX technique:
 a) micro crack incubation in intermetallic particles results in major crack growth; b) element mapping of aluminum;  c) element mapping of copper; d) element mapping of iron; e) element mapping of magnesium.

In Merati's study (Merati, 2005), the population density of intermetallic particles was 3,158 particles per mm², and the average particle size was 3.4 µm. Since only iron rich particles were found to contribute to crack nucleation, the EDAX technique was conducted to ascertain population density of iron rich particles (Figure 3.3). The result indicated that the population of Al₇Cu₂Fe particles is 53.2% of all particles. Therefore, the population density of iron rich intermetallic particles is approximately 1,680 per mm². Base on the observed population density, the average spacing between Al₇Cu₂Fe particles is 27.5 µm. This conclusion is based on an assumption that all the particles are evenly distributed and the particle-centered zone is in a circular shape. The average size and spacing of Al₇Cu₂Fe particles were used in the following simulations using the developed SVE model and damage criterion to determine nucleation growth and subsequent coalescence into major cracks. Figure 3.4 shows iron rich intermetallic sites, which are represented by white dots in the SVE model. The rectangular zones with different colors
represent the grain with variable orientations. The intermetallic sites represented by white dots are evenly distributed in the horizontal and vertical direction of SVE model. In the simulation, the damage index to capture the fatigue damage evolution is calculated and used to predict crack growth and direction for each intermetallic site. The rectangular zones with variable colors represent grains with different orientations.

Figure 3.3 EDAX analysis to identify element composition for intermetallic particles.
3.3. Damage criterion for nucleation of micro cracks

In order to study multiscale damage effects, it is necessary to take into account crystal dislocation micromechanics, material microstructure, and macroscale behavior in the continuum description of finite strain plasticity. Taylor (1938) found that crystal dislocation provides an atomistic interpretation of the slip mechanics and strain hardening. His work was followed by many other researchers including Hill (1966) and Asaro (1977). Their work showed that crystal plasticity is important to incorporate micromechanical features of plastic flow into macroscopic analysis. In this research, single crystal plasticity theory is used to describe material behavior in an SVE model based on the several advantages that it has over other techniques.

In this work, micro crack nucleation is governed by a developed damage criterion, which is modified from Jiang’s model (Jiang, 2000). The original damage criterion is as follows:

\[ dD = \frac{\sigma_m}{\sigma_0} - 1 \cdot \left[ 1 + \frac{\sigma_n}{\sigma_f} \right] dY, \]  \hspace{1cm} (3.1)

where,

\[ dY = \beta \sigma_n d\varepsilon^p + \frac{1 - \beta}{2} \sigma_s d\gamma^p. \]  \hspace{1cm} (3.2)

In Equation (3.1) and (3.2), \( dY \) represents the plastic strain energy increment and \( dD \) represents the damage parameter increment in a material plane. \( \sigma_n \) represents the normal stress, and \( \sigma_s \) represents the shear stress on a material plane. The quantities \( \varepsilon^p \) and \( \gamma^p \) represent plastic strains corresponding to \( \sigma_n \) and \( \sigma_s \) respectively. The symbols \( \beta \) and \( m \) are...
are material constants (see Table 3.1). The symbol \( < > \) is the MacCauley bracket (i.e., \( \langle x \rangle = 0.5(x + |x|) \)). The quantity \( \sigma_{mr} \) is a material memory parameter, and \( \sigma_0 \) is the endurance limit of the material and can in essence be considered to be the ‘no-damage’ level of the fatigue parameter. \( \sigma_f \) represents the true fracture stress. More details of this damage model can be found in Jiang’s work (Jiang, 2000).

**Table 3.1 Material parameters for Al 2024-T351 (Luo, 2009; Needs, 1987)**

<table>
<thead>
<tr>
<th>m</th>
<th>( \beta )</th>
<th>( \sigma_0 )</th>
<th>( \sigma_f )</th>
<th>( \gamma )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.5</td>
<td>0.32</td>
<td>220 MPa</td>
<td>950 MPa</td>
<td>2.323 J/m²</td>
</tr>
</tbody>
</table>

Face centered cubic (FCC) crystal structures, such as Al 2024-T351, are of interest in this work; therefore, four slip planes \{1 1 1\} are considered. At the intermetallic particles, where micro cracks tend to nucleate, the four slip planes are representative of probable crack planes. At each intermetallic particle, the crack growth direction can be affected by slip in any combination of the four slip planes, including all. In Jiang’s criterion (Jiang, 2000), the incremental fatigue damage is dependent on the orientation of the material plane. However, since the micro crack can initiate and grow in any of the four slip planes, the critical plane is defined as the material plane where the fatigue damage accumulation first reaches a critical value. In this research, the damage increment will be applied to each of the four material planes for each nucleation point, instead of only one single plane considered in Jiang’s original study. For FCC structures, the angle between any two slip planes is always 70.53° (see Figure 3.5 (a)). In order to accommodate multiple slip planes, the original fatigue damage criteria and plastic strain energy, equations (3.1) and (3.2), are reformulated to include the dependence on multiple slip planes, equations (3.3)
and (3.4). The degree in which the material planes are dependent is taken into account by incorporating a dependent factor, \( \delta \), in Equation (3.4). For example, for two mutually perpendicular material planes, the fatigue damages, described in Equation (3.1), are totally independent. However, if the two material planes have the same orientation, they are dependent and contribute equally to the plastic strain energy (see Figure 3.5 (b)). In this case the slip planes are not independent and the dependent factor is used to quantify the degree of dependence. For two perpendicular planes, of which the cosine value of their interior angle is zero, the dependent factor is defined as one, since the fatigue damages in the two planes are totally independent (see Figure 3.5 (c)). For two planes with the same orientation, of which the cosine value of their interior angle is one, the dependent factor is defined as two, because the fatigue damages are dependent. For this research, the cosine value of the angle between any two slip planes (70.53°) is 1/3, and the total dependent factor for the four material directions is determined to be 4/3 based on a linear fit. The modified fatigue damage criterion, which has been developed to accommodate the polycrystalline plasticity theory, can be described as:

\[
dD_i^{(a)} = \left( \frac{\sigma_{\alpha}}{\sigma_0} - 1 \right) > \left( 1 + \frac{\sigma_{\alpha}^{(a)}}{\sigma_f} \right) dY_i^{(a)} \\
\]

\[
dY_i^{(a)} = \frac{1}{\delta} \left[ \beta \sigma_{\alpha}^{(a)} (d\varepsilon)^{(a)} + 1 - \frac{\beta}{2} \sigma_{\alpha}^{(a)} (d\gamma_p)^{(a)} \right] \\
\]

where, \( dD_i^{(a)} \) represents the damage increment in the \( a \)th slip plane of the \( i \)th intermetallic particle, the dependent factor \( \delta \) can be calculated using Equation (3.5):

\[
\delta = 1 + (2 - 1) \cdot \frac{\cos(\theta) - \cos(90^\circ)}{\cos(0) - \cos(90^\circ)} \\
\]

58
The “1” and “2” on the right hand side of Equation (3.5) represent the dependent factor for 90° and 0, respectively; θ represents the angle between two slip planes, which is 70.53°. Using this linear fit calculation described by Equation (3.5), the dependent factor δ for FCC structure is 4/3 (when θ=70.53°).

Figure 3.5 a) slip planes in FCC unit cell; b) two perpendicular material planes which are totally independent; c) two parallel material planes which are totally dependent; d) two material planes with an arbitrary degree which are partly dependent.

In Luo’s work (Luo, 2010), an assumption is made that the cumulative damage due to plastic deformation in the meso RVE should be greater than the minimum energy for...
creating two free surfaces of a crack. This assumption was used to estimate the crack growth using the accumulated damage. For aluminum, the surface energy density \( \gamma \) that corresponds to the energy variation per unit area due to the creation of surface at room temperature is 2.323 J/m\(^2\) (Needs, 1987). In order to initiate a crack, the minimum energy required should be \( 2 \times \gamma \times L \), where 2 indicates that there are two free surfaces for one crack, and \( L \) is the crack length. So there is a link between the fatigue damage \( D \) and the crack length \( L \):

\[
DA = 2\gamma L. \tag{3.6}
\]

So the modified incremental micro crack length for intermetallic particles could be described as:

\[
dL_{i}^{(a)} = \frac{dD_{i}^{(a)} A}{2\gamma} \tag{3.7}
\]

In Equation (3.7), symbol \( A \) represents the plastic zone size around the nucleation points. Using the von Mises yield criterion (Guerra-Rosa, 1984), the plastic zone in plane stress state as a function of \( \omega \) is described in Equation (3.8) as,

\[
r_{p}^{\theta} = \frac{K_{i}^{2}}{4\pi\sigma_{ys}^{2}} (1 + \frac{3}{2} \sin^{2} \omega + \cos \omega) \tag{3.8}
\]

The corresponding plastic zone size can be derived using integral calculus and can be expressed as:

\[
A \approx 0.0765 \cdot \frac{K_{i}^{4}}{\sigma_{ys}^{4}} \tag{3.9}
\]

Since the stress states in nucleation points vary, the plastic zone size is different for different nucleation points. Finite element simulation has been used to determine the
plastic zone size. A 2-D finite element model with 29,230 CPS4 elements is generated. In this model, a small crack with the initial length, 1 μm, is embedded at the center of an square Aluminum plate. The material property is assumed as isotropic and homogeneous. Part of the model is shown in Figure 3.6. Static tensile load is applied on the edges of the plate and perpendicular to the crack surface. This model is used to calculate the plastic zone size for different stress states. The results show that the plastic zone size in finite element method simulation (see Figure 3.6) matches very well with the theoretical value, which is given in Equation (3.9).

![Figure 3.6 Plastic zone around the micro crack.](image)

Critical reserved shear stress (CRSS) is an important material parameter, and is applied as a critical criterion in governing slip (Stoller, 2000). CRSS is the component of shear stress, resolved in the direction of slip, necessary to initiate slip in a grain. It is a constant for a given crystal. The ease of slip on different crystal systems is usually quantified by the CRSS, which is measured in stage I deformation on unconstrained single-crystal specimens where a unique slip system is activated. Therefore Equation
(3.7), which is used to describe the relation between the incremental micro crack length and the incremental damage index, is available only when the shear stress in the slip direction is greater than the CRSS value.

Figure 3.7 shows the result of one simulation. In this simulation case, a finite element model of the lug joint specimen is constructed. A SVE model is embedded at a structural hot spot to capture the damage. Finite element meshes are used to model the remaining parts of the component. The lug joint specimen is force controlled cyclically loaded using a sinusoidal waveform with a load range between 489 N and 4890 N (load ratio 0.1) at a rate of 20 Hz. The incremental growth of the micro crack length as a function of time for the three nucleation points (N1, N2, and N3) in each of the four slip planes (slip1, slip2, slip3 and slip4) are calculated. In this case, micro cracks increase in length only in slip plane 1 for nucleation point N1 (the black line) and slip plane 3 for nucleation point N3 (the brown line). In the other 10 slip planes of the three nucleation points, the micro crack does not increase in length because the shear stress in the slip plane fails to reach the CRSS value so there is no damage increment. Furthermore, in the nucleation directions mentioned above, the micro crack length increases steadily, cycle by cycle. This conclusion provides a basis to use a linear fit to extrapolate the micro crack length increment versus time. Finally, the growth of a micro crack will stop when it reaches a critical value, 27.5 µm, which is the average length of spacing between neighboring intermetallic particles. The corresponding physical phenomenon is that the intermetallic particles have effects in both nucleation and obstruction of micro crack growth. In other
words, the micro crack starts from one intermetallic particle and ends in another
intermetallic particle.

![Micro crack diagram](image)

Figure 3.7 Micro crack length increase cycle by cycle in slip directions.

3.4. **Damage criterion for coalescence of micro cracks**

In order to model coalescence of micro cracks and the formation of major crack, a
hypothesis is presented in this section. First, the micro cracks in the nucleation points are
projected in an arbitrary direction. Then, the major crack orientation is assumed to be in
the direction in which the sum of length projections of the micro cracks increases at the
highest rate. As shown in Figure 3.8, the micro cracks $AB$, $BC$, $CD$, etc. are projected in
the direction of the arrow line. The corresponding length projections are $A'B', B'C'$, $C'D'$,
etc., respectively. The major crack length is therefore the sum of the
projections $A'B'$, $B'C'$, $C'D'$, etc. in the prescribed arrow line direction $\overrightarrow{A'H'}$. Therefore,
the major crack is calculated in Equation (3.10):
\[ L_{\text{total}} = \sum_{i=1}^{n} \sum_{\alpha=1}^{4} \left| L_{i}^{(\alpha)} \cos(\theta - \varphi_{i}^{(\alpha)}) \right| \quad (3.10) \]

where, \( \varphi_{i}^{(\alpha)} \) is the direction of the \( i^{\text{th}} \) slip plane in \( \alpha^{\text{th}} \) nucleation point, corresponding to the micro crack length \( L_{i}^{(\alpha)} \). \( \theta \) is the prescribed direction for micro crack projection, which is assumed to be the probable major crack direction. The range of \( \theta \) is from \(-\pi/2\) to \( \pi/2 \) because the crack grows on two opposite sides of the nucleation point and combines in the middle to form a single crack. Therefore, the crack is represented by a line, described by only an angle, as opposed to a vector. By solving for the maximum value of, \( L_{\text{total}} \) which is a function of \( \theta \), the major crack direction \( \theta \) and the corresponding major crack length \( L_{\text{total}} \) could be calculated.

Figure 3.8  Schematic procedure of projection of micro cracks to major crack.

3.5. **Damage criterion for crack formation in thermal mechanical fatigue**

Crack initiation and propagation due to TMF loading is one of the major causes of failure and leads to damage and degradation in aerospace components. TMF loading is the overlay of a cyclical mechanical loading, which leads to fatigue of a material, with a cyclical thermal loading. Fatigue damage is primarily due to cyclic creep caused by vibration loading and temperature cycling. In this research, plastic deformation refers to
that occurring over almost an instantaneous time scale due to dislocation slip; creep deformations refer to those occurring over longer time scales due to diffusion-assisted mechanisms such as grain boundary sliding, dislocation glide/climb, and mass transport through the grain boundary. Furthermore, there are interactions between vibration and temperature damage accumulation rates due to temperature dependent changes in material properties.

A varying temperature condition was generated to simulate a TMF loading case. The temperature range of thermal cycling is between 100 °C and 200 °C. One thermal fatigue cycle takes 60 minutes. It takes 20 minutes to increase the temperature from 100 °C to 200 °C at a linear heating rate. Then the temperature is held at 200 °C for 10 minutes and then decreased to 100 °C in 20 minutes in a linear cooling rate. The value of the linear heating rate in the temperature increasing stage is equal to the linear cooling rate in the temperature decreasing stage. Finally, the temperature is held at 100 °C for 10 minutes, after which the next thermal cycle starts. The variation of temperature in one complete thermal cycle is shown in Figure 3.9. Compared with thermal cycling, the frequency of mechanical fatigue is much higher, which is 20 Hz (see Figure 3.10). The time for one thermal cycle is 72,000 times of that for one mechanical cycle. Therefore, in the temperature increasing/decreasing stages, the change in temperature is only 0.083 °C through one mechanical cycle, which is 0.05 second. There is little effect on the mechanical response and damage evolution of the material from the temperature difference in one mechanical cycle. So the temperature is assumed to remain constant.
during one fatigue cycle. The temperature is selected to be the averaged value in the simulation.

Figure 3.9 Variable temperature condition for thermal mechanical fatigue tests.

Figure 3.10 Variable mechanical load condition for thermal mechanical fatigue tests.
The thermal effects on damage evolution include mechanical responses (thermal creep, elastic modulus and yield strength etc.) and material properties (thermal expansion factor, density etc.). Generally speaking, temperature will change the dislocation motion, which plays a critical role in determining the inelastic behavior of a metal and its flow stress under different load conditions. To deform a metal beyond the elastic limit means to activate and move its dislocations through the crystal. The approach in this section will lead to an improved understanding of the fatigue damage characteristics under varying temperatures. The damage criterion will be taking into account thermal effect and will be modified to capture crack growth in a TMF load.

In the subroutine UMAT introduced in chapter 2, a power law is used to describe the strain rate in the flow rule to calculate the slip increment in polycrystal elastoplasticity, as shown in equations (2.15), (2.16) and (2.17). The relation between shear strain rate and shear stress (Harper, 1957) can also be described in the form of the power law in Equation (3.11):

$$\dot{\gamma} = A_0 \cdot \tau^n$$  \hspace{1cm} (3.11)

To apply the SVE model and damage criteria to thermal fatigue issues, the Harper–Dorn creep model is used, where the grain boundary sliding effect and diffusional flow theory are considered (Harpor, 1957; Kloc, 1977; Ruano, 1988; Wang, 1996; Langdon, 2002). The relation between the applied stress and the steady-state creep rate for Harper–Dorn creep is phenomenologically described by:
\[ \dot{\gamma} = \frac{A \cdot D \cdot G \cdot b}{k \cdot T} \cdot \left(\frac{\tau}{G}\right)^n \]  

(3.12)

where \( D \) is the diffusion coefficient for lattice self-diffusion, \( G \) is the shear modulus, \( b \) is the Burgers vector, \( k \) is Boltzmann’s constant, \( T \) is the absolute temperature, \( \tau \) is the applied shear stress, and \( A \) is a dimensionless constant of the order of \( 10^{-11} \). The parameters for this material can be found in Table 3.2. In Equation (3.12), the diffusion parameter \( D \) is dependent on temperature and can be expressed as:

\[ D = D_0 \cdot \text{Exp}\left(-\frac{Q}{R \cdot T}\right) \]  

(3.13)

Then taking into account temperature effect on creep, a temperature dependent term, \( \exp\left(-\frac{Q}{R \cdot T}\right) \), is added in Equation (3.12), where \( Q \) is the activation energy and \( R \) is the gas constant. \( A_s \) is material constant, which can be calculated by comparing Equation (3.12) and Equation (3.13) at room temperature (Wilshire, 2008; Warren, 2006; Syed, 2004; Clech, 2004).

\[ \dot{\gamma} = A_s \cdot \left(\frac{\tau}{G}\right)^n \cdot \exp\left(-\frac{Q}{R \cdot T}\right) \]  

(3.14)

Other material properties, such as Young’s modulus, yield strength, and CRSS are also dependent on temperature and should be modified in the TMF model. The temperature dependent Young’s modulus of Al 2024-T351 can be found in Gibson’s work (Gibson, 1997). An increase in temperature expands the crystal lattice, reduces the stiffness of the bonds, and therefore, causes a drop in the modulus. The temperature dependence is well approximated in a linear fit:

\[ E = E_0 \cdot \left(1 - \alpha_m \cdot \frac{T}{T_m}\right) \]  

(3.15)
where $E_0$ is the value of the modulus at absolute zero temperature, $T_m$ is the melting temperature and $\alpha_m$ is a constant, of which the value is close to 0.5, meaning that the modulus drops by a factor of about 2 in the temperature interval between absolute zero and the melting point.
Table 3.2 Creep dependent parameters for Al 2024 (Kassner, 2007; KLOC, 1997; Yavari, 1982)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>A: Dimensionless constant</td>
<td>3.5E-11</td>
</tr>
<tr>
<td>D: Diffusion coefficient</td>
<td>1.86E-4</td>
</tr>
<tr>
<td>R: Gas constant</td>
<td>8.314 Jmol⁻¹K⁻¹</td>
</tr>
<tr>
<td>Q: Activation energy</td>
<td>143.4 kJ/mol</td>
</tr>
<tr>
<td>G: Shear modulus</td>
<td>3.022E4-16×T MPa</td>
</tr>
<tr>
<td>b: Burgers vector</td>
<td>2.86E-10 m</td>
</tr>
<tr>
<td>k: Boltzmann constant</td>
<td>1.381 × 10⁻²³ JK⁻¹</td>
</tr>
<tr>
<td>n: Stress exponent</td>
<td>3</td>
</tr>
</tbody>
</table>

The yield strength decreases with increasing temperature for Al 2024 T 351 (Gibson, 1997). On a microscopic scale, thermal energy activates dislocations and causes them to move a little more easily; this imparts a temperature dependence to the yield strength. Kinetic models (Kocks, 1975) lead to equations for yield by thermal plasticity, which simplify to a form:

\[
\tau_{ys} = \frac{G_s}{G_s^0} \cdot \tau_{ys}^0 \cdot (1 - \frac{A \cdot T}{T_m} \ln \frac{\dot{\gamma}_{0s}}{\dot{\gamma}})
\]  

(3.16)

where \( \tau_{ys}^0 \) is the yield strength at absolute zero temperature, \( A \) is a constant of general order of 0.04, and \( \dot{\gamma}_{0s} \) is a kinetic constant of about \( 10^6 \) /s. The equation summarizes the experimental observations, namely, at near room temperature, the yield strength...
decreases linearly with increasing temperature, and logarithmically with decreasing strain rate.

When a single crystal specimen is loaded, the applied stress is resolved on the slip planes in the material at grain level. The resolved shear stress, $\tau_s$ on any given plane is determined by the angle between the plane normal and the applied stress direction. Yielding occurs as a result of dislocation slip when the resolved shear stress on one of the planes exceeds a critical value. The relationship between applied stress and resolved shear stress is the same in a polycrystalline material, but is complicated by the fact that maximum resolved shear stress will vary from one grain to another. In addition, material compatibility and continuity act to limit the deformation of any one grain that may be favorably oriented for slip. By applying a simple compatibility criterion and assuming that all the grains in the material deformed uniformly, Taylor (1938) derived a relationship between yield strength and the resolved shear stress in polycrystalline material. Such an analysis amounts to determining an effective average reciprocal Schmid factor for the polycrystalline material. The average value obtained by Taylor for FCC aluminum was about 3.06 and has since been termed the Taylor factor (Stoller, 2000). Therefore, the temperature dependent CRSS can be calculated by temperature dependent yield strength:

$$CRSS = \frac{1}{m \tau_{ss}} \quad (3.17)$$
where $m$ is the Taylor factor, with a value of 3.06. For aluminum alloys, the yield strength, which is a temperature dependent material property, decreases with increasing temperature (Lipski, 2012).

The thermal expansion factor of Al 2024-T351 increases with increasing temperature, a phenomenon studied by Fridman (Fridman, 1975), and as shown in Table 3.3. In the temperature range between 100 °C and 200 °C, the change of the thermal expansion factor is around $2 \times 10^{-6}/^\circ$C. Also, in this approach, the mechanical load is force control instead of displacement control. So the thermal expansion has little effect on stress distribution and damage evaluation, and is ignored in the TMF model.

Table 3.3 Thermal expansion factor of Al 2024-T351 (Fridman, 1975).

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>20</th>
<th>77</th>
<th>127</th>
<th>227</th>
<th>327</th>
<th>427</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermal Expansion ($10^{-6}/^\circ$C)</td>
<td>23.0</td>
<td>24.1</td>
<td>24.9</td>
<td>26.5</td>
<td>28.2</td>
<td>30.4</td>
</tr>
</tbody>
</table>

Based on the thermal effects discussed above, the damage criterion will be modified to capture damage accumulation under variable temperature. All the temperature dependent factors (Young’s modulus, yield strength and CRSS) were updated in the subroutine UMAT. In this simulation, a finite element model of the lug joint specimen is constructed. A SVE model is embedded at a structural hot spot to capture the damage. Finite element meshes are used to model the remaining parts of the component. Comparison between different working temperatures is constructed to study the thermal effect on damage evolution. The material for the specimen is Al 2024-T351. The lug joint specimen is cyclically loaded using a sinusoidal waveform with a load range between 489
N and 4890 N (force control, load ratio 0.1) at a rate of 20 Hz. The simulation results are shown in Figure 3.11. The damage accumulation in ten cycles at room temperature and 200 °C are shown in Figure 3.11 (a) and (b), respectively. The result shows that the damage will increase with increasing temperature.

![Figure 3.11 Distribution of damage accumulation in slip system {1 1 1} <1 1 0> at (a) room temperature and (b) 200°C.](image)

3.6. Simulation Result and Experimental Validation

To validate the SVE model and the physics based damage criterion, a series of experiments were conducted, including uniaxial cyclic loading on lug joint specimens and biaxial FALSTAFF loading on cruciform specimens. The simulations were conducted using the same properties and conditions as the experiment. The SVE models were constructed in the hot spots where there is high stress concentration to be able to capture the damage accumulation.

3.6.1. Case 1: Uniaxial Cyclic Loading on Lug Joint Specimens

A uniaxial fatigue test on lug joint specimens was conducted to validate the prediction capabilities of fatigue crack growth of the SVE model and the damage
criterion. Lug joint specimens were machined from a bulk Al 2024-T351 plate with the rolling direction lengthwise along the lug joint (see Figure 3.12b). The specimens were cyclically loaded in a servo hydraulic desktop test frame using a sinusoidal waveform with a load range between 489 N and 4890 N (load ratio 0.1) at a rate of 20 Hz. MTS Bionix 370.02 test frame (with the maximum loading capability 22.2 kN) was used to conduct the fatigue test (Figure 3.13). To validate the multiscale model, the number of cycles necessary to achieve a 1 mm crack was obtained experimentally and a total of five specimens were tested. The experimental results are summarized in Table 3.4. A final image at failure of one specimen illustrating the crack angle is shown in Figure 3.12 (a). The mean deviation for the number of cycles to produce a 1 mm crack was in the range from 68 K to 98 K cycles. Among the five tests, there are two tendentious crack directions: around -4º (specimens 1 and 2) and -28º (specimens 3, 4 and 5). The reasons that there is no single probable crack direction include the effect of the microstructural polycrystalline, geometry of specimen, loading condition, and stress distribution in the hot spot.
Figure 3.12 Lug joint specimen for fatigue test: a) crack initiates in the shoulder of lug joint and b) geometric dimension.
Figure 3.13 Experimental test frame for fatigue loading (MTS Bionix 370.02).

<table>
<thead>
<tr>
<th>Sample</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fatigue life (No. of cycles)</td>
<td>92K</td>
<td>98K</td>
<td>68K</td>
<td>83K</td>
<td>82K</td>
</tr>
<tr>
<td>Crack direction (degrees)</td>
<td>-4</td>
<td>-4</td>
<td>-29</td>
<td>-28</td>
<td>-28</td>
</tr>
</tbody>
</table>

Table 3.4 Experimental results of fatigue life and crack direction

For the numerical simulation, a widely used commercial finite element software ABAQUS and a subroutine UMAT that implements single crystal plasticity and the energy based damage criterion were used. A finite element model of the lug joint specimen was constructed using: (i) SVE of the microstructure, which is explicitly modeled and meshed at a structural hot spot; and (ii) finite element mesh of the remaining parts of the component (Figure 3.14). This avoids the need for homogenization/localization schemes to connect the two length scales. The microscale bridges to the mesoscale through the subroutine UMAT governing the stress-strain
response of an element within the SVE. This multiscale model is applied to solve the problem of efficiently predicting crack initiation and direction within the component. Three simulation test cases were constructed with different SVE models based on the statistical orientation pool. Figure 3.15 shows the most probable major crack direction and corresponding increment of crack length per loading cycle. Results of fatigue cycles prediction to reach 1 mm crack length and probable crack directions are shown in Table 3.5.

Figure 3.14 Boundary conditions and implementation of a two-scale mesh at the structural hot spot of an aluminum lug joint.
The fatigue life prediction and the estimated crack direction are both within the same order of magnitude compared with the experimental results. The average fatigue life to reach 1 mm crack is 84.6K cycles for the experiment and 79.8K cycles for the simulation. The error of fatigue life prediction is about 5.7%. From the experimental results, two probable crack directions, approximately -4° and -28°, are found. And the estimated crack direction is around -2° and -32°. The error of crack direction between experiment and simulation is less than four degrees. The results indicate that the multiscale damage
model can successfully capture the fatigue crack growth and direction and is expected to provide good estimates of fatigue life of Al 2024-T351.

The error in fatigue life prediction can be attributed to several possible factors. First, one possible reason is that the magnitude of the surface energy density (in Equation 3.7) of a bulk homogenized material is most likely not the same as that within a grain. As a result, a difference between local information in grains and average global information in SVE is expected. Second, the micro crack nucleates and grows first in grains, of which the growth rate of damage accumulation in the slip directions is relatively higher. Loading conditions vary across different positions of the structural component. The same grain orientation under different loading conditions shows significantly different sensitivities. The stochasticity in grain orientation distribution in both actual specimens and SVE models is another reason for the difference. Finally, in the simulation, the material property corresponds to an ideal and healthy state. There are no flaws and voids in the modeling before loading. Also the intermetallic particles are constructed with the same size, and arranged in the SVE model with the same spacing distance. So the presence of defects, flaws, and large intermetallic particles in the real material will affect the fatigue life.

**3.6.2. Case 2: Biaxial FALSTAFF Loading on Cruciform Specimens**

FALSTAFF loading typically occurs at the wing root area of a fighter-type aircraft. For this reason, it has been widely used in numerous fatigue research programs (Schijve, 2004). A modified block of FALSTAFF loading, including 79 cycles, is used as shown in Figure 3.16. To approach the fatigue crack initiation and growth under biaxial
FALSTAFF loading, the root mean square method (RMS) is introduced to simplify the complex loading history. In previous studies, the RMS model was shown to be a simple, reliable, and efficient method to approach random loading (Kim 2006).

Figure 3.16 FALSTAFF loading (79 cycles)

In previous study by Mohanty (2010), cruciform specimens were subjected to biaxial fatigue loading. The cruciform specimens were machined from a bulk Al 2024-T351 plate with the rolling direction along one symmetrical axis. The specimens were cyclically loaded under force controlled biaxial FALSTAFF loading with a frequency of 20 Hz. The loading is shown in Figure 3.16. An example of the cruciform specimen is shown in Figure 3.17. The area of the center span is 62.66 mm by 62.66 mm, and the thickness is 2.54 mm. The diameter of the center hole is 6.35 mm. A 1 mm width notch was introduced at the center hole along a 45° angle with respect to the vertical direction. Since there is high stress concentration at the tip of the notch, the probability of crack
Initiation is greatly increased, therefore creating a structural hot spot. Following this observation, the SVE model is embedded in the hot spot location of the cruciform. The length of the notch is 1.5 mm. Therefore the SVE size is designed to be $3 \text{ mm} \times 3 \text{ mm}$ to cover the whole length of the notch. The notch tip is almost at the center of the SVE model.
Figure 3.17 Cruciform specimen: a) a round hole in center for test; b) a 45° notch at the center hole for fatigue test; c) geometric dimension of cruciform; d) geometric dimension of the center.

Before conducting the fatigue life prediction simulation, validation of mechanical and damage responses were performed to ensure the RMS model could be used to accurately represent the FALSTAFF loading. The RMS method, which is also known as the quadratic mean method, is a statistical measure of the magnitude of a varying quantity. It can be calculated for a series of discrete values. In this approach, there are 79 sinusoids cycles in one block of FALSTAFF loading (see Figure 3.16). So there are 79 maximum and 79 minimum loading values, which can be used to represent the variability of the loading. The RMS model is used to simplify the complex loading history. The RMS values for the 79 maximum loading values and the 79 minimum loading values are calculated respectively. The tests were assumed to be under constant amplitude loading. The following relationships are used to obtain the RMS loadings:

\[
\text{Load}_{\text{max}, \text{rms}} = \left[ \frac{1}{N} \sum_{i=1}^{N} (\text{Load}_{\text{max}, i}) 2^{-1/2} \right]^{1/2}
\]

\[
\text{Load}_{\text{min}, \text{rms}} = \left[ \frac{1}{N} \sum_{i=1}^{N} (\text{Load}_{\text{min}, i}) 2^{-1/2} \right]^{1/2}
\]

Using Equations (3.17) and (3.18), the complex FALSTAFF loading is converted into a simplified loading condition based on the RMS model, as shown in Figure 3.18.
In a previous study on damage criteria, the fatigue damage was determined to be significantly dependent on the plastic strain energy (Jiang, 2000; Luo, 2011). Therefore, the accumulation of plastic strain energy density can be used as an important criterion to validate the RMS model. For comparison, two simulations were conducted with the same cruciform finite element model, but under two different loading conditions, i.e., FALSTAFF and RMS loading.

The distributions of plastic strain energy density after 79 loading cycles is shown in Figure 3.19. The square blocks represent the SVE area. From this result, the plastic strain energy shows similar distributions for FALSTAFF and RMS loadings. This indicates that RMS methods can provide a good representation of local damage accumulation. Furthermore, the average value of plastic strain energy density is another index to
measure the total response to damage accumulation. The accumulated average plastic strain energy density within the SVE model during 79 cycles (one repeating block) for FALSTAFF and RMS loading are shown in Figure 3.20. The FALSTAFF and RMS models show a linear increase of plastic strain energy accumulation. After 79 loading cycles, the average plastic strain energy density is 32.59 MPa for FALSTAFF and 32.87 MPa for the RMS model. The difference between FALSTAFF and the corresponding RMS model is only 0.85%. Therefore, the RMS model can be used to simply and accurately represent the complex loading case.

Figure 3.19 Distribution of plastic strain energy density in a) RMS model after 79 cycles; b) FALSTAFF model after 79 cycles
A series of experiments of biaxial FALSTAFF loading on cruciform specimens were conducted using an MTS biaxial tension-torsion test system (with the maximum loading capability 97.9 kN) as shown in Figure 3.21. The cruciform specimens were machined from a bulk Al 2024-T351 plate with the rolling direction along one symmetrical axis. The specimens were cyclically loaded under biaxial FALSTAFF loading with a frequency of 20 Hz. To validate the multiscale model, the number of cycles necessary to achieve a 3 mm crack was obtained experimentally. A total of four specimens were tested (see Figure 3.22). The crack generated from the notch tip, which was oriented at 45º from the loading direction. The experimental results are summarized in Table 3.6 (Mohanty, 2010). The average cycle number to produce a 3 mm crack was 42.0K cycles, and the mean crack direction was 58.8º.
Table 3.6 Experimental results of fatigue life and crack direction (Mohanty, 2010)

<table>
<thead>
<tr>
<th>Sample</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>Average</th>
</tr>
</thead>
<tbody>
<tr>
<td>Crack direction (degrees)</td>
<td>57</td>
<td>56</td>
<td>56</td>
<td>66</td>
<td>58.8</td>
</tr>
<tr>
<td>Average fatigue life (No. of cycles)</td>
<td>42.0K</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
The simulations were conducted using the same properties and conditions as the experiment. Three simulation models with individually generated SVE models were implemented. The SVE model (3 mm × 3 mm) was placed at the notch tip as shown in Figure 3.23. The fatigue life prediction to reach a 3 mm crack (same size as SVE length) and respective crack directions are listed in Table 3.7. Compared with the experimental results, the accuracy of fatigue life prediction is 9.8% and the accuracy of probable crack direction prediction is 9.2°.
Figure 3.23 Loading conditions and implementation of SVE model at the structural notch tip of an Al 2024-T351 cruciform.

Table 3.7 Fatigue cycles prediction to reach a 3 mm crack and corresponding direction

<table>
<thead>
<tr>
<th>Model</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>Average</th>
</tr>
</thead>
<tbody>
<tr>
<td>Probable crack direction (degrees)</td>
<td>76</td>
<td>75</td>
<td>52</td>
<td>68</td>
</tr>
<tr>
<td>Fatigue life (No. of cycles)</td>
<td>25.0K</td>
<td>47.0K</td>
<td>66.3K</td>
<td>46.1K</td>
</tr>
</tbody>
</table>

There are also several additional possible factors for errors in biaxial FALSTAFF experiments. First, the RMS model is introduced in the analysis to simplify the loading condition. Although the validation of the RMS model shows the difference from FALSTAFF loading condition as being only 0.85%, loading history can also affect the fatigue life and crack direction, especially in the context of the high loading points in the FALSTAFF model. Also, the pre-implemented notch in the middle circle can be considered to be an existing major crack, which leads to higher stress and damage concentration in the hot spot. In addition to the nucleation and coalescence of micro
cracks inside materials, there is also the macro crack propagation effect at the notch in the hot spot. So, the final crack can also be attributed to the major crack propagation effect. This observation can also explain why the accuracy in case 2 is lower than in case 1.

3.6.3. Case 3: TMF Loading on Lug Joint Specimens

In the TMF test, a lug joint specimen having the same dimension and material as in case 1 was used. The experiments here were conducted under simultaneous mechanical loading and thermal cycling (see Figure 3.9 and Figure 3.10). The specimens were cyclically loaded using a sinusoidal waveform with a load range between 489 N and 4890 N (load ratio 0.1) at a rate of 20 Hz. It takes one hour for one temperature cycle, and the fatigue frequency is much higher than thermal frequency. So the temperature is considered to be constant in each fatigue cycle. To validate the multiscale model, the number of cycles necessary to achieve a 1 mm crack was obtained experimentally.

In order to get material properties including Young’s modulus and a yield strength of Al 2024-T351 from the experiments, a series of tensile tests under different temperatures were conducted. The dog bone specimen was designed and used in the thermal tensile test. The dimension of the dog bone specimen is shown in Figure 3.24(a). The temperatures in the tensile tests are room temperature, 100 °C, 150 °C, 200 °C and 250 °C. All the final cracks take place in the middle of the specimens (see Figure 3.24(b)). The thermal tensile test was conducted using the Instron material test frame 985 with a thermal chamber (see Figure 3.25).
Figure 3.24  Dog bone specimen for tensile test at different temperatures: a) geometric dimension and b) crack takes place in the middle of dog bone specimen.
Figure 3.25 Instron material test frame 985 with thermal chamber.

The stress-strain curves of the tensile tests as shown in Figure 3.26, show that the yield strength decreases with increasing temperature. The CRSS can be calculated based on yield strength using Equation 3.16. The CRSS decreases with increasing temperature as well. The Young’s modulus decreases slightly with increasing temperature. In the TMF test, the temperature range is between 100 °C and 200 °C. The related material properties in this temperature range are listed in Table 3.8. The material properties in other temperatures are calculated using the linear interpolation method.
Taking into account the variable temperature conditions in the TMF test (see Figure 3.9), three damage models are used to solve this thermal mechanical fatigue case: I) cycled loading in 100°C, II) cycled loading in 200°C and III) cycled loading in the temperature varying between 100°C and 200°C. For the two constant temperature conditions, the damage increment and crack growth rate governing the function in Equations (3.3) and (3.6) can be used directly based on temperature dependent material properties (i.e., Young’s modulus, yield strength, CRSS, and creep parameters). The crack coalescence criterion described in Equation (3.9) can be used directly as well. For the
variation temperature stages (between 100 °C and 200 °C), a set of temperature dependent models were applied under different temperatures, respectively. The weight averaged method was used to get the comprehensive effect in one thermal cycle, as shown in Equation (3.19):

\[ L = \frac{L_1 t_1 + L_2 t_2 + L_3 t_3}{t_1 + t_2 + t_3} \]  (3.19)

where \( L \) is the comprehensive crack growth rate, \( L_1, L_2 \) and \( L_3 \) are crack growth rates at stage 1 (100°C), stage 2 (100°C - 200°C), and stage 3 (200°C), respectively. \( t_1, t_2 \) and \( t_3 \) are weight factors, which are equal to the time length of stage 1, stage 2, and stage 3, respectively.

The crack growth rates in different stages are listed in Table 3.9. It shows that the crack grows faster at higher temperatures. The time lengths of the three different stages are used as weight factors to calculate the average crack growth rate in one block (one hour). The simulation result shows that the predicted fatigue life is 67.6K cycles to form a 1mm crack. Thermal mechanical fatigue tests were conducted and the average fatigue life was seen to be 62.4K cycles. The error between simulation and experiment is 7.7%. The simulation result shows a good match with the experimental results.

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Time in one thermal cycle (min)</th>
<th>Crack growth rate (mm/cycle)</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>10</td>
<td>5.03E-10</td>
</tr>
<tr>
<td>100 - 200</td>
<td>40</td>
<td>5.92E-10</td>
</tr>
<tr>
<td>200</td>
<td>10</td>
<td>6.79E-10</td>
</tr>
</tbody>
</table>
Compared with the fatigue test conducted under room temperature, some material properties needed to be updated in the TMF test, which resulted in temperature dependent damage accumulation. However, the damage indexes in the 12 slip systems are changed proportionally and in the same ratio. Therefore, it can be concluded that the temperature only affects the crack growth rate, but not the crack direction, which is determined by equation (3.9). For the TMF test, the estimated crack direction is the same as case 1, which is around -2° and -32°. From the experimental results (see Figure 3.27), two cracks grow simultaneously at the shoulders of the lug joint specimen. The averaged crack direction in the experiment is -29°. The error in crack direction between experiment and simulation is 3 degrees. The results indicate that the thermal fatigue damage model can capture the thermo-mechanical fatigue crack growth.

Figure 3.27 Crack initiation takes place in shoulders of lug joint specimen in TMF test.

3.7. Summary
In this chapter, a physics and slip based multiscale damage criterion is developed to predict fatigue life and crack direction in aluminum alloy based complex components. Three different length scales are considered in this study. At the microscale, a damage criterion based on single crystal plasticity theory is developed to approach micro crack nucleation, which occurs in iron-rich intermetallic particles and grows into the surrounding grains. At the mesoscale, a computationally efficient SVE model is constructed to represent material property and mechanical response in the hot spot. The fatigue life and corresponding crack direction are predicted by the simulation. At the macroscale, a finite element analysis of components (lug joint and cruciform specimens) is conducted with the meso SVE bridging two-scale meshes. Results indicate that the physics based damage criterion is capable of capturing nucleation and coalescence of micro cracks in different scales. It also provides the possibility of bridging energy-based damage in intermetallic particles and crack initiation in structural components. Compared with a conventional RVE model, the SVE model significantly improves the preprocessing efficiency as well as computational efficiency through reduced number of meshes. The temperature dependent creep effect on the slip mechanism is also considered. The power law that is used to describe the strain rate in the flow rule to calculate the slip increment in the subroutine UMAT is modified to solve the thermal mechanical fatigue problem. The simulation results from the developed multiscale damage criterion show good correlation with the experimental results while ensuring computational efficiency. The results show that the multiscale damage criterion can successfully capture crack initiation and predict fatigue life.
4. Development of Spring-bead Based Network Model to Simulate a Self-sensing Polymeric Material Response

4.1. Background

Mechanically sensitive mechanophores are covalently linked into polymers to lead to specific chemical reactions upon mechanical loading. Mechanophores open a novel way for designing multifunctional self-sensing materials (Chang, 1987; Thostenson, 2006; Wu, 2008). To model polymeric systems integrated with nanoparticles, numerous different approaches have been developed. These include homogenization techniques, molecular dynamics (MD) simulation, Monte Carlo (MC) simulation and the Mori-Tanaka approach. The high computational cost associated with large-scale MD simulations limits its use beyond the nanoscale whereas the use of micromechanical homogenization techniques in a multiscale framework can lead to the propagation of large errors across length scales. A major challenge is how to scale material behavior from the nano-, micro-, and mesoscales to the macroscale in order to investigate the effect of the self-sensing material at the structural scale. Despite the accuracy of MD simulations, computational inefficiency prohibits their use within a multiscale analysis framework. In order to maximize computational efficiency and maintain high accuracy while investigating the material behavior of polymers, a novel multiscale modeling framework was developed in this research. The simulation techniques include MD simulation at the atomistic scale, spring-bead model at the microscale, crosslinked network model at the mesoscale, and FE simulation at the macroscale.
This chapter presents a spring-bead model and a network model which are developed to bridge nanoscale information to higher length scales for modeling epoxy polymers embedded with smart particles (see Figure 4.1). Because mechanical properties are determined by inter/intra-molecular potential energy and there is no reported literature on the mechanical properties of the self-sensing polymer, MD simulation is the most appropriate approach to understanding the material properties of the self-sensing polymer at the microscale. A series of MD simulations are performed to capture the generation of crosslinked bonds in the self-sensing polymer; this information is further used to construct the probability distribution of crosslinking degrees. At the mesoscale, the material is partitioned into discrete mass beads which are linked using linear springs. By integrating multiple spring-bead models, a crosslinked network model is generated to represent the elastic material properties at the mesoscale. The spring-bead based network model is integrated with FE model to characterize the mechanical properties at the macroscale. The developed methodology is computationally efficient and provides a possible means to bridge various length scales without significant loss of accuracy.
Figure 4.1 Modeling of self-sensing polymer materials at the microscale, mesoscale, and macroscale.

4.2. **MD simulation of bond clusters at the microscale**

4.2.1 **Self-sensing behavior of the smart material**

MD simulation is used to characterize the mechanical properties of this self-sensing polymer at the molecular level. A stochastic approach is used to estimate the most likely crosslinking degree of the polymer system. Some relevant research efforts (Bandyopadhyay, 2011; Li, 2010; Tack, 2008) estimated the crosslinking degree indirectly by comparing the $T_g$ obtained from MD simulations, and from differential scanning calorimetry (DSC). In this study a direct approach to estimate the local crosslinking degree is introduced; this direct method mimics the curing process based on inter/intra molecular potentials. The inter/intra molecular potentials are determined by a force field, which is a set of functions and parameters achieved from experimental or quantum mechanical studies to describe material properties at the molecular level. The Merck molecular force field (MMFF), which was developed for general organic research and pharmaceutical development that requires the most accurate results, is used for the epoxy-based systems used in this study (Yang, 2012; Halgren, 1996). The MD simulations are performed using the Large-scale Atomic Molecular Massively Parallel Simulator (LAMMPS) package (Plimpton, 2007).
Figure 4.2 Schematic of UV-initiated cyclobutane generation and damage-induced cinnamoly group generation.

The self-sensing material modeled in this work comprises Tris-(Cinnamoyloxymethyl)-Ethane (TCE) monomer to synthesize cyclobutane - a mechanophore formed by exposing the TCE monomer to UV light (wavelengths of range 330-380 nm), as shown in Figure 4.2. With local damage, the physical discontinuities break the covalent bonds in cyclobutane. Subsequently, the cyclobutane transforms into the TCE monomer, which consists of cinnamoyl groups that emit visible light of wavelengths ranging from 450 nm to 600 nm under UV excitation (Chung, 2004; Cho, 2008, 2010). Figure 4.3 shows the results observed from this self-sensing material surface of a specimen during a uniaxial loading test. The UV fluorescence images were taken at different stages of load increment. There is no fluorescence observed in the initial range of the loading (see Figure 4.3a); fluorescence can be observed when micro cracks initiate in the specimen (the green scatter points in Figure 4.3b). The intensity of the fluorescence keeps increasing with the growth of the micro cracks (the green zone in Figure 4.3c). The mechanophore response is a result of the transmission of external force at the macroscale to the debonding of covalent links at the molecular level (Kingsbury, 2011; Silberstein,
This observation provides evidence that the self-sensing material has the potential to capture various levels of damage progression. MD simulation is adopted to further understand the interactions between the epoxy/hardener and the self-sensing material, which could affect the color changing phenomena significantly. Two important features of the material are required from the MD simulation to construct the spring-bead model that can represent various crosslinking degrees at the microscale: statistical distribution of crosslinking degree and corresponding mechanical properties.

Figure 4.3 Fluorescence observation in self-sensing polymer with increasing load: a) no crack and no fluorescence observed; b) micro crack and slight fluorescent intensity; c) major crack and higher fluorescent intensity.

4.2.2 Statistical crosslinking degree in MD simulation

The molecular structures of the epoxy resin and the hardener that form the polymer used in this study are Di-Glycidyl Ether of Bisphenol F (DGEBF) and Di-Ethylene Tri-Amine (DETA), respectively (see Figure 4.4a and 4.4b). The smart particle responsive to mechanical loading is TCE (see Figure 4.4c). A stochastic approach is proposed to capture the variability of the crosslinking degree and the mechanical properties of the polymer system; an RVE model is constructed with molecules (of the resin, the hardener, and the smart particle) distributed randomly in the initial configuration (Figure 4.4d). The RVE size is 14 nm × 14 nm × 14 nm. The weight percentages of the components in
this self-sensing polymer are 70.9% for DEGBF, 19.1% for DETA, and 10.0% for TCE. Table 4.1 shows the respective chemical formulae, weights, and numbers of component molecules.

![Figure 4.4 Components of self-sensing polymer: a) epoxy resin, b) hardener, c) smart material to form, and d) RVE model.](image)

**Table 4.1 Components in the self-sensing polymer**

<table>
<thead>
<tr>
<th></th>
<th>Formula</th>
<th>Weight</th>
<th>Molecule number in one RVE</th>
</tr>
</thead>
<tbody>
<tr>
<td>DGEBF</td>
<td>C₁₉H₂₀O₄</td>
<td>313 g/mol</td>
<td>650</td>
</tr>
<tr>
<td>DETA</td>
<td>C₄H₁₃N₃</td>
<td>103 g/mol</td>
<td>550</td>
</tr>
<tr>
<td>TCE</td>
<td>C₃₂H₃₀O₆</td>
<td>510 g/mol</td>
<td>50</td>
</tr>
</tbody>
</table>

The epoxy based polymer is an extensively crosslinked structure; additionally, the extent of crosslinking significantly affects the mechanical properties. The crosslinking degree is defined as the percentage of actual crosslinked covalent bonds over all potential crosslinked bonds. It is important to estimate the crosslinking degree accurately to capture the mechanical properties at the microscale. The crosslinking degree in the network structure is defined in Equation (4.1):
\[ \theta\% = \frac{N_{\text{Actual}}}{N_{\text{Ideal}}} \]  

(4.1)

where \( \theta \) is the crosslinking degree, \( N_{\text{Actual}} \) and \( N_{\text{Ideal}} \) are the number of the actual and all potential crosslinked covalent bonds in a certain zone, respectively. A schematic of the epoxy network structure is shown in Figure 4. Covalent bonds (represented are represented by a black solid line in Figure 4.5c. The blue ellipse R (Figure 4.5a) and the red circle H (Figure 4.5b) represent the epoxy resin and hardener, respectively. For epoxy resin particles there are two active sites (yellow points in Figure 4.5a), and for hardener particles there are five active sites (purple points in Figure 4.5b). A covalent bond can be generated when the distance between the active sites of the epoxy resin and the hardener is shorter than a critical value. The two active sites can share their electrons to stabilize the potential energy. The process of bond formation between the epoxy resin and the hardener molecules is also known as “curing” in polymer science.

Figure 4.5 Schematic of crosslinked structure of epoxy resin and hardener: a) molecular structure of epoxy resin with two active sites; b) hardener with five active sites; c) epoxy resin and hardener are crosslinked to generate polymer structure. Black
solid lines represent covalent bonds.

Figure 4.6 Statistical distribution of crossing-linking degrees based on MD simulations (N = 500).

A total of 500 MD simulations were performed, each with a randomly generated initial configuration (42,350 atoms in each RVE) at standard room conditions (300K and 1atm). The RVE size is 14 nm × 14 nm × 14 nm. The 500 repeating MD models ensure that the simulation results can characterize the statistical distribution of material properties. In the simulation, each RVE was cured using a bond formation command in LAMMPS and a crosslinking cut-off radius of 4.0 Angstroms; this cut-off radius was selected because it is more than twice the length of a carbon-nitrogen covalent bond (Varshney, 2008; Yu, 2009). The resulting crosslinking degree is unique for each RVE due to the random initial configuration. The frequency distribution of resulting crosslinking degrees (Figure 4.6) from the 500 MD simulations is statistically smooth. The simulation results indicate a quasi-normal distribution with crosslinking degrees
ranging between 40% and 65%. The average crosslinking degree is 52.72% for the polymer system containing the self-sensing material. These results are used to construct the statistical network model at the mesoscale.

4.2.3 Mechanical properties of self-sensing polymer in MD simulation

MD simulations were performed on the crosslinked polymeric systems to obtain the tensile, compressive, and shear moduli. Uniaxial tensile/compressive tests were simulated on the atomistic systems with different crosslinking from 30% to 70%. The resulting RVEs with different crosslinking degrees were equilibrated at zero-atmospheric pressure to relieve residual stresses. The equilibrated RVEs were deformed along x, y, and z axes independently under the Isothermal-Isobaric ensemble (300K and zero atm on the other axes). Figure 4.7 shows the raw stress-strain data and a local regression model with a simple filter to minimize data noise. Based on the filtered stress-strain data, the Young’s modulus of the polymer system is calculated from the slope of the linear fitting functions in the elastic region (~ 10% strain). To determine the bulk modulus, triaxial deformation tests were simulated on the polymer RVEs. The hydrostatic pressure on each RVE was varied from zero atm to 5000 atm at room temperature; the change in volume was measured to obtain the bulk modulus based on Equation (4.2):

\[ K = \frac{\Delta p}{\Delta V/V_0} \] (4.2)

where \( K \) is the bulk modulus, \( V_0 \) is the original volume of the RVE, \( \Delta p \) and \( \Delta V \) are the change of pressure and change of RVE volume, respectively. From the Young’s modulus \( E \), and the bulk modulus \( K \) obtained from MD simulation, the shear modulus \( G \) of the
polymer system can be calculated using Equation (4.3) based on the assumption of isotropy:

\[ G = \frac{3KE}{9K - E} \]  

(4.3)

Figure 4.8 shows the variation of elastic properties with crosslinking degrees based on MD simulation results. These results provide the input for the spring-bead model at the microscale and the network model at the mesoscale. The moduli as a function of crosslinking degree \( \theta \) are described in Equations (4.4), (4.5), and (4.6) using linear fitting functions:

\[ E_{\text{tensile}} = 0.01456\theta + 0.911 \]  

(4.4)

\[ E_{\text{compressive}} = 0.01857\theta + 0.839 \]  

(4.5)

\[ G_{\text{shear}} = 0.00507\theta + 0.309 \]  

(4.6)

where \( E_{\text{tensile}}, E_{\text{compressive}}, \) and \( G_{\text{shear}} \) are the tensile, compressive, and shear moduli, respectively; \( \theta \) represents the crosslinking degree.
Figure 4.7 Uniaxial deformation test in MD simulation: a) tensile load and b) compressive load of self-sensing polymer.
Figure 4.8 Relationship between crosslinking degrees and a) tensile modulus, b) compressive modulus and c) shear modulus.
4.3. Development of spring-bead model to represent bond clusters at the microscale

Micromechanical techniques allow the mechanical behavior of polymers to be analyzed through the continuum approximation of heterogeneous microstructures. The variation of microstructural properties leads to variable macroscopic properties. Because the mechanical behavior in nanocomposites is affected more by discrete phenomena, the application of continuum mechanics is not a suitable option at the microscale. The FE method is the most widely used numerical methods for discretizing the continuum mechanical description of a material (Buxton, 2002). The FE method incorporates a complex preprocessed mesh which allows detailed investigations of complex geometries at hot spots, while enabling complex constitutive relations to be incorporated. However, the accuracy and efficiency of FE method are dependent on mesh sizes, and therefore limitations exist on the level of complexity that can be simulated (Tomar, 2004). In order to simulate more heterogeneous microstructures, a simpler technique may be adopted. The spring-bead model is considered as a two-dimensional or three-dimensional network of interconnecting one-dimensional linear springs. The continuous material is lumped into discrete beads. The neighbor springs are linked together by the nodes fastened in the centers of the beads. The principal advantages of the model are the ease with which the microstructural heterogeneity can be incorporated through the local variation in spring characteristics, and the simulation of crack propagation through the iterative removal of springs.

In this work a spring-bead model is developed to characterize the elastic deformation of a crosslinked cluster of polymer chains with inputs from MD simulations that define
local material properties. At each iteration step in the simulation, forces in the springs are applied to the nodes at the center of the beads, and the equilibrated nodal displacements throughout the system are calculated. Different from the traditional FE method for obtaining stress and strain, the spring-bead model provides the displacements of the nodes and forces in the springs. The equivalent strain and strain energy of spring-bead based network model can be defined and calculated using the displacements of nodes and the spring characteristics. Furthermore, the results from the network model can be scaled up to obtain the structural response at the macroscale using FE analysis (see Figure 4.1).

In this spring-bead model (see Figure 4.9 (a)), each of the two beads serves as half of the mass of the bond cluster; the linear spring is used to represent the mechanical response (tensile and compressive) of the bond cluster, and the potential energy stored in the spring due to extension or compression captures the elastic strain energy in the deformed material. The spring-bead model can be further simplified as shown in Figure 4.9 (b), where the spring is replaced by a line with linear force-extension behavior. The relation between the force and relative displacement is shown in Figure 4.9 (c). Variable spring stiffness (ratios of force to relative displacement) is used to represent bond clusters with different crosslinking degrees. It should be noted that the architecture of this spring-bead model is dependent on the size of the bond cluster. To represent a bond cluster with a larger size, the mass of beads will be enhanced, and the spring stiffness will be increased as well. The linear relation between force and relative displacement can be expressed in Equation (4.7):

$$ F = k \cdot \Delta u $$

(4.7)
where, $F$ is the attractive/exclusive force in the spring, $\Delta u$ is the relative displacement of the two beads compared to their original state, and $k$ represents the spring stiffness. The elastic energy stored in the spring can be expressed as:

$$E = \frac{1}{2} \cdot k \cdot (\Delta u)^2$$ (4.8)

where, $E$ is the elastic energy stored in the spring. The elastic energy is used to calculate the equivalent strain energy density of the network model.

The existing set-up of the spring-bead model can be extended to characterize the elastic-plastic material behavior by replacing the linear springs with appropriate nonlinear ones. Dampers can also be added in the spring-bead model to represent the viscoelastic and viscoplastic properties of some materials. However, experimental tensile tests of the self-sensing polymer material exhibit brittle behavior. There is no obvious plasticity region observed from these experimental tensile tests. Therefore, the spring-bead model and the subsequent network model developed in this study use linear springs to capture the mechanical response of the self-sensing polymer.

Figure 4.9 a) Spring-bead model; b) simplified spring-bead model; c) mechanical
response of spring-bead models with different crosslinking degrees.

4.4. Development of network model at the mesoscale

The spring-bead model can only carry load in the uniaxial direction of the spring. At each point in the amorphous polymer material, there should be tensile, compressive, and shear load carrying ability in all directions. Therefore, it is important that the network model with crosslinked springs and beads accurately represents the load carrying capacity in all directions. The construction, evaluation and the parametric studies of different network models are discussed in this section. Different kinds of network models, named according to the number of neighbor beads surrounding each bead (i.e., a 6 neighbor based network model implies that each bead is connected with six neighbor beads using springs), are designed and compared. The network model, consisting of a series of beads and springs connected to neighboring beads, is used to represent larger crosslinked polymer chains and capture the omnidirectional mechanical responses of the material. In addition, the network model serving as a simplified mechanical equivalent of MD simulations leads to significant reduction in computational resources compared to MD simulations.

Different combinations of spring-bead arrangements are studied to understand the mechanical behavior of the material. Several combination strategies (including 3, 4, 6, 8, and 12 neighbor based connections) are shown in Figure 4.10. The bead located at the center of the grey area is used to represent the total mass of the corresponding area. The spring stiffness is equivalent to the strength of the related bond cluster calculated from MD simulation. In the candidate network models, the spring length is defined as 0.8 μm; this value is also used as the lower bound if there is more than one kind of spring. For
example, there are two kinds of springs for 8 neighbor based network model (see 4.10d). The short spring length is defined as 0.8 μm in the 8 neighbor based network model. The density of springs and beads in the network models are listed in Table 4.2. It must be noted that complex network models with more neighbors will reduce simulation efficiency; therefore network models with more than 12 neighbors are not considered in this approach.

Figure 4.10 Different arrangements of spring-bead models to form a: a) 3 neighbor based; b) 4 neighbor based; c) 6 neighbor based; d) 8 neighbor based; e) 12 neighbor based network model.

The candidate network models are listed in Figure 4.10. The optimal arrangement is the one that is capable of carrying tensile, compressive, and shear loads. Among the candidate combinations, the 3 and 4 neighbor based models are not stable structures because they do not exhibit shear load carrying capacity. For the remaining three
candidate network models shown in Figure 4.11 (6, 8, and 12 neighbor based arrangements), the optimized configuration is evaluated by how well a candidate model can represent the mechanical response at the mesoscale.

Figure 4.11 The 6, 8, and 12 neighbor based network models

The self-sensing polymer is assumed to be homogeneous and isotropic at the mesoscale and macroscale. Therefore, the representation of isotropic property is considered to be an important criterion for evaluating the optimal network configuration. In all the network models proposed above, the springs are aligned along specific directions, depending on the type of the network configuration. For example, in the 8 neighbor based network model (see figure 4.11b), all the springs are at an angle of 0°,
$45^\circ$, $90^\circ$, or $135^\circ$. Consequently, the mechanical response of all combined network models is dependent on orientations.

A 6 neighbor based network model is constructed with springs of uniform length whereas the 8 and the 12 neighbor based network models are made up of two types of springs (long and short). Since changes in the spring stiffness will lead to different mechanical properties, the polymer material at different crosslinking degrees can be represented effectively by appropriately varying the $k_1$ (long spring) or $k_2$ (short spring) values. This feature provides the possibility of generating an equivalent isotropic network model using a specific ratio of spring stiffness. Additionally, an isotropy index is defined to describe the orientation-dependence of mechanical property in the network model:

$$I(\theta) = \frac{E_x}{E(\theta)}$$

(4.9)

where, $E_x$ represents Young’s modulus in the principal direction (x-direction of the network model in Figure 4.11), $E(\theta)$ represents the Young’s modulus along an arbitrary direction at an angle $\theta$ with respect to the x-direction, $I(\theta)$ is the isotropy index that shows the variation of material property along different directions. For a perfectly isotropic material, the isotropy index $I(\theta)$ is equal to 1. An isotropic index approaching unity is indicative of good isotropic material property representation.

The evaluations of candidate network models are listed in Table 2. The 6 neighbor based network model fails to represent good isotropic property because it uses a single spring configuration; the average isotropy index of a 6 neighbor based network model is 1.149 and the root mean square deviation (RMSD) between different directions is 7.45%.
For the 8 and the 12 neighbor based network models, a parametric approach was adopted to find the relation between the RMSD of mechanical property in different directions and the stiffness ratio of long springs to short springs. From the simulation results, it can be observed that the average isotropy index is a continuously increasing function of stiffness ratio of springs. For the 8 neighbor based network model, the RMSD is 0.04% when the stiffness ratio is 0.6002 (see Figure 4.12a). The maximum difference between mechanical properties along different directions is 0.08%. For the 12 neighbor based configuration, the minimum isotropy index is 1.149 and the RMSD value is 7.45%. Therefore, the 12 neighbor based network model cannot adequately represent the isotropic property.

![Figure 4.12 Isotropic representation of a) 8 neighbor based, and b) 12 neighbor based network models corresponding to stiffness ratio of long spring to short spring.](image)

To summarize the results in this section, the 3 and the 4 neighbor based network models cannot carry loads owing to their unstable structures, whereas the 6 and the 12 neighbor based network models lack good isotropic representation capability. In addition,
the 12 neighbor based network model consists of a high number of springs and beads, which will increase simulation time and cost. The 8 neighbor based network model is the optimal one considering structural stability, representation of isotropic property, and computational efficiency. The 8 neighbor based network model is equivalently isotropic when the ratio of long spring stiffness $k_2$ to short spring stiffness $k_1$ is given as 0.6002. It must be noted that a 2D spring-bead based network model represents a polymer plate of unit thickness (1 μm). The spring stiffness will be redefined by multiplying a factor (ratio of material thickness to 1 μm) to represent different material thickness.

Table 4.2 Configuration and evaluation of network models with different combination methods.

<table>
<thead>
<tr>
<th>Network model</th>
<th>Number of beads per 100 μm$^2$</th>
<th>Number of springs per 100 μm$^2$</th>
<th>Evaluation</th>
<th>Optimal isotropic index</th>
</tr>
</thead>
<tbody>
<tr>
<td>3 neighbors</td>
<td>120</td>
<td>181</td>
<td>Not stable</td>
<td>Not applicable</td>
</tr>
<tr>
<td>4 neighbors</td>
<td>156</td>
<td>313</td>
<td>Not stable</td>
<td>Not applicable</td>
</tr>
<tr>
<td>6 neighbors</td>
<td>180</td>
<td>541</td>
<td>Anisotropic</td>
<td>1.1490</td>
</tr>
<tr>
<td>8 neighbors</td>
<td>156</td>
<td>625</td>
<td>Optimal model</td>
<td>1.0008</td>
</tr>
<tr>
<td>12 neighbors</td>
<td>180</td>
<td>1081</td>
<td>Anisotropic</td>
<td>1.1490</td>
</tr>
</tbody>
</table>

4.5. Optimization of mechanical equivalence between MD model and network model

The network model integrated results from molecular level simulations to the mesoscale. Mechanical equivalence of the network model with the actual MD system also validates the approximation at the microscale. The next step is to determine the spring strengths that ensure minimal deviation of the mechanical properties obtained
from the network model and MD simulation. A multiobjective optimization technique is used to address this problem. The methodology also helps to establish a relation between spring stiffness ($k_1$ or $k_2$) and the local crosslinking degree.

To obtain the relation between spring stiffness $k_1$ and corresponding crosslinking degree $\theta$, a set of parametric studies is performed. First, a series of 8 neighbor based network models is generated. The size of the square network model is 8 μm × 8 μm. The lengths of the short and long springs are 0.8 μm and 1.131 μm, respectively. The stiffness ratio of the springs is kept to be 0.6002 to ensure that the mechanical properties of the network model is isotropic. The equivalent tensile, compressive, and shear strengths of network models are calculated for different spring stiffness. The simulation results and fitting curves indicate a linear relation between equivalent modulus of network model and spring stiffness $k_1$ (see Figure 4.13). The moduli (GPa) as functions of $k_1$ (N/m) are described by Equations (4.10), (4.11), and (4.12):

\[
E'_{\text{tensile}} = 0.001494k_1 + 0.003286 \quad (4.10)
\]
\[
E'_{\text{compressive}} = 0.001476k_1 - 0.000210 \quad (4.11)
\]
\[
G'_{\text{shear}} = 0.000423k_1 + 0.000469 \quad (4.12)
\]

The calculated value of all three moduli from the network model must match the corresponding values obtained from the MD simulation at a fixed crosslinking degree (Equations 4.4, 4.5 and 4.6). A multiobjective optimization algorithm is formulated where the objective is to minimize the deviation for each loading condition.

\[
F_1(x) = \frac{f_T(k_1)}{E'_{\text{tensile}}} - 1 \quad (4.13)
\]
It must be noted that the objectives are competing as well as coupled; i.e., the design variable, $k_1$, has a different degree of impact on each of the three objective functions, and the minimization of one objective could lead to an increase in the value of another objective. Therefore, a robust technique is required to determine the optimal spring stiffness at each crosslinking degree. The Kreisselmeier-Steinhauser (KS) function approach is used to solve the multiobjective optimization problem. Using the KS function, a composite envelope function is formulated to transform the original multiple objectives and constraints to a single unconstrained objective function (Chattopadhyay, 1991, 1994). The first step in formulating the objective function in this approach involves the transformation of the original objective functions into reduced objective functions. The reduced objective functions are of the form:

$$F^*(x) = \frac{F_k(x)}{F_{k_0}} - 1 - g_{max} \leq 0 \quad k = 1, 2, \ldots, n_{obj}$$  

(4.16)

where, $F_{k_0}$ corresponds to the value of $F_k$ calculated at the start of each iteration; ‘$g_{max}$’ is the maximum value among all the constraints and remains constant throughout the iteration. The KS function combines the objectives and constraints ($n_{obj} + m = M$) to form the single objective function, described in Equation (4.17):

$$\bar{F}(x) = g_{max} + \frac{1}{\rho} \log \sum_{k=1}^{M} e^{\rho(g_k(x) - g_{max})}$$  

(4.17)
The algorithm attempts to satisfy the constraints of the reduced objective function by maximizing $F_k$. The multiplier “$\rho$” is analogous to the draw-down parameter of penalty function formulations and controls the distance from the surface of the KS objective function to the surface of the maximum function value. A large value of ‘$\rho$’ causes the KS function to closely follow the surface of the largest constraint function; a small value causes the inclusion of violated constraints to the KS function (Haftka, 1992).
Figure 4.13 Fitting curves of modulus as a function of spring stiffness: a) tensile modulus; b) compressive modulus; c) shear modulus.
Figure 4.14 compares the performance of the optimization algorithm with respect to the results from MD simulation. The optimal $k_I$ value overestimates the values of the tensile and compressive moduli at lower crosslinking degrees. However, at the most likely crosslinking degree (~ 52.72%), which is the average crosslinking degree in the 500 MD simulations, the error between the tensile and the compressive responses are quite balanced. The norm of the maximum constraint violation is within the specified tolerance of $1 \times 10^{-4}$.

Figure 4.14 Comparison between MD simulation and optimization results.
Figure 4.15 Linear fitting curve of spring stiffness based on optimization results.

Figure 4.15 illustrates the variation of optimal spring stiffness with crosslinking degree. The relationship is a close linear approximation; this result is consistent with the inference from MD simulation that the tensile, compressive, and shear moduli vary linearly with crosslinking degree. The linear fitting expression of the optimal spring stiffness $k_1$ using the crosslinking degree $\theta$ is shown in Equation (4.18):

$$k_1 = 123.17 \cdot \theta + 117.35 \quad (4.18)$$

4.6. Equivalent strain and strain energy in network model

The network model is constructed by crosslinked springs and discrete beads, instead of continuous material. Therefore the traditional concepts of strain and strain energy density are not available for this modeling. New concepts of strain and strain energy are required before the discussion and evaluation of network model in next chapter. In traditional continuous materials, strain is defined as a geometrical measure of deformation representing the relative displacement between particles in a material body.
In spring-bead based network model, the “equivalent strain” in one spring is defined as the deformation in term of original and relative displacement between the two beads linked by this spring, as shown in Equation (4.19):

$$\varepsilon_i = \left| \frac{\Delta L_i}{L_i} \right|$$  \hspace{1cm} (4.19)

where, $L_i$ is the original length of the $i$th spring, $\Delta L_i$ is the change of the same spring length, and $\varepsilon_i$ is the equivalent strain of the $i$th spring. For each bead in the 8 neighbor based network model, there are eight beads linked to it directly using springs (see Figure 4.16). The averaged equivalent strain in the bead centered subzone (the grey square zone in Figure 4.16) is defined as the averaged value of the strain in the eight neighbor springs linking to the centered bead. For the 8 neighbor based network model, the length of the square subzone side is equal to the shorter spring length. The equivalent strain in the subzone is defined as:

$$\bar{\varepsilon} = \frac{1}{N} \cdot \sum_{i=1}^{N} \varepsilon_i$$  \hspace{1cm} (4.20)

where $\varepsilon_i$ is the equivalent strain in the $i$th spring, which is defined in equation (4.19), $\bar{\varepsilon}$ is the averaged equivalent strain in the subzone (grey zone in Figure 4.16), and $N$ is the number of neighbor springs linked to the center bead. For the 8 neighbor based network model, $N$ is equal to 8.
Figure 4.16 Beads, springs, and subzone in 8 neighbor based network model.

The equivalent elastic strain energy in spring is defined as the strain energy stored due to the deformation of the spring, which can be calculated using equation (4.21):

$$U_i = \frac{1}{2} \cdot E_i \cdot (\varepsilon_i)^2$$  \hspace{1cm} (4.21)

where $E_i$ is the spring stiffness of the $i$th spring, $U_i$ is the elastic strain energy stored in the spring when the equivalent strain of the spring is $\varepsilon_i$. The equivalent elastic strain energy density in the subzone is defined as:

$$\bar{U} = \frac{1}{2A} \cdot \sum_{i=1}^{N} U_i$$  \hspace{1cm} (4.22)

where $U_i$ is the elastic strain energy in the $i$th spring, $A$ is the area of the subzone (grey area in Figure 4.16) and $\bar{U}$ is the corresponding equivalent elastic strain energy density in the subzone, which is equal to the density of half of the energy stored in all surrounding springs. $N$ is the number of neighbor springs around linked with the center bead. For the 8 neighbor based network model, $N$ is equal to 8. The factor $1/2$ in Equation (4.22) indicates that each spring is equally shared by the subzone and one of its neighbor
subzones. So the total elastic strain energy in each spring is divided into two equal parts in the calculation of the equivalent strain energy density.

4.7. Summary

In this chapter, a spring-bead based network model was developed to represent the mechanical properties of self-sensing polymeric material. At the microscale, the spring-bead model was developed to represent mechanical properties and mass of cluster bonds. MD simulation was implemented to provide necessary information to construct the spring-bead model. At the mesoscale, a computationally efficient network model was developed; these models were implemented in a general purpose finite element solver to obtain the mechanical properties. Parametric studies and multiobjective optimization were conducted to construct an optimal combination of an 8 neighbor based network model and determine the corresponding spring stiffness. Compared to MD simulations, the spring-bead based network model can significantly improve the simulation efficiency while maintaining sufficient accuracy.
5. **Multiscale Modeling of Self-sensing Polymer using Statistical Network Model**

5.1. **Background**

Discrete material techniques, such as the spring-bead based network model, have been developed to study polymer material (Iwata, 2003; Schwarz, 2006; Indei, 2012). Spring-bead chains are crosslinked to generate the network model to represent the larger scale material behavior of polymer. In epoxy based self-sensing polymers the crosslinking bond clusters between the resin and the hardener molecules generate a larger scale of network structure. The heterogeneous crosslinked microstructure at the microscale has significant effect on the local mechanical properties (Flory, 1943; Krumova, 2000; Fan, 2007). Therefore to design and synthesize polymers with multifunctional capabilities it is important to develop a fundamental understanding of the effects of nano- and microscale variability on material properties and response such as Young’s modulus, heterogeneous stress/strain distribution and damage precursor. Parametric studies of the variability, such as the crosslinking degree, chain flexibility and chain length, are important to enhance the accuracy of the network models (Espuche, 1995; Chzarulatha, 2003; Park, 2006) discussed in Chapter 4. Among all variability the crosslinking degree (or crosslinking density), which represents the degree of microscopic covalent bonds, plays an important role in influencing the mechanical properties (Zosel, 1993; Espuche, 1995; Halary, 2000; Berger, 2004). In this research the computationally
efficient network model is used to investigate this effect. In particular, the impact of crosslinking degree on damage initiation is studied.

A series of simulations are performed to study the effects of the crosslinking degree on the strain distribution. In addition, a preliminary investigation has been made to evaluate the damage initiation under monotonic loading and correlating this information to the mechanophore fluorescence under loading. This information is expected to help understand and further improve the sensitivity of the self-sensing polymer to predict damage initiation.

5.2. **Parametric study of statistical network model**

5.2.1 **Heterogeneous and homogeneous distribution of crosslinking degree**

The influence of heterogeneous distribution of the crosslinking degree on the mechanical properties is studied. A set of four 8 neighbor based network models (size: 1mm × 1mm) were generated. There are 100 (10 × 10) subzones in each of the four network models. As shown in Figure 5.1(a), the schematic network model consists of two subzones (A and B) representing two different crosslinking degrees. The degree of heterogeneity, which is defined as the difference in crosslinking degrees between neighbor subzones, for all four network models is present in Table 5.1. It can be seen that although the average crosslinking degree value remain the same, 52.72%, the degree of heterogeneity increases gradually from model 1 to model 4. The crosslinking degree value is directly related to the material properties, which are represented by spring stiffness in the spring-bead based network model. The spring stiffness in subzone A and B, for all four models, are shown in Figure 5.1(b). The increasing difference in spring
stiffness between neighbor subzones also indicates that the material properties changes from homogeneous to heterogeneous.

Figure 5.1 a) Specific network model to study effect of degree of heterogeneity and b) spring stiffness in subzone A and B of the network model 1, 2, 3 and 4.

Table 5.1 crosslinking degree and degree of heterogeneity in the four network models

<table>
<thead>
<tr>
<th></th>
<th>crosslinking degree in A</th>
<th>crosslinking degree in B</th>
<th>Heterogeneous degree</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model 1</td>
<td>52.72%</td>
<td>52.72%</td>
<td>0</td>
</tr>
<tr>
<td>Model 2</td>
<td>51.72%</td>
<td>53.72%</td>
<td>2%</td>
</tr>
<tr>
<td>Model 3</td>
<td>50.72%</td>
<td>54.72%</td>
<td>4%</td>
</tr>
<tr>
<td>Model 4</td>
<td>49.72%</td>
<td>55.72%</td>
<td>6%</td>
</tr>
</tbody>
</table>

Simulations were conducted using uniaxial tensile load applied to all four network models. The loading was strain control and the maximum loading strain was 5%. The average equivalent strain which is defined as the average deformation of springs in one subzone is used to evaluate the strain in the network models. The simulation results are shown in Table 5.2 and Figure 5.2. In model 1, 2, and 3, where the degree of heterogeneity is not more than 4%, the average equivalent strain is nearly the same (equal
to 0.0339). The average strain decreases significantly in model 4 in which the degree of heterogeneity is 6%. It can be observed that the difference between maximum and minimum equivalent strain in the network models is influenced by the degree of heterogeneity as well (see Table 5.2). The difference between maximum and minimum equivalent strain increases with degree of heterogeneity (see Figure 5.2).

Table 5.2 Equivalent strain in network models to study degree of heterogeneity effect

<table>
<thead>
<tr>
<th></th>
<th>Model 1</th>
<th>Model 2</th>
<th>Model 3</th>
<th>Model 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Average crosslinking degree</td>
<td>0.0339</td>
<td>0.0339</td>
<td>0.0339</td>
<td>0.0322</td>
</tr>
<tr>
<td>Maximum crosslinking degree</td>
<td>0.0357</td>
<td>0.0357</td>
<td>0.0357</td>
<td>0.0350</td>
</tr>
<tr>
<td>Minimum crosslinking degree</td>
<td>0.0327</td>
<td>0.0326</td>
<td>0.0320</td>
<td>0.0288</td>
</tr>
<tr>
<td>Difference between maximum and minimum crosslinking degree</td>
<td>8.4%</td>
<td>8.7%</td>
<td>10.4%</td>
<td>17.7%</td>
</tr>
</tbody>
</table>

Figure 5.2 The difference in neighbor crosslinking degree influences the difference
between maximum and minimum equivalent strain in the network model.

Based on this parametric study of heterogeneous distribution in crosslinking degree (see Figure 5.2), a larger degree of heterogeneity leads to a higher difference in equivalent strain; the effect is more pronounced where the degree of heterogeneity is greater than 4% for the cases studied. It must be noted that in brittle material, strain gradient plays an important role in singular or non-singular stress concentrations and local damage (Li, 2011). It has been found that a higher local strain gradient can promote damage initiation (Geers, 1998; Francfort, 1998). From the simulations and analyses of results since increasing degree of heterogeneity increases the strain gradient, from damage evolution perspective it is preferable to reduce the degree of heterogeneity.

5.2.2 Homogeneous and statistical distribution of crosslinking degree

At the microscale of the self-sensing polymer, the crosslinking degrees are statistically distributed. This is also the reason why traditional FE model cannot well represent the heterogeneous microstructure and one motivation to develop the network model. To represent the statistical distribution of crosslinking degrees at the microscale, a statistical network model was developed, which is shown in Figure 5.3(a). To validate microstructural representation capability of the statistical network model, a homogeneous network model was constructed with no variation in the crosslinking degree (Figure 5.3(b)) and compared to the statistical network model. The same size and geometry as the model used in section 5.3.1 (10 × 10 subzones in 1mm × 1mm) is maintained. In Figure 5.3(a) and 5.3(b) the numbers in the variable subzones represent the weight percentage of the corresponding local crosslinking degrees. Note that the variable crosslinking degrees
in the statistical network model is defined by the probability density function (PDF) obtained from the MD simulation (see Figure 4.6). For the homogeneous network model, uniform crosslinking degree which is equal to the averaged value of all crosslinking degrees in the statistical network model (52.72%) is used for all subzones.

![Crosslinking degree distribution](image1)

a) Crosslinking degree distribution in statistical network model and b) homogeneous network model (unit: %).

Uniaxial tensile test was performed in both statistical and homogeneous network models. The loading was strain control and the maximum loading strain was 5%. The simulation results are shown in Figure 5.4(a) and 5.4(b), which provide the equivalent strain distribution in the statistical and homogeneous network models, respectively. Results of the average, maximum and minimum equivalent strain in the statistical and homogeneous network models are presented in Table 5.3.
Figure 5.4 Equivalent strain distribution in a) statistical network model and b) homogeneous network model.

As shown in Table 5.3, the average values of equivalent strain in statistical network model and homogeneous network model are close. This implies that the overall mechanical property of the statistical network model corresponds well with the homogeneous model under monotonic loading. The difference between maximum and minimum strain for statistical network model (which is 10.36%) is greater than the corresponding value for homogeneous network model (which is 8.40%). This observation implies that the statistical distribution of crosslinking degrees results in a larger distinguishable disorder in strain distribution; indicating that there is a high strain gradient. This increase in strain gradient can lead to early damage initiation in the homogeneous microstructure.

Table 5.3 Equivalent strain in statistical and homogeneous network models

<table>
<thead>
<tr>
<th>Equivalent</th>
<th>Statistical</th>
<th>Homogeneous</th>
</tr>
</thead>
<tbody>
<tr>
<td>Average</td>
<td>0.0338</td>
<td>0.0339</td>
</tr>
<tr>
<td>Maximum</td>
<td>0.0357</td>
<td>0.0357</td>
</tr>
</tbody>
</table>
5.2.3 Effect of spring length in network model

As discussed in chapter 4, the two steps in developing a network model are: i) designing the configuration variables including arrangement, spring size, and spring stiffness; ii) bridging MD simulation and network model using mechanical equivalence optimization. In the first step the definition of spring stiffness is related to the spring length. In the second step the mechanical equivalence provides the network model with the most proximate mechanical properties of the MD simulation. Technically, the spring length has negligible effect on the mechanical properties of the network model due to the mechanical equivalence optimization conducted in the second step of the development of the network model. To understand the spring length effect on the material behavior representation two network models with different spring lengths were generated. The sizes of the two network models are 8 μm × 8 μm and 1 mm × 1 mm, respectively; the corresponding spring lengths in the two network models are 0.8 μm and 0.1 mm, respectively. Based on the simulation results shown in Table 5.4, the material characteristics including tensile modulus, compressive modulus and shear modulus represented by the two network models are close (all errors are less than 1%), validating the hypothesis that there is negligible effect of the spring length on the mechanical properties of network model.

Although the spring length appears to have minor influence on the mechanical properties of the network model, shorter spring lengths are expected to capture the local
effects. The tradeoff is between increased accuracy and computational complexity. The spring length therefore plays a similar role as the mesh size in an FE model. As a compromise, spring elements of variable lengths can be used in different locations in a multiscale simulation. Shorter springs (under 1 μm) are used in the “hot spots” where the probability of damage initiation is high. Large springs (around 0.1 mm) are used in the zone surrounding the hot spot. This arrangement provides a trade-off between simulation efficiency and accuracy. Finite elements with bulk homogeneous material properties are used in the remaining part of the structure to improve the simulation efficiency. Numerical results are presented and discussed in section 5.3.

Table 5.4 Mechanical properties in network models of different spring lengths.

<table>
<thead>
<tr>
<th></th>
<th>Tensile Modulus</th>
<th>Compressive Modulus</th>
<th>Shear Modulus</th>
</tr>
</thead>
<tbody>
<tr>
<td>Network model of short springs (0.8 μm)</td>
<td>1.778 GPa</td>
<td>1.752 GPa</td>
<td>0.502 GPa</td>
</tr>
<tr>
<td>Network model of long springs (0.1 mm)</td>
<td>1.769 GPa</td>
<td>1.744 GPa</td>
<td>0.503 GPa</td>
</tr>
<tr>
<td>Maximum error</td>
<td>0.51%</td>
<td>0.46%</td>
<td>0.20%</td>
</tr>
</tbody>
</table>

5.3. Multiscale integration based on statistical network model

5.3.1 Validation of statistical network model

A set of three meso statistical network models were constructed to validate the simulation accuracy (see Figure 5.5 (b), 5.5 (c) and 5.5 (d)). The weight percentage of the crosslinking degrees in the three network models is controlled by the PDF function obtained from MD simulation in chapter 4. The probability distribution of crosslinking degrees in the three statistical network models is shown in Figure 5.5 (a). For each network model, the same size and geometry as the model used in section 5.2.1 (10 × 10
subzones in 1mm × 1mm) is maintained. There are 121 beads, 220 short springs, and 200 long springs in the 8 neighbors based network model. The lengths of the short and long springs in the network models are 0.1 mm and 0.1414 mm respectively. The numbers shown on the square subzones in Figure 5.5 (b), 5.5 (c), and 5.5 (d) represent the local crosslinking degrees.

![Graph showing weight percentage of crosslinking degrees](image)

![Subzones with local crosslinking degrees](image)
Figure 5.5  a) The probability distribution of crosslinking degree in the statistical network model, b) network model 1, c) network model 2, and d) network model 3.

Simulations were conducted using uniaxial strain controlled tensile load; the maximum loading strain was 10%. The average equivalent strain in the three network models was calculated. It was observed that the average equivalent strain in the three statistical network models was very close and the error was less than 1% (see Figure 5.6). The results establish the validity and robustness of the representative models. It must be noted that one deficiency of the developed network model is that it only captures the mechanical properties, and does not take into account the thermal and chemical properties of the mechanophores as in a MD simulation. This undoubtedly improves the computational efficiency significantly. For a similar uniaxial tensile loading simulation 20 hours of runtime is required using MD modeling whereas a network model completes the simulation in 4 minutes. The simulation efficiency is improved by 300 times using the network model.
Figure 5.6 Average equivalent strain in three statistical network models v.s. loading strain.

To validate the statistical network model, experimental investigations and their correlations with the network model are discussed. Three statistical representative network models were generated (see Figure 5.5 (b), (c) and (d)). A set of uniaxial compressive experiments were performed to determine the Young’s modulus of this self-sensing material. An MTS Bionix 370.02 test frame (with the maximum loading capability 22.2 kN) was used to conduct the compressive tests. The results from the experiments and the simulations, shown in Table 5.4, show very good correlation in Young’s modulus prediction.

Table 5.5 Simulation and experimental results of Young’s modulus

<table>
<thead>
<tr>
<th>Young’s modulus (GPa)</th>
<th>Model 1</th>
<th>Model 2</th>
<th>Model 3</th>
<th>Experiment</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.77</td>
<td>1.76</td>
<td>1.77</td>
<td>1.82</td>
<td></td>
</tr>
</tbody>
</table>
5.3.2 Local strain and crosslinking degree in the network model

Simulations were conducted with the statistical network model to study the relation between local strain and crosslinking degree using biaxial strain controlled tensile load; the maximum loading strain was 10% in both directions. The statistical network model 1 is used in the simulation (see Figure 5.7 (a)). The distribution of equivalent strain is shown in Figure 5.7 (b). There is an obvious relation between local strain and crosslinking degree: high strain concentration (the red band in Figure 5.7 (b)) occurs mostly where there is low crosslinking degree (the red square zone in Figure 5.7 (a)), especially in areas where the crosslinking degree is below 52.72%, which is the average crosslinking degree in the model). These results are physically meaningful; lower material stiffness leads to a higher strain under the same external loads. The locations with high strain concentration also correlate to potential local defects. The damage evaluation based on MD & network simulations will be discussed in section 5.4.

Figure 5.7 Simulation of statistical network model under biaxial tensile load: a) crosslinking degree distribution in network model and b) distribution of equivalent strain in network model.
5.3.3 Comparison between network model and FE model

The spring-bead based network model was developed to represent the self-sensing polymer at the mesoscale. To capture the material behavior from mesoscale to macroscale a coupled network and FE model is required. To bridge different length scales the meso network model is explicitly modeled and embedded at the hot spot within a FE mesh of the structure. A notched dog bone specimen was designed for simulation under uniaxial tensile loads. The dimension of the notched dog bone specimen is shown in Figure 5.8. The network model and FE model were used concurrently to represent the material properties at the notch tip and the remaining section respectively (see Figure 5.9 (a)). A FE model without embedded springs and beads was developed (see Figure 5.9 (b)). To validate the network model based multiscale modeling approach two measures were considered: hot spot location and far field distributions. To ensure the network model is representative of the bulk material and mechanical properties both measures must remain consistent with or without a network model implemented in the FE model.

![Dimensional drawing of dog bone specimen for simulation.](image)

Figure 5.8 Dimensional drawing of dog bone specimen for simulation.
Comparison of the strain distributions obtained using the two models are shown in Figure 5.9. In both network model (Figure 5.9 (a)) and FE model (Figure 5.9 (b)) the high strain concentrations are observed near the notch tip. However, the strain distribution in the network model shows larger variability due to the variability in the crosslinking degree. The local strain distribution obtained using the network model is expected to provide more accurate estimate of the local defects at the microscale. Figure 5.10 (a) and 5.10 (b) show the comparison of strain distributions outside the hot spots in the simulations, with and without a network model. The good correlation between network model and FE model is observed, validating the accuracy of the network model with the FE model outside of the hot spot (notch tip).
5.4. Damage estimation using statistical network model

5.4.1 Evaluation of self-sensing intensity of smart polymer

In this research TCEs were used as stress-sensing particles to detect the defects in the self-sensing polymer. The epoxy resins are brittle with a propensity to crack if exposed to sufficient deformation, leading to irreversible damage in the form of micro cracking. In the high strain concentration locations of the material the force can be transferred through the bulk material to individual polymer chains, and then to the cleavable bonds on the mechanophore units. The local deformation in these regions exceeds the critical limitation of the polymer chains and results in the permanent deformation under rupture of crosslinking bonds (Buehler, 2008). This early damage precursor can be detected through the employment of TCE-containing polymers. Note that the fluorescence response of the mechanophore results from the rupture of the covalent bonds in cyclobutane. It is also related to the onset of permanent strain (deformation) of the bonds.
at the microscale. The fluorescence intensity is also directly dependent on the density of the breaking bonds. Therefore, there is a correlation between the local strain and the color changing phenomena. This relation between fluorescence intensity obtained in the experiments and the strain field predicted by in the simulation using the network model was studied.

Uniaxial compressive tests were performed to obtain the fluorescence intensities of the self-sensing material under different loads. A Test Resources Electromechanical System (with the maximum loading capability 4.4 kN) was used to conduct the compressive tests and the stress-strain curves were obtained. The tests were performed with strain control in longitudinal direction at loading rate of 1 mm/min. The maximum loading strain was 10% to ensure that the material remained in elastic stage. To monitor the fluorescence from defects in the polymer the cubic samples of polymer blends were compressed to different strains and observed under the fluorescence microscope (Nikon Elipse TE300 inverted video microscope) by exposure to 330-380 nm UV light. An image processing program, ImageJ, was used to process the fluorescent micrographs and capture the fluorescence intensities. The micrographs were taken at the same location of the specimen surface, with the size 427 μm × 325 μm. The integrated fluorescence intensity was calculated through the summation of all pixel values in the image. A quasi-linear relation was observed between the fluorescence intensity density and the loading strain (see Figure 5.11 (a)). Figure 5.11 (b) and 5.11 (c) show the microscopic images of the specimen surface and the corresponding fluorescence responses, when the loading
strain is 4% and 6% respectively. The relation between fluorescence intensity density and the loading strain can be described using a linear fit:

\[ I = 117.35 \cdot \varepsilon + 123.17 \]  

(5.1)

where \( I \) represents the observed fluorescence intensity density, and \( \varepsilon \) is the loading strain.

Figure 5.11 Fluorescence observation of self-sensing polymer. a) Integrated intensity density v.s. loading strain in fluorescence observation, b) Microscopic images and detected fluorescence of specimen at 4% strain, and c) Microscopic images and detected fluorescence of specimen at 6% strain.

Next, simulations were performed using statistical network model 1, as shown in Figure 5.5(b). Uniaxial compressive loads of same magnitude were applied to the network model. The equivalent strain in the network model was calculated and shows a quasi-linear relation between the average equivalent strain and the loading strain (Figure 5.12 (a)). The distribution of equivalent strain in the network model under different loading strain is shown in Figures 5.12 (b) - (e). The simulation result shows that the strain distribution is influenced by the local crosslinking degree. Also, both local and
average equivalent strain increases linearly with loading. A linear fit is used to describe the relation between average equivalent strain and global loading strain:

\[ \bar{\varepsilon} = 0.694 \cdot \varepsilon - 0.00081 \]  

(5.2)

where \( \varepsilon \) is the loading strain, and \( \bar{\varepsilon} \) is the average equivalent strain in the statistical network model. As shown in Equations (5.1) and (5.2) both the fluorescence intensity and the strain in the network model exhibit a quasi-linear relationship with respect to the loading strain (see Figure 5.11(a) and Figure 5.12(a)). By combining Equation (5.1) and (5.2), a relation between average strain \( \bar{\varepsilon} \) in the network model and fluorescence intensity density \( I \) from experimental observation can be obtained as follows.

\[ I = \textcolor{red}{169.09} \cdot \bar{\varepsilon} + \textcolor{red}{123.17} \]  

(5.3)

Equation (5.3) can be used as an indirect means to evaluate the observed fluorescence intensity of the self-sensing material. Since the network model does not take into account the chemical properties of the mechanopohore polymer, this simple strain based damage index can be used to simulate the change in fluorescence intensity with increase in mechanical strain.
a) 

![Graph showing the relationship between Average Equivalent Strain and Global Strain.](image)

b) 

![Heatmap illustrating a specific pattern or data distribution.](image)
Figure 5.12  Network model based simulation results: a) Average equivalent strain in network model; and equivalent strain distribution at different global strain at b) 3%, c) 5%, d) 8%, and e) 10%.

5.4.2 Strain based damage evaluation to predict failure

In the MD simulation uniaxial tensile loads were implemented on a series of representative volume element (RVE) models with different crosslinking degrees. The RVE size, molecular constitutes and number and MD simulation conditions have been discussed in chapter 4. The simulation results showed that the stress in the RVE model increased in a fluctuating curve with strain (see Figure 5.13). One important conclusion from the MD results is that the first fluctuation of the stress-strain curves takes place where the strain value is around 8% for a range of crosslinking degree. This phenomenon indicates that there is a notable microstructural defect resulting from the rupture of polymer chains at the fluctuation point. The relation between the fluctuation of the mechanical response and the damage initiation was also found in experiments and simulations conducted by other researchers. Kingsbury et al. (2011) obtained the
threshold fluctuation point of the stress-strain curve of self-sensing polymer material experimentally. It also corresponded with the onset of the mechanochemical activation in the fluorescence observation. Silberstein et al. (2013) found a non-equilibrium state resulting in local force fluctuations in glassy polymers. In the MD simulation results there is good agreement between the onset of strain softening (first fluctuation) and the onset of mechanophore activation.

![Stress-strain curve](image)

Figure 5.13 Tensile mechanical responses of self-sensing polymer at variable crosslinking degrees based on the MD simulation.

The self-sensing polymer material used in this research is brittle, which was also validated in the tensile tests. There is no obvious plastic stage in the tensile experiments. The material shows elastic behavior until failure. For brittle material the micro cracks initiating at the microscale can propagate to form a macro crack and result in structural failure. Based on the damage analysis in the MD simulation the micro cracks initiate when the local strain exceeds 8%, associated with the observed initial force fluctuation.
The material is assumed to fail when the local strain exceeds the critical value. The key issue in damage estimation is to capture this local strain using the network model. Therefore simulations were conducted using the network model 1 under a uniaxial tensile load. The equivalent strain distribution from the simulation results is shown in Figure 5.14. It is observed that the local equivalent strain increases with load. From the simulation result the loading strain is 11.2% when the maximum local equivalent strain exceeds 8%. This implies that the tensile fracture strain for this self-sensing material is 11.2% based on the strain based damage evaluation.
Figure 5.14 Equivalent strain distribution in statistical network model 1 at different loading strain: a) 5%, b) 8%, c) 10%, and d) 11.2%.

Experiments were conducted to validate this phenomenon. A set of three uniaxial tensile tests were conducted. A Test Resources Electromechanical System (with the maximum loading capability 4.4 kN) was used to conduct the tensile tests. From the experimental results the material shows elastic behavior until failure (see Figure 5.15). The average permanent tensile strain is 10.6% based on experimental observation. The error in the permanent tensile strain prediction, between experiment and simulation, is 5.36%. These observations provide confidence in the use of the computationally efficient network model to evaluate damage initiation in the self-sensing polymer material.

![Stress vs Strain Graph](image)

Figure 5.15. Experimental results of tensile tests.

5.5. Summary

In this chapter, a series of parametric studies are performed using network model to understand the microstructural behavior of the self-sensing material. The results show
that the local crosslinking degree has a significant effect on the material behavior at the microscale. A high crosslinking degree leads to low local strain, indicating stronger material performance. A larger degree of heterogeneity increases the strain gradient, which leads to higher local defects. The results of this parametric study can be used to provide design guidelines to improve the material performance. Using information from experimentally observed fluorescence intensity and the equivalent strain obtained from the statistical network model a simple relationship is established to relate the self-sensing phenomenon with the mechanical response. This strain based damage formulation was used to compare the material behavior and the results were compared with those obtained using MD simulations. Good agreement is observed between simulation and experiment.
6. Summary and Future Directions

The research presented in this dissertation is focused on multiscale modeling and damage evaluation in both metallic and polymeric materials. The objective is to develop methodologies that bridge different length scales ensuring accuracy and efficiency of simulation. The proposed framework aims to reduce computational cost by developing an efficient multiscale model and provide data for prognosis. The summarized novel points, important observation and future directions are discussed in the following sections, respectively.

6.1. Metallic material

For metallic material (Al 2024-T351), the methodology initiates at the microscale where extensive material characterization is conducted to capture the microstructural variability. A statistical volume element (SVE) model is developed to represent the critical variability at the mesoscale. A damage criterion based on single crystal plasticity theory is developed to predict the crack growth rate and crack direction simultaneously.

6.1.1 Innovative nature of this research

In this thesis, novel contributions are made to multiscale modeling and damage evaluation of metallic alloys. They can be summarized as follows:

1) A statistical volume element model is constructed to represent the material properties. Geometric and crystallographic features including grain orientation, misorientation, size, shape, principal axis direction and aspect ratio are captured by material characterization. The material characterization using EBSD scans is performed to obtain the crystallographic and geometric features of grains. EDAX and SEM
techniques are used to characterize the intermetallic particle information, including particle size, population density and spacing between neighbor particles. Simplified grain shapes are constructed because they offer ease of assembly, reduction in preprocessing time, and reduction in the total number of elements used. This approach provides a computationally efficient alternative to traditional techniques using RVE models while maintaining statistical accuracy.

2) For metallic material, a physics based multiscale damage criterion is developed to simulate the fatigue crack initiation. Two stages of crack initiation, including crack nucleation at the microscale and formation of major crack at the mesoscale are captured. The crack growth rate and probable directions are estimated using the multiscale damage criteria simultaneously.

3) Single crystal plasticity theory is used to capture the dislocation on the slip planes of the face centered cubic (FCC) structure. At the intermetallic particles, where micro cracks tend to nucleate, the four slip planes constitute probable crack planes. At each intermetallic particle, the crack growth direction can be affected by slip in a combination of any or all of the four slip planes.

4) A dependent factor is introduced to take into account the relation of the damage increments between different slip planes. The dependent factor for FCC structure is calculated using the cosine values of the angle between any two slip planes. The modified damage criteria accommodate multiple slip planes and prevent the overestimation of damage accumulation.
5) The multiscale model is further extended to estimate crack initiation under thermal mechanical fatigue (TMF) loading. The thermal effects on damage evolution including mechanical responses (thermal creep, elastic modulus and yield strength etc.) and material properties (thermal expansion factor, density etc.) are considered. The Harpor Dorn creep model (Harpor, 1957; Kloc, 1977; Ruano, 1988; Wang, 1996; Langdon, 2002), which accounts for the grain boundary sliding effect and diffusional flow theory, is used to apply the SVE model and damage criteria to thermal fatigue issues.

### 6.1.2 Important observations

1) The SVE model was developed by capturing grain orientation and misorientation while implementing the average response of geometrical features, including grain principal axis direction, grain size, grain shape, and aspect ratio. The results obtained show that the model can represent the material properties and capture the damage evolution as accurately as the RVE model.

2) Before constructing the SVE model, a series of parametric studies were conducted to understand the influence of grain features on the mechanical response. The inference is that the principal axis direction and the grain shape are the most effective features. The aspect ratio has the weakest influence on the mechanical response of the SVE.

3) For Al 2024, there are two physically and chemically distinguishable types of intermetallic particles, Al$_7$Cu$_2$Fe ($\beta$-phase) and CuMgAl$_2$ ($S$-phase). From the SEM observation, all micro cracks are incubated from $\beta$-phase particles. So the iron-rich intermetallic particles alone are considered to influence crack nucleation. These features of the effective intermetallic particles ($\beta$-phase), including population density and particle
size, were obtained and used to construct the nucleation sites in the SVE model. The results indicate that the developed multiscale model can capture micro crack nucleation at the microscale and growth at the mesoscale.

4) Experiments were conducted to validate the developed multiscale model. Lug joints were tested under uniaxial fatigue loads and uniaxial TMF loads. Cruciform specimens were tested under biaxial FALSTAFF loading. The results from the multiscale model showed very good correlation with the test results.

6.1.3 Future directions

The developed multiscale model can be further extended by constructing 3D SVEs and corresponding physics based damage criterion to predict crack growth in complex structures. Element deletion approach can be implemented for progressive damage simulations using a user-defined element (UEL) subroutine that interfaces with the Abaqus software. With some modifications, the methodology developed can be applied to other metallic materials such as Al 7075 and Al 6061.

6.2. Self-sensing polymer part

For the self-sensing polymer material, a spring-bead based network model is constructed to bridge the MD model at the microscale and the FE model at the macroscale. Parametric study using the network model is implemented to investigate the influence of the microscopic variability on the material behavior. The high efficiency network model can also capture the self-sensing phenomenon and estimate the damage evolution.

6.2.1 Innovative nature of this research
In this thesis, novel contributions are made to multiscale modeling and damage evaluation of a self-sensing polymer. They can be summarized as follows:

1) A spring-bead based network model is developed to represent material properties of self-sensing polymer. MD simulation results including the statistical distribution of crosslinking degree and corresponding mechanical properties is used to construct the spring-bead model. Various arrangements of spring-bead models are designed and compared to obtain the optimal network model configuration. Among the candidate combinations, the 8 neighbor based network model is found to be optimal, considering structural stability, representation of isotropic property, and computational efficiency. KS function is introduced to bridge the mechanical properties of the MD model and network model using the mechanical equivalence optimization.

2) Parametric study using the network model is performed and the results describe the influence of microscopic variability on material behavior. A highly heterogeneous microstructure combined with a large difference between neighbor crosslinking degrees can increase the probability of damage evolution. A relation between crosslinking degree distribution and strain distribution is observed: high strain concentration is observed in areas of low crosslinking degree. This result indicates that a lower value of material stiffness (or low crosslinking degree) leads to higher potential local defects.

3) The network model can effectively represent the self-sensing phenomenon of the smart polymer using the equivalent strain index. A linear fit between average equivalent strain in network model and observed fluorescence intensity is obtained. The molecular dynamics simulation and network model based simulation are implemented to estimate
the damage evolution of the material. The microscopic strain threshold is obtained from MD simulation results and used to estimate the global fracture limit.

6.2.2 Important observations

1) The multiscale approach bridges the high accuracy MD model at the microscale and high efficiency FE model at the macroscale. Statistical distribution of crosslinking degree of the polymer is captured in the network model to represent the heterogeneous material properties at the microscale.

2) A series of parametric studies based on network model were performed to understand the influence of microscopic variability such as the distribution of crosslinking degree on material behavior. The results indicate that the local crosslinking degree has a significant effect on the material behavior at the microscale. A high crosslinking degree leads to low local strain, which indicates stronger material performance. It also implies that a larger difference between neighbor crosslinking degrees can increase the strain gradient, leading to potential local defects. The results of the parametric study can help to understand the microstructural behavior and enhance the material performance by controlling the effective microscopic variability in the material design process.

3) Compared to MD simulations, the spring-bead based network model enhances the simulation efficiency by 300 times without compromising the accuracy. A comparison of the experimental and simulation results shows that the spring-bead based network model can capture the global mechanical properties of the self-sensing polymer.
4) A strain based damage criterion has been developed to predict damage initiation in the self-sensing material. From MD simulation results, the first fluctuation in the linear stress-strain curves takes place at the strain value of around 8% for all crosslinking degrees. This indicates that there is a notable microstructural defect resulting from the elongation of bonds in the polymer chains. From the network model based simulation, the loading strain is 11.2% when the maximum local equivalent strain exceeds 8%. This concludes that the tensile fracture strain for this self-sensing material is 11.2% based on the strain based damage evaluation.

5) The statistical network model is also capable of capturing the self-sensing phenomenon using a relation between local equivalent strain in network model and the observed fluorescence intensity. A governing function is obtained to describe the relation between equivalent strain index and the fluorescence intensity density. Good agreement is obtained between the experiment and simulation, of which the error is lower than 4%.

6.2.3 Future directions

The developed network model can be further extended to characterize complex material behavior including elasticity, plasticity, viscosity and thermomechanics by introducing a set of series-parallel connected nonlinear damper-spring models. The network model can also be used to simulate crack propagation by removing springs in the crack path. 3D crosslinked network model of the polymer can also be developed to extend the applicability of the simulation framework.
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