WAVELET TRANSFORMATION BASED MULTI-TIME SCALE METHOD FOR FATIGUE CRACK INITIATION IN POLYCRYSTALLINE ALLOYS

DISSERTATION

Presented in Partial Fulfillment of the Requirements for the Degree Doctor of Philosophy in the Graduate School of the Ohio State University

By
Pritam Chakraborty, MS
Graduate Program in Mechanical Engineering

The Ohio State University
2012

Dissertation Committee:
Professor Somnath Ghosh, Advisor
Professor June K. Lee
Professor Jack Joseph McNamara
Professor Vish V. Subramaniam
ABSTRACT

Fatigue crack nucleation in polycrystalline alloys is strongly influenced by the crystallographical and morphological features of the underlying microstructure. This necessitates the incorporation of microstructural effects in the fatigue crack nucleation models developed for these alloys. Crystal plasticity based finite element (CPFE) simulations of statistically equivalent microstructures coupled with a physically motivated crack nucleation law captures the microstructural effects and can accurately predict fatigue life of polycrystalline alloys. However, fatigue analysis for large number of cycles by single time scale CPFE simulations is computationally exhaustive. To alleviate this problem, a wavelet transformation based multi-time scale (WATMUS) method is developed in the present work. In the WATMUS method, the wavelet based transformation of variables decouples the slow monotonic evolution from the fast oscillatory behavior and permits integration in time steps of cycles to provide significant computational benefit. This method has no assumption of periodicity in the evolution of variables and hence can be used to decouple the strongly non-linear crystal plasticity equations. The accuracy and efficiency of the WATMUS method is compared with conventional single time scale integration scheme through cyclic CPFE simulations of Ti-6242.

The load and microstructure sensitive fatigue behavior of Ti-6242 is investigated using a physically motivated non-local crack initiation law and the proposed WATMUS method based CPFE simulations. The crack nucleation model is based on dislocation pile up and stress concentration at grain interfaces, caused by inhomogeneous plastic deformation in
the microstructure. The dislocation pile up length and stress concentration increases with load cycles, causing macroscopic crack nucleation. The number of cycles to nucleate a crack and the microstructural feature characteristics at the initiation site, predicted by the model shows good agreement with experimentally observed values.

A variable is defined based on experimentally observed crystallographical feature characteristics at the crack initiation site to relate the sensitivity of fatigue crack nucleation to the underlying microstructure. From cyclic CPFE simulations on different statistically equivalent microstructures of Ti-6242, a correlation between this local microstructural variable and number of cycles to nucleate a crack is observed. Additionally, the sensitivity of crack nucleation to the characteristics of the applied load is studied by performing WAT-MUS based CPFE simulations on a statistically equivalent microstructure. The predicted number of cycles to nucleate a crack agrees with experimentally observed trends.
Dedicated to my Father, Mother, Elder Sister and Brother
ACKNOWLEDGMENTS

I would like to express my deepest thanks to my advisor Prof. Somnath Ghosh. His guidance, encouragement and support is the single largest factor in the success of the research presented in this dissertation. His vision and never ending attitude to extend the frontiers of research has inspired me immensely.

In addition I would like to thank Prof. J. K. Lee, Prof. V. V. Subramaniam and Prof. J. J. Mcnamara for being on my committee. I want to thank Jim Giuliani for his help in working with the super-computers. My deepest thanks to my friend and lab-mate Daniel for his constant help and support during the PhD period. I would like to thank Josh, Erik, Shahriyar, Deepu, Masoud, Anand, Piyush, Srinath, Santosh, Hyun Sik, Sajedur, Kapil, Bodhayan and all the previous members of our lab for the good time I spent with them. I would also like to thank my friends at Columbus for making my stay so memorable.

I would like to acknowledge Dr. Clark Cooper, Program Manager US National Science Foundation (grant # CMMI-0800587), Dr. Julie Christodoulou, Program Manager Office of Naval Research (grant # N00014-05-1-0504), Dr. David Stargel, Program Manager Air Force Office of Scientific Research (DCT grant # FA9550-09-1-0452) and Ohio Supercomputer Center (grant # PAS813-2) for supporting this effort.

My special thanks to my fiancee Sugata for her endless support and encouragement. Finally I would like to express my heartfelt gratitude to my parents, my sister and my brother for their unwavering support and motivation.
VITA

1979 . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . Born - Mumbai, India

2002 . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . B. E. in Mechanical Engineering, Jadavpur University, Kolkata, India.

2004 . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . M. Tech. in Mechanical Engineering, Indian Institute of Technology Kanpur, India.

2006 . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . Research Engineer at GE Global Research Center, Bangalore, India.

2006-2011 . . . . . . . . . . . . . . . . . . . . . . . . . . . . Graduate Research Assistant, The Ohio State University, Columbus, Ohio.

PUBLICATIONS


FIELDS OF STUDY

Major Field: Mechanical Engineering

Specialization: Computational Mechanics of Materials: Prof. Somnath Ghosh
# TABLE OF CONTENTS

Abstract ................................................................. ii
Dedication ................................................................. iii
Acknowledgments ......................................................... v
Vita .............................................................................. vi
List of Figures ............................................................. x
List of Tables ............................................................... xiv

<table>
<thead>
<tr>
<th>CHAPTER</th>
<th>PAGE</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Introduction ......................................................... 1</td>
</tr>
<tr>
<td>1.1</td>
<td>Organization of the thesis ......................................... 6</td>
</tr>
<tr>
<td>2</td>
<td>Wavelet Transformation based Multi-time Scale Method ........ 8</td>
</tr>
<tr>
<td>2.1</td>
<td>Extrapolation based methods ..................................... 10</td>
</tr>
<tr>
<td>2.2</td>
<td>Multi-time scale methods ......................................... 11</td>
</tr>
<tr>
<td>2.2.1</td>
<td>1-d viscoplastic model ............................................ 12</td>
</tr>
<tr>
<td>2.2.2</td>
<td>Asymptotic expansion based methods ............................ 15</td>
</tr>
<tr>
<td>2.2.3</td>
<td>Almost Periodic Temporal Homogenization (APTH) operator</td>
</tr>
<tr>
<td></td>
<td>based method ....................................................... 17</td>
</tr>
<tr>
<td>2.2.4</td>
<td>Method of parameterized locally invariant manifolds .......... 20</td>
</tr>
<tr>
<td>2.3</td>
<td>Wavelet transformation based multi-time scale method for first order</td>
</tr>
<tr>
<td></td>
<td>ODEs ................................................................. 24</td>
</tr>
<tr>
<td>2.3.1</td>
<td>Wavelets overview ................................................ 26</td>
</tr>
<tr>
<td>2.3.2</td>
<td>Coarse scale rate equations ..................................... 28</td>
</tr>
<tr>
<td>2.4</td>
<td>Wavelet transformation based multi-time scale method for initial boundary value problems involving damage .......... 35</td>
</tr>
<tr>
<td>2.4.1</td>
<td>Selection of evolving coefficients .............................. 38</td>
</tr>
<tr>
<td>2.4.2</td>
<td>Representation using reduced set of coefficients and compari-</td>
</tr>
<tr>
<td></td>
<td>son of accuracy between discrete wavelet and Fourier transforms 39</td>
</tr>
</tbody>
</table>

viii
2.4.3 Quasi-Newton Method ........................................ 41
2.4.4 Non-uniform discrete wavelet transform ...................... 42
2.4.5 Automatic selection of cycle jumps ............................ 44
2.5 Conclusions .................................................... 45

3 Numerical Examples ................................................ 58
3.1 Kinetics of phase transforming material .......................... 59
  3.1.1 Case 1: Constant load ........................................ 60
  3.1.2 Case 2: Cyclic load .......................................... 62
3.2 1d viscoplastic model with heterogeneous properties ............ 65
3.3 Crystal plasticity based FE model for Ti-alloys .................... 71
3.4 Crystal plasticity based FE model for nickel based superalloys .... 89
3.5 Conclusion ....................................................... 98

4 Microstructural Sensitivity of Crack Initiation in Ti-6242 ........... 104
4.1 Non-local crack initiation model ................................ 105
4.2 Calibration and validation of critical stress intensity factor $R_c$ .... 111
  4.2.1 Calibration .................................................. 112
  4.2.2 Validation .................................................. 113
4.3 Microstructural sensitivity of fatigue crack nucleation ............. 114
4.4 Sensitivity of crack nucleation to load characteristics ............. 117
4.5 Conclusion ....................................................... 119

5 Conclusions and Future Work ........................................ 128

Bibliography ........................................................ 131
### LIST OF FIGURES

<table>
<thead>
<tr>
<th>FIGURE</th>
<th>PAGE</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.1</td>
<td>Evolution of plastic variables obtained from single time scale integration of the 1-d viscoplastic model for 200 cycles: (a) $\epsilon^p$ (b) $g^c$ and corresponding magnified view</td>
</tr>
<tr>
<td>2.2</td>
<td>Evolution of stress in the viscoplastic model: (a) Overall response (b) Variations at specific cycles</td>
</tr>
<tr>
<td>2.3</td>
<td>Evolution of plastic strain in the viscoplastic model: (a) Average response (b) Oscillatory response at specific cycles</td>
</tr>
<tr>
<td>2.4</td>
<td>Coarse scale response from APTH operator based multi-time scale method: (a) Coarse scale time step $\Delta t=2$ sec (b) Coarse scale time step $\Delta t=3$ sec</td>
</tr>
<tr>
<td>2.5</td>
<td>Evolution of viscoplastic variable subjected to cyclic strain: (a) Single time scale response (b) Magnified view of response over few cycles (c) High frequency fine time scale response over one load period (d) Coarse time/Cycle scale evolution corresponding to the value at start of cycle</td>
</tr>
<tr>
<td>2.6</td>
<td>Wavelet transformation of an oscillatory signal. High and low resolution basis functions capture the fast and slow change of the signal</td>
</tr>
<tr>
<td>2.7</td>
<td>Relative error $\epsilon$ in log scale as described in equations 2.55 and 2.56, of coarse scale integration for the viscoplastic model using different coarse scale rate equations defined in section 2.3.2 with varying $\Delta N$ and $\Delta N_p=2$: (a) $\epsilon_0^p$ (b) $\epsilon^p$ over a cycle</td>
</tr>
<tr>
<td>2.8</td>
<td>Comparison of local error in $\epsilon_0^p$ obtained from coarse scale integration using rate equation (i) defined in section 2.3.2 with different $\Delta N$ and $r=1$.</td>
</tr>
<tr>
<td>2.9</td>
<td>Comparison of coarse scale evolution for different $\Delta N$ and $r=1$ using coarse scale rate equation (i) defined in section 2.3.2: (a) $\epsilon_0^p$ with cycles (b) Reconstructed $\epsilon^p$ at cycle 963 from coarse variables</td>
</tr>
</tbody>
</table>
2.10 Comparison of global error in $\epsilon_0^p$ at cycles 259 and 963 obtained from coarse scale integration with different $\Delta N$ and $r=1$ using coarse scale rate equation (i) defined in section 2.3.2. ........................................ 51

2.11 Evolution of a nodal displacement degree of freedom within cycle: (a) 10 (b) 8000. ................................................................. 52

2.12 Coefficients from discrete wavelet transform at 10th cycle. .................. 53

2.13 Number of evolving coefficients based on different values of $\eta$. ............... 53

2.14 Comparison of reconstructed and exact response at 8000th cycle for different set of evolving coefficients: (a) $n_{evol}$=43 (b) $n_{evol}$=65. .................... 54

2.15 Coefficients from discrete Fourier transform at 10th cycle. .................... 55

2.16 Number of evolving coefficients based on different values of $\eta$. ............... 55

2.17 Comparison of reconstructed and exact response at 8000th cycle for different set of evolving coefficients: (a) $n_{evol}$=49 (b) $n_{evol}$=87. .................... 56

2.18 Comparison of error $e = \frac{|y(N,\tau)-\tilde{y}(N,\tau)|}{|y(N,\tau)|}$ in reconstruction for different set of evolving coefficients between discrete wavelet and Fourier transform. ........ 57

3.1 Evolution of volume fraction $\lambda$ under constant applied stresses as obtained from single time scale and method of parameterized invariant manifold [Acharya and Sawant, 2006]. ........................................ 61

3.2 Comparison of evolution of coarse scale variable $\lambda_0$ obtained from WAT-MUS methodology and single time scale solution for 2 different time period: (a) T=0.5 sec (b) T=1 sec. ........................................ 63

3.3 Evolution of volume fraction $\lambda$ under cyclic applied stresses. ............... 64

3.4 Comparison of evolution of coarse scale variable $\lambda_0$ obtained from WAT-MUS methodology and single time scale solution. ...................... 64

3.5 1-d viscoplastic finite element model with 2 elements. ......................... 65

3.6 Evolution of $\epsilon_0^p$ of element 1 from 1d viscoplastic finite element model: (a) Single time scale response for 2000 cycles (b) Response in 800th cycle. 68

3.7 Comparison of evolution of $\epsilon_0^p$ with cycles in the 1st element. ............ 69

3.8 Comparison of $\epsilon_0^p$ in the 1st element at 2000th cycle. .................... 69

3.9 Variation of number of evolving coefficients solved in the modified cycle scale FE method with cycles. ........................................ 70
3.10 Microstructure of forged Ti-6242 alloy: (a) SEM image (b) Schematic of the lathe structure in the $\alpha + \beta$ colonies. 71

3.11 Microstructural distribution of c-axis orientation. 77

3.12 FE model of statistically equivalent microstructure of Ti-6242: (a) Mesh (b) Boundary conditions. 79

3.13 Comparison of evolution of coarse internal variables: (a) $F_{0,22}^p$ (b) $g_0^\alpha$. 81

3.14 Relative error $e(N, \tau) = \frac{\|y(N, \tau) - \tilde{y}(N, \tau)\|}{\|y(N, \tau)\|}$ of fine scale evolution of internal variables at 211$^{th}$ cycle reconstructed from coarse scale variables ($\tilde{y}(N, \tau)$) and single time scale solution ($y(N, \tau)$): (a) $F_{22}^p$ (b) $g^\alpha$ (c) $\sigma_{22}$. 82

3.15 Comparison of distribution of $\sigma_{22}$ (MPa) in the microstructure at $N = 211$ and $\tau = 1$ sec as obtained from WATMUS and single time scale simulation (a) WATMUS (b) Single time scale. 83

3.16 Comparison of distribution of $F_{22}^p$ in the microstructure at $N = 211$ and $\tau = 1$ sec as obtained from WATMUS and single time scale simulation (a) WATMUS (b) Single time scale. 84

3.17 Comparison of stress distribution in the microstructure along a material line at $N = 211$ and $\tau = 1$ sec as obtained from WATMUS and single time scale simulation: (a) $\sigma_{22}$ (b) relative error in $\sigma_{22}$. 85

3.18 Evolution of coarse internal variables from WATMUS CPFE simulation: (a) $F_{0,22}^p$ (b) $g_0^\alpha$. 86

3.19 Oscillatory response of internal variables at a material point at 300,000$^{th}$ cycle, reconstructed from coarse variables obtained from WATMUS CPFE simulation: (a) $F_{22}^p$ (b) $g^\alpha$. 87

3.20 Evolution of oscillatory stress $\sigma_{22}$ with cycle at a material point. 88

3.21 Evolution of $\sigma_{22}$ along a material line in the microstructure with cycles. 88

3.22 Microstructure of nickel based superalloy René 104 showing the $\gamma$ and $\gamma'$ phase [Karthikeyan et al., 2006]. 90

3.23 Schematic of dwell load for one cycle. 97

3.24 FE model to demonstrate the accuracy of WATMUS method for nickel based super alloys: (a) FE mesh (b) Euler angle distribution. 99

3.25 Comparison of coarse scale evolution of internal variables at a material point: (a) $F_{0,22}^p$ (b) $s_0^\alpha$. 100
3.26 Relative error in the reconstructed response at a material point: (a) $F_{22}^p$ (b) $\sigma_{22}^2$. .............................................................. 101

3.27 Distribution of $F_{22}^p$ in the microstructure at $N = 700$ and $\tau = 121$ sec: (a) Single time scale simulation (b) WATMUS simulation. ............................... 102

3.28 Distribution of $\sigma_{22}^2$ in the microstructure at $N = 700$ and $\tau = 121$ sec: (a) Single time scale simulation (b) WATMUS simulation. ............................... 103

4.1 Stress variation along a material line in the microstructure. A and C are the hard regions, B and D are the soft regions. (a) $\sigma_{22}^2$ distribution and its evolution with cycles (b) Schmid factor (SF) distribution along the material line. ............................................................... 121

4.2 Schematic of micro crack formation due to dislocation pile up at a hard soft grain interface [Anahid et al., 2011]. ......................................................... 122

4.3 Volume averaged stress-strain plot of statistically equivalent microstructure 1 (MS1) obtained from constant strain rate CPFE simulations. ............... 122

4.4 Evolution of maximum nodal R evaluated in every cycle (N) at $\tau = 121$ sec of MS1. .............................................................. 123

4.5 Volume averaged stress-strain plot of statistically equivalent microstructure 2 (MS2) obtained from constant strain rate CPFE simulations. ............... 123

4.6 Evolution of maximum nodal R evaluated in every cycle (N) at $\tau = 121$ sec of MS2. .............................................................. 124

4.7 Softness index (SI) distribution for MS1 and MS2. ................................ 124

4.8 Comparison of softness index distribution and yield strength of MS1 and MS3: (a) Softness index (SI) distribution (b) Volume averaged stress-strain obtained from constant strain rate FE simulations. ......................... 125

4.9 Distribution of volume fraction of hard grains and corresponding surface area fractions of neighboring soft grains in MS1, MS2 and MS3. ............. 126

4.10 Comparison of evolution of $R$ at the crack nucleation site for MS1, MS2 and MS3. .............................................................. 126

4.11 Evolution of $R$ with Cycles for 4 different fatigue load cases A,B,C and D described in section 4.4. .............................................................. 127

4.12 Evolution of $R$ with Cycles for 4 different fatigue load cases A,E,F and G described in section 4.4. .............................................................. 127

xiii
## LIST OF TABLES

<table>
<thead>
<tr>
<th>TABLE</th>
<th>PAGE</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.1</td>
<td>Slip plane normal $n^a$ and direction $m^a$ for APB shearing</td>
</tr>
<tr>
<td>3.2</td>
<td>Twin plane normal $n^a$ and direction $m^a$ for microtwinning</td>
</tr>
<tr>
<td>3.3</td>
<td>The values of latent hardening matrix $q^{a\beta}$ based on interactions between different systems</td>
</tr>
<tr>
<td>3.4</td>
<td>Parameters for APB shearing based inelastic deformation in activation energy based model</td>
</tr>
<tr>
<td>3.5</td>
<td>Parameters for microtwinning based inelastic deformation in activation energy based model</td>
</tr>
<tr>
<td>3.6</td>
<td>Parameters for microtwin nucleation model</td>
</tr>
<tr>
<td>4.1</td>
<td>Comparison of number of cycles to crack initiation as predicted from the model and experiments for MS2.</td>
</tr>
<tr>
<td>4.2</td>
<td>Comparison of microstructural features at crack initiation as predicted from the model and experiments for MS1 and MS2.</td>
</tr>
<tr>
<td>4.3</td>
<td>Microstructural features at crack initiation site as predicted from the model for MS3.</td>
</tr>
</tbody>
</table>
CHAPTER 1
INTRODUCTION

Polycrystalline materials like Ti-alloys or nickel based superalloys are widely used in automotive and aerospace industry due to their desirable mechanical properties. During service, these materials are exposed to cyclic loading conditions which results in their fatigue failure. The fatigue life in these alloys shows large scatter due to strong influence of the underlying microstructure. Hence for accurate predictions, the sensitivity of fatigue behavior to the polycrystalline microstructure should be considered. Conventional lifing methods only consider macroscopic parameters like applied stresses, cyclic frequency, loading waveform, etc. to determine fatigue life and fatigue strength [Suresh, 1998, Laird, 1976, Fleck et al., 1994, Hashimoto and Pereira, 1996]. For example, in the total life approaches like the stress-life and strain-life methods, the cycles to failure is determined based on stress amplitude and accumulated strain respectively [Coffin, 1973]. These approaches have been modified to consider notch effects and fatigue failure under variable amplitude loading (Palmgren-Miner rule of cumulative damage). Defect or damage tolerance approaches are also widely used to determine the number of cycles to propagate an initial crack to a critical size [Paris, 1964]. Parameters such as threshold stress intensity factor, fracture toughness, limit load, allowable strain or allowable compliance are defined to characterize fatigue behavior of a material. In these conventional approaches, the effect of microstructure on fatigue behavior is addressed macroscopically through shifts in data curves obtained from extensive testing. Hence the predictions of these methods can suffer from significant
error due to the absence of underlying physical mechanisms and information of the material microstructure in their representations. Mechanistic calculations of polycrystalline microstructures can prove effective in capturing the microstructural influence on fatigue behavior and has been used in the present work.

For the mechanistic calculations, crystal plasticity based finite element models of statistically equivalent microstructures have been used in [Mineur et al., 2000, McDowell and Dunne, 2010, Chu et al., 2001, Ghosh et al., 2010, Dawson, 2000, Dawson and Marin, 1997] to study the deformation behavior of polycrystalline alloys. In the crystal plasticity models, the overall plastic deformation of polycrystalline aggregates is dictated by slip on individual slip systems in each grain [Kalidindi et al., 1992, Anand and Kothari, 1996, Balasubramanian, 1998]. The amount of slip on a slip system in a grain depends on the grain orientation and slip resistances. Kinematic hardening and grain size effects are incorporated in crystal plasticity based evolution laws to model fatigue [Morrissey et al., 2001, Goh et al., 2001, Goh et al., 2003] and creep [Venkataramani et al., 2007] response in metallic alloys. The morphological and crystallographical features of the microstructure are represented in a statistical sense in the crystal plasticity based finite element models [Deka et al., 2006, Hasija et al., 2003, Venkatramani et al., 2006, Venkataramani et al., 2007]. These representative microstructures satisfy the distributions of orientation, misorientation, size, shape of grains and microtexture obtained from OIM scans of samples of the polycrystalline alloy [Groebert et al., 2008a, Groebert et al., 2008b]. The use of statistically equivalent representation not only reduces the number of grains in the finite element simulations but also captures some of the key features of the microstructure that affects its macroscopic and microscopic response.

Although CPFE simulations accurately capture the deformation behavior of polycrystalline alloys, the use of conventional time integration schemes for the non-linear damage evolution laws at large applied stresses and strains require very fine time steps. This can
lead to exorbitant computational requirements when fatigue analysis needs to be performed for large number of cycles, since reduced time steps may be required at every cycle of the loading process. To resolve this computational prohibitiveness, fatigue life predictions are performed in [Bennett and McDowell, 2003, Sinha and Ghosh, 2006, Turkmen et al., 2003] by extrapolating the results based on few number of cycles. However extrapolation can lead to considerable error and cannot be used for fatigue life predictions where accuracy in the evolution of local microstructural variables is of utmost importance. Hence for accurate predictions, it is desirable to perform simulations till the onset of the failure event being analyzed. Multi-time scale methods based on decoupling the low and high frequency responses and integrating the low frequency response with coarser time steps, can be used to perform accelerated finite element simulations for large number of cycles. However, the existing multi-time scale methods like the method of separation of motions [Blekhman, 2000, Thomsen, 2004], asymptotic expansion based methods [Yu and Fish, 2002, Manchiraju et al., 2007, Manchiraju et al., 2008] and almost periodic temporal homogenization operator based method [Oskay and Fish, 2004b, Oskay and Fish, 2004a], assumes local periodicity or almost periodicity of the variables in the temporal domain and hence cannot be used to decouple the response of crystal plasticity variables which show non-periodic evolutions and spatial localizations. The multi-time scale method based on parameterized locally invariant manifolds, described in [Acharya and Sawant, 2006, Acharya, 2005, Sawant and Acharya, 2005], has no assumption of periodicity or almost periodicity. However the method involves a parameterization procedure to obtain the coarse scale evolution and hence has limited applicability. In the present work, a wavelet transformation based multi-time scale (WATMUS) method is developed that overcomes the drawbacks of the existing methods and performs accelerated CPFE simulations.

WATMUS based CPFE simulations of statistically equivalent microstructures are used in the present work to study the microstructurally driven load dependent fatigue behavior
of Ti-alloys at temperatures where diffusion mediated deformation mechanisms are absent [Bache, 2003, Evans et al., 1994, Sinha et al., 2004]. From the different stages in the fatigue failure of metallic materials [Suresh, 1998], crack nucleation is the life limiting phenomenon in Ti-alloys [Rokhlin et al., 2005] and the focus of the current study. The microstructure of Ti-alloys have different phases depending on the heat treatment and work done on them [Lutjering and Williams, 2007]. The α phase has hexagonal close packed (hcp) crystal structure which is strongly anisotropic in its plastic response and the β phase has body centered cubic (bcc) structure with a fairly homogeneous plastic behavior. Strongly anisotropic plastic behavior of the α phase is due to widely differing resistances to slip on different slip systems. For instance, the resistance to dislocation glide of the \(<c+a>\) slip systems on the pyramidal plane is 3–4 times higher than the \(<a>\) slip systems on the basal or prismatic planes [Hasija et al., 2003, Deka et al., 2006, Venkataramani et al., 2007]. Depending upon the orientation of a grain relative to the loading direction, different slip systems experience different levels of driving force or resolved shear stresses for slip. Since the basal and prismatic \(<a>\) slip systems have lower slip deformation resistances, grain orientations that cause more resolved shear stresses on them experience more plastic deformation (soft grains) than those that activates the pyramidal \(<c+a>\) slip systems (hard grains). At the shared boundary of hard and soft grain pairs in the microstructure, the compatibility condition results in large elastic strains and stresses in the hard grain. This microstructure dependent stress concentration is considered as the driver for crack nucleation [Bache, 2003, Venkataramani et al., 2006, Venkataramani et al., 2007]. The CPFE simulations of statistically equivalent microstructures of Ti-alloys captures this stress rise accurately and hence a crack nucleation law is developed based on it [Anahid et al., 2011].

In the physically motivated non-local crack nucleation model, it is assumed that at the interfaces of hard soft grains, micro-cracks develop due to dislocation pile-up in the soft
grain and their growth into a macroscopic crack nucleus is aggravated by the high stresses in the adjacent hard grains. Since the length scale of micro-cracks are much smaller than the grain dimensions, the stresses in the hard grain are considered as far field stresses and a stress intensity factor similar to linear elastic fracture mechanics is constructed based on the micro-crack length and the local stresses. Crack nucleation is assumed to happen when stress intensity factor at any material point at the hard soft grain interfaces exceeds some critical stress intensity factor. The critical stress intensity factor is a material parameter and is calibrated from dwell fatigue experiments on samples of Ti-6242. The cycles to crack nucleation as predicted from this model is validated with experiments [Anahid et al., 2011].

A comparison of the non-local crack initiation model with some of the existing models to predict crack nucleation in Ti-6242 is performed in [Anahid et al., 2011]. These models are based on local stress, energy and void growth and their predictions are compared with experimentally observed life. In the stress based models [Stroh, 1954, Kirane and Ghosh, 2008] the effect of evolving plastic strain accumulation in the adjacent soft grain is neglected and crack nucleation is only related to the local stresses at a material point. However from CPFE simulations it is observed that stress evolution saturates early and thus the stress based models show error in their predictions. Also the stress based model proposed in [Stroh, 1954] considers only mode I crack formation. In the energy based model [Lin et al., 1986, Yao et al., 2007], nucleation of crack is assumed to happen at a cycle when the associated Gibb’s free energy reaches a maximum. However when this model is applied to Ti-6242, the predictions differ from the experimentally obtained values [Anahid et al., 2011]. Also the model predicts initiation in microstructures insensitive to crack nucleation. The void growth model proposed in [Bhat and Fine, 2001] is based on the evolution of a parameter that depends on the ratio of hydrostatic stress and Von Mises stress, and equivalent plastic strain. The cycles to crack initiation for Ti-6242 as predicted by this model also differs from the experiments [Anahid et al., 2011]. The non-local crack
nucleation model captures the physical mechanism causing crack initiation in Ti-6242 and hence more accurate in its prediction.

In the present work, the sensitivity of fatigue crack nucleation to the morphological and crystallographical features of the underlying microstructure and the characteristics of the applied load for Ti-6242 is studied. The WATMUS method based CPFE simulations of statistically equivalent microstructures subjected to cyclic loading is performed. The crack nucleation model developed in [Anahid et al., 2011] is used to study the microstructural sensitivity of fatigue life in Ti-6242. Premature failure under dwell load as compared to normal cyclic load has been observed in Ti-6242 [Sinha et al., 2004, Williams, 2006, Bache, 2003]. CPFE simulations under normal cyclic load and dwell load with maximum stress at 95% of yield stress is performed to demonstrate the fidelity of the crack nucleation model to capture this behavior.

1.1 Organization of the thesis

The organization of the thesis is as follows. In chapter 2, the limitations of some of the existing multi-time scale methods and the general framework of the WATMUS method to perform cycle scale integration of initial boundary value problems is presented. In chapter 3, four different numerical examples are solved using the proposed multi-time scale methodology. In the first example, cycle scale rate equations are derived and solved for evolution of volume fraction of phase transforming material. In the second example the method is applied to solve a 1-d viscoplastic model with heterogeneous properties. In the third example, the single time and coarse scale framework for CPFE model for Ti-alloys is presented. The coarse scale problem is solved and compared with single-time scale solutions to demonstrate the accuracy and efficiency of the proposed multi-time scale method. In the fourth example the WATMUS method is used to perform CPFE simulations for nickel based superalloys. The crack nucleation model and a study of sensitivity of crack
nucleation to microstructural features and load characteristics is presented in chapter 4.
The thesis is concluded in chapter 5.
CHAPTER 2
WAVELET TRANSFORMATION BASED MULTI-TIME SCALE METHOD

Crystal plasticity based finite element (CPFE) simulations of statistically equivalent microstructures under cyclic loading conditions are desirable to accurately capture the fatigue behavior of polycrystalline alloys. In crystal plasticity models, the evolution of variables are governed by spatio-temporal differential equations which are integrated using finite element method where the domain is discretized into a finite number of elements and spatial distributions of variables are approximated using piecewise polynomial functions. Temporal evolution is obtained by equilibrating the spatially discretized system at certain time points. When spatio-temporal gradients are large, accuracy of the numerical integration scheme permits very fine time steps and this can significantly increase the computational requirements.

Due to exorbitant computational expense associated with CPFE simulations for large number of cycles, variables are extrapolated from few cycles of simulation to perform fatigue life predictions in [Bennett and McDowell, 2003, Sinha and Ghosh, 2006, Turkmen et al., 2003]. However extrapolation can lead to considerable error and cannot be used where accuracy in evolution of variables is of utmost importance. Multi-time scale methods based on decoupling the low and high frequency responses and integrating the low frequency response with coarser time steps, can be used to perform accelerated simulations with sufficient accuracy for large number of cycles. However, the existing multi-time
scale methods like the method of separation of motions [Blekman, 2000, Thomsen, 2004], asymptotic expansion based methods [Yu and Fish, 2002, Manchiraju et al., 2007] and almost periodic temporal homogenization operator based method [Oskay and Fish, 2004b], assumes local periodicity or almost periodicity of the variables in the temporal domain. These assumptions restrict the applicability of these methods to problems having slow or dominant time average evolution of variables. The multi-time scale method based on invariant manifolds proposed in [Acharya and Sawant, 2006] has no assumption of periodicity. However the method involves parameterization of evolution of coarse variables from underlying fine scale evolution. The extension of this methodology to solve initial boundary value problems [Sawant and Acharya, 2005] scales up the parameterization process immensely and makes it ineffective. A wavelet transformation based multi-time scale (WATMUS) method has been developed in the present work that overcomes the drawbacks of the existing methods and performs accelerated simulations for large number of cycles with sufficient accuracy. The method has no assumption on the characteristics of evolution of the variables, excludes any calibration process and hence proves advantageous over the existing multi-time scale methods.

This chapter provides a detailed description of the WATMUS method to solve initial boundary value problems, where the temporal evolution is governed by non-linear 1st order rate equations. Extrapolation based method is presented in section 2.1. Some of the existing multi-time scale methods in the context of 1-d viscoplastic model are discussed in section 2.2. The WATMUS method for first order non-linear ODEs is described in section 2.3. An overview of wavelets justifying its use in the proposed multi-time scale method is given in section 2.3.1. Section 2.3.2 describes the different rate equations of the coarse variables and compares them through the 1-d viscoplastic model. The extension of the methodology to initial boundary value problems is described in section 2.4. An adaptive criterion to select the evolving coefficients to reduce the size of the global system is described in section 2.4.1.
and a comparison between discrete wavelet and Fourier transformation is made in section 2.4.2. Section 2.4.3 describes the Quasi-Newton method employed to solve the wavelet coefficients. Section 2.4.4 presents the automatic time stepping algorithm to accelerate the fine scale integration in the coarse scale framework. An adaptive criteria to predict cycle jumps based on the rate of evolution of coarse variables is described in section 2.4.5, followed by conclusion in section 2.5.

2.1 Extrapolation based methods

In extrapolation based methods, single time scale cyclic simulations are performed for few cycles and then the variables are extrapolated for large number of cycles based on them. High cycle fatigue problems have been studied in [Bennett and McDowell, 2003], where extrapolation is performed based on two complete strain cycles and response is assumed to stabilize thereafter. Fretting fatigue in titanium alloys also have been studied in [Goh et al., 2001, Goh et al., 2003] using this method. Fatigue life prediction of HSLA steels are performed by using CPFE simulations and extrapolation based methods [Sinha and Ghosh, 2006]. Functional relationships are derived for the local variables affecting the fatigue life in terms of number of cycles and macroscopically applied stress or strain. The accuracy of extrapolation based methods is strongly dependent on the time or cycle from which extrapolation is performed and can be completely inaccurate and inefficient if stabilization of response happens after a large number of cycles [Joseph et al., 2010, Joseph, 2010]. Also these methods are macroscopic and cannot capture local evolution of variables with sufficient accuracy.
2.2 Multi-time scale methods

In initial boundary value problems with plasticity, the equilibrium equations,
\[ \frac{\partial \sigma_\zeta^{ji}}{\partial x_j} = 0 \] (2.1)
in conjunction with first order rate laws of internal variables,
\[ \dot{y}_\zeta^\alpha = f_\alpha(y_\zeta^\beta, F_{ij}^\zeta, t) \] (2.2)
are integrated for specified initial and boundary conditions to obtain spatio-temporal evolution. The effect of body forces and inertia are neglected in the equilibrium equations. In equation 2.1, \( \sigma_\zeta^{ji} \) is the stress tensor and depends on deformation gradient \( F_{ij}^\zeta \) and internal variables \( y_\zeta^\alpha \). In equation 2.2, \( \alpha \) is the number of internal variables and \( f_\alpha \) are non-linear functions that govern their evolution. Under cyclic loading conditions, the evolution of variables exhibit dual-time behavior with a high frequency fine time and a low frequency coarse time scale component. Multi-time scale methods are used to decouple the dual-time components, so that integration is performed in the coarse time scale where the response is monotonic and significant benefit in computational time can be achieved.

In the existing multi-time scale method like the asymptotic expansion and almost periodic temporal homogenization operator based methods, proposed in [Yu and Fish, 2002, Manchiraju et al., 2007, Oskay and Fish, 2004b], the coarse time \( t \) is related to the fine time \( \tau \) by the relation \( t = \epsilon \tau \) where \( \epsilon \ll 1 \) and forms the basis of decoupling the scales. The method based on invariant manifolds developed in [Acharya and Sawant, 2006] does not assume inherent scale separation. However a coarse phase space needs to be formed from the underlying fine evolution through parameterization. A 1-d viscoplastic model is described in the next section to highlight the de-merits of these methods. The 1-d viscoplastic constitutive equations are similar to the crystal plasticity material model used in this work. It also provides a simplified representation to analyze the existing multi-time scale methods and develop the framework of the WATMUS method.
2.2.1 1-d viscoplastic model

A homogeneous 1-d viscoplastic bar of length \( L = 1 \) mm, fixed at one end \((u(x = 0, t) = 0)\) and with cyclic displacement \((u(x = L, t) = u_L(t))\) at the other end is considered. The equilibrium equation after neglecting body force and inertia can be represented as,

\[
\frac{\partial \sigma^\zeta}{\partial x}(x, t) = 0 \Rightarrow \sigma^\zeta(x, t) = \dot{\sigma}^\zeta(t) \tag{2.3}
\]

In the viscoplastic law, stress rate \( \dot{\sigma}^\zeta \) is related to strain rate \( \dot{\varepsilon}^\zeta \) and plastic strain rate \( \dot{\varepsilon}^p \) by

\[
\dot{\sigma}^\zeta = E(\dot{\varepsilon}^\zeta - \dot{\varepsilon}^p) \tag{2.4}
\]

where \( E = 200 \) GPa is the elastic modulus. The initial conditions for stress and plastic strain are \( \sigma^\zeta(x, t = 0) = 0 \) and \( \varepsilon^p(x, t = 0) = 0 \) respectively. The evolution of plastic variables are governed by

\[
\begin{align*}
\dot{\varepsilon}^p &= \dot{a} \left| \frac{\sigma^\zeta}{g^\zeta} \right|^{\frac{1}{m}} \text{sign}(\sigma^\zeta) \tag{2.5a} \\
g^\zeta &= h |\dot{\varepsilon}^p| \tag{2.5b}
\end{align*}
\]

where \( g^\zeta, h, m \) and \( \dot{a} \) are the hardness, modulus of hardening rate, rate sensitivity exponent and reference plastic strain rate respectively. An uniform initial hardness value of \( g^\zeta(x, t = 0) = 320 \) MPa is considered. The values of the parameters in the viscoplastic law shown in equation 2.5 are \( h = 100 \) MPa, \( m = 0.02 \) and \( \dot{a} = 0.0023 \) sec\(^{-1}\).

The evolution of plastic strain is homogenous \((\varepsilon^p(x, t) = \dot{\varepsilon}^p(t))\) for spatially constant initial hardness of the bar. This can be shown by considering a case when \( \dot{\sigma}^\zeta(t) > 0 \) and equation 2.5b can be represented as

\[
\begin{aligned}
\frac{\partial g^{\zeta \text{ref}}}{\partial t} &= \frac{m + 1}{m} h \dot{a} \dot{\sigma}^\zeta \left| \frac{\sigma^\zeta}{g^\zeta} \right|^{\frac{1}{m}} \tag{2.6}
\end{aligned}
\]

Integration of equation 2.6 gives

\[
\begin{aligned}
g^{\zeta \text{ref}}(x, t) &= \left( \frac{m + 1}{m} h \dot{a} \int_0^t \dot{\sigma}^\zeta dt + g^{\zeta \text{ref}}(x, t = 0) \right)^{\frac{m}{m + 1}} \tag{2.7}
\end{aligned}
\]
Since \( g^\xi(x, t = 0) \) is constant in the bar, the evolution of hardness is homogenous \( (g^\xi(x, t) = \hat{g}^\xi(t)) \) and from equation 2.5a only temporal evolution of plastic strain happens in the bar \( (e^p^\xi(x, t) = \hat{e}^p^\xi(t)) \). Strain is uniform in the bar \( (\epsilon^p^\xi(x, t) = \hat{\epsilon}^p^\xi(t)) \) and spatial variation of displacement, after substituting the boundary conditions, is linear as shown below.

\[
\hat{\epsilon}^\xi(t) = \frac{\partial u^\xi}{\partial x} = \hat{\epsilon}^\xi(t)x
\]

(2.8)

The externally applied displacement at \( x = L \) is considered to be periodic with time period \( T = 1 \) sec \( (u^\xi(L, t) = 0.008 \sin(2\pi t) \text{ mm}) \). The temporally evolving periodic strain is obtained from equation 2.8 as \( \hat{\epsilon}^\xi(t) = 0.008 \sin(2\pi t) \). Since the rate equations are non-linear, single time scale integration of the viscoplastic model is performed by using a backward Euler scheme with a constant time step \( \Delta t = 0.0078125 \text{ sec} \). The single time scale evolution of plastic strain and hardness is shown figure 2.1.

Due to the cyclic nature of the applied displacement and the corresponding strain, the plastic variables has dual-time behavior with rapid oscillations within time period of each load cycle and a slow monotonic evolution spanning across cycles. Multi-time scale methods can be used to decouple the slow or coarse scale evolution from the oscillatory behavior, where the coarse scale rate laws are derived from the underlying single time scale rate equations. The single-time scale rate equations shown in equations 2.2 and 2.5 can be represented as,

\[
\dot{y}^\xi(t) = f(y^\xi, v^\xi, t)
\]

(2.9)

where \( f \) is some non-linear function, \( y^\xi \) is the variable having an oscillatory single-time scale response and \( v^\xi \) is some oscillatory (periodic or non-periodic) or monotonic external signal. Some of the existing multi-time scale methods are discussed with respect to the autonomous ODE shown in equation 2.9 and intial boundary value problems, in the following sections. The assumptions and methodology to obtain coarse scale rate equations...
Figure 2.1: Evolution of plastic variables obtained from single time scale integration of the 1-d viscoplastic model for 200 cycles: (a) $\epsilon^p$ (b) $g^\zeta$ and corresponding magnified view
for each of these multi-time scale algorithms are presented. Their limitations when used to
decouple viscoplastic and crystal plasticity models are also discussed.

2.2.2 Asymptotic expansion based methods

In asymptotic expansion based methods [Yu and Fish, 2002, Manchiraju et al., 2007], the
response variables are expanded in an asymptotic series based on different orders of con-
tribution as shown below.

\[ y^\xi(t) = y(t, \tau) = y_0(t, \tau) + \eta y_1(t, \tau) + \eta^2 y_2(t, \tau) + \ldots = \sum_{n=0}^{N} \eta^n y_n \] (2.10)

where \( \eta << 1 \). In [Yu and Fish, 2002] the dual-time relation \( t = \eta \tau \) in conjunction with
series expansion is used to obtain the modified rate equations in terms of \( y_n \) as shown below.

\[ \frac{dy^\xi}{dt} = \frac{\partial y_0}{\partial t} + \frac{\partial y_1}{\partial \tau} + \frac{1}{\eta} \frac{\partial y_0}{\partial \tau} + \eta \left( \frac{\partial y_1}{\partial t} + \frac{\partial y_2}{\partial \tau} \right) + \ldots = f(y, t, \tau) \] (2.11)

The time averaged variable

\[ \bar{y}(t) = \frac{1}{T} \int_{t}^{t+T} y^\xi dt \] (2.12)

with slow evolution is formed and equivalent rate equations in coarse scale are obtained
assuming local periodicity of \( y_n \) where \( n=1, \ldots, N \). However the assumption of local peri-
odicity made in [Yu and Fish, 2002] is not valid for evolving microstructural variables in
viscoplastic and crystal plasticity simulations under cyclic loading and hence cannot be
used for decoupling.

In [Manchiraju et al., 2007, Manchiraju et al., 2008] local periodicity of \( y_n \) is not as-
sumed and the variables are decomposed into

\[ y^\xi(t) = y(t, \tau) = \bar{y}(t) + \tilde{y}(t, \tau) \] (2.13)
where \( \bar{y} \) and \( \tilde{y} \) are the cycle averaged (equation 2.12) and oscillatory response respectively. The cycle averaged variables evolve with coarse time \( t \) and the oscillatory response is expanded in an asymptotic series as shown below.

\[
\tilde{y}(t, \tau) = \tilde{y}_0(t, \tau) + \eta \tilde{y}_1(t, \tau) + \eta^2 \tilde{y}_2(t, \tau) + \ldots
\] (2.14)

The rate equations of \( \dot{y} \tilde{z} \) can then be represented as

\[
\dot{y} = \frac{\partial \bar{y}}{\partial t} + \frac{1}{\eta} \frac{\partial \tilde{y}_0}{\partial \tau} + \eta \frac{\partial \tilde{y}_1}{\partial t} + \eta \frac{\partial \tilde{z}_1}{\partial \tau} + \ldots = f(y, t, \tau) \] (2.15)

where the dual-time scale relationship and the asymptotic series expansion of the oscillatory response has been used. Equating the different orders of \( \eta \) in equation 2.15 yields the condition that the zero-th order oscillator of \( \tilde{y} \) is zero as shown below.

\[
\eta^{-1} \text{ order: } \frac{\partial \tilde{y}_0}{\partial \tau} = 0 \Rightarrow \tilde{y}_0 = 0
\] (2.16)

For the viscoplastic problem described in section 2.2.1 this implies that \( \tilde{\epsilon}_0^p = 0 \) and \( \tilde{g}_0 = 0 \). Substituting these conditions in the relation for stress gives

\[
\sigma^\varepsilon(t) = \sigma(t, \tau) = E(\tilde{\epsilon} + \tilde{\epsilon} - \tilde{\epsilon}^p + \eta \tilde{\epsilon}_1^p)
\]

\[
\Rightarrow \tilde{\sigma} = E(\tilde{\epsilon} - \eta \tilde{\epsilon}_1^p)
\] (2.17)

Since \( \eta \ll 1 \), the oscillatory stress \( \tilde{\sigma} \) in equation 2.17 only depends on the oscillatory characteristics of the applied strain \( \tilde{\epsilon} \). Based on this observation, the coarse scale rate equation of \( \tilde{\epsilon}^p \) for the viscoplastic model is calibrated from fine scale simulations of two consecutive cycles for different \( \tilde{\epsilon}^p, \tilde{g}, \tilde{\epsilon} \) and given \( \tilde{\epsilon} \). For crystal plasticity models a similar calibration is performed at slip system level.

Asymptotic expansion based method is valid when oscillatory response is a perturbation to the overall evolution of variables which is predominantly average. In the 1-d viscoplastic model described in section 2.2.1, the applied strain is periodic with zero average. The stress
response is shown in figure 2.2 and has a ratio \( R = \sigma_{\text{min}}/\sigma_{\text{max}} \to -1 \). Under these conditions \((R \to -1)\), the average evolution of plastic variable \( \dot{e}^p \) is nearly zero and the oscillatory response is dominant as shown in figure 2.3. Also the waveform of plastic oscillation and stress in each cycle changes with progressing cycles of applied strain. Though equation 2.17 suggests that stress oscillator remains unchanged for temporally periodic applied strain, it is not true when the applied strain are completely reversible. Since asymptotic series expansion of variables can only be used where average evolution is dominant, it fails to decouple the coarse and fine evolutions when local stress ratio \( R = \sigma_{\text{min}}/\sigma_{\text{max}} \to -1 \). The WATMUS method does not assume inherent scale separation and hence works for all stress ratios.

2.2.3 Almost Periodic Temporal Homogenization (APTH) operator based method

In APTH operator based dual-time scale method [Oskay and Fish, 2004b], the variables are assumed to evolve in an almost periodic manner. Such near periodicity can arise in constitutive laws due to damage or hardness evolution. The almost periodic variable is represented in terms of a periodic function and a small change which depends on the \( \tau \)-scale as shown below.

\[
y^\varepsilon(t) = y(t, \tau) = y_p(t, \tau) + \epsilon \tau \tilde{y}
\]

(2.18)

where \( \epsilon \ll 1 \). An almost periodic operator \( \mathcal{M}(y) \) is defined to obtain the coarse scale variables from the underlying fine scale variables. The coarse scale evolution is defined as

\[
\frac{\partial \mathcal{M}(y)}{\partial t} = \frac{1}{T} \int_{t}^{t+T} \dot{y}^\varepsilon dt'
\]

(2.19)

Such a definition of coarse scale rate equation of almost periodic variables results in the condition of weak convergence similar to periodic fields as shown below.

\[
\lim_{\varepsilon \to 0} \int_{t}^{t+T} \dot{y}^\varepsilon(t') dt' \to \int_{t}^{t+T} \mathcal{M}(y(t', \tau)) dt'
\]

(2.20)
Figure 2.2: Evolution of stress in the viscoplastic model: (a) Overall response (b) Variations at specific cycles
Figure 2.3: Evolution of plastic strain in the viscoplastic model: (a) Average response (b) Oscillatory response at specific cycles
To solve the coarse scale initial boundary value problems, the coarse scale evolution at any cycle (equation 2.19) is obtained by solving equilibrium equations along with fine scale integration of almost periodically evolving variables over that cycle. Once the coarse scale rate at any cycle is evaluated, the coarse variable at the next cycle is obtained by performing a forward integration as follows.

\[
\mathcal{M}(y)\bigg|_{n+1} = \mathcal{M}(y)\bigg|_n + \frac{\partial \mathcal{M}(y)}{\partial t} \bigg|_n \Delta t \tag{2.21}
\]

The use of such a staggered global local approach to perform coarse scale integration shows stability issues similar to explicit integration schemes, when the evolution is not almost periodic. The APTH operator based method is used to decouple the coarse and fine evolutions of the 1-d viscoplastic problem described in section 2.2.1. The coarse plastic variables \(\mathcal{M}(\epsilon^p)\) and \(\mathcal{M}(g)\) are integrated using equation 2.21. Two different coarse scale time steps are considered. When the coarse scale time step \(\Delta t = 2\) sec the method converges and a comparison is shown in figure 2.4(a). However when \(\Delta t > 2\) sec, the method diverges and is shown in figure 2.4(b). The explicit nature of the APTH operator based method restricts the coarse scale time steps and can diverge when cyclic evolutions are large. Hence it cannot be used as a general method to decouple coarse and fine scale evolution in crystal plasticity problems. The WATMUS method provides an implicit framework and hence stability issues can be avoided.

### 2.2.4 Method of parameterized locally invariant manifolds

The method of invariant manifolds is originally proposed by [Muncaster, 1983] in which the temporal evolution laws of a spatially reduced coarse description of a system is derived from the underlying fine evolution. The evolution of the fine system \(y\) is governed by first order rate equations. The coarse system \(Y(t)\) is obtained from the fine system through a
Figure 2.4: Coarse scale response from APTH operator based multi-time scale method: (a) Coarse scale time step $\Delta t=2$ sec (b) Coarse scale time step $\Delta t=3$ sec.
unique mapping function \( \pi : (y) \rightarrow Y \). An inverse mapping function \( G(Y) \rightarrow y \) from coarse to fine system is obtained from

\[
DG\left[D\pi(G)\left[h(G)\right]\right] = h(G) \tag{2.22}
\]

where \( h \) are functions governing the evolution of the fine system. The inverse map \( G \) must be unique and invariant under translations of time. The first order rate equations of the spatially reduced coarse system can then be represented in terms of \( G \).

The method developed in [Acharya and Sawant, 2006, Sawant and Acharya, 2005] extends the theory proposed in [Muncaster, 1983] to decouple temporal scales. In this method, coarse time variables are obtained by averaging the evolution of the corresponding fine time variables as shown below.

\[
\bar{y}(t) = \frac{1}{T} \int_{t}^{t+T} y dt' \tag{2.23}
\]

where \( y \) is the fine time scale variable whose evolution is governed by equation 2.9, \( \bar{y} \) is the equivalent coarse representation and \( T \) is some time period. From equation 2.23, the rate equation of the coarse variables can be expressed as

\[
\frac{d\bar{y}}{dt} = \frac{1}{T} \left[y(t+T) - y(t)\right] \tag{2.24}
\]

where \( y \) is a forward shift of the fine variable \( y(t) \), is introduced and is shown below.

\[
\tilde{y}(t) = y(t+T) \tag{2.25}
\]

The evolution of coarse variable \( \bar{y}(t) \) can be represented in terms of the corresponding fine variables \( y(t) \) and \( \tilde{y}(t) \) as shown below.

\[
\frac{d\bar{y}}{dt} = \frac{1}{T} \left[y(t+T) - y(t)\right] \tag{2.26}
\]

A fine time scale variable \( y_f(t) \), which is a forward shift of the fine variable \( y(t) \), is introduced and is shown below.

\[
\tilde{y}_f(t) = f(y(t), y(t+T)) \tag{2.25}
\]
To relate the evolution of coarse variables to their underlying fine variable, functions $G$ and $G_f$ are defined as

$$y^\xi(t) = G(\bar{y})$$
$$y^\xi_f(t) = G_f(\bar{y})$$

(2.27)

The inverse mapping functions $G$ and $G_f$ also satisfy the first order partial differential equations shown below.

$$\frac{\partial G_f}{\partial \bar{y}} \frac{1}{T} [G_f - G] = f(G_f, v^\xi(t + T))$$
$$\frac{\partial G}{\partial \bar{y}} \frac{1}{T} [G_f - G] = f(G, v^\xi(t))$$

(2.28)

The above equation can be solved to obtain the mapping functions $G$ and $G_f$ for a system whose coarse trajectories are sought for. The coarse scale evolution equations can then be represented as

$$\frac{d\bar{y}}{dt} = \frac{1}{T} \left[ G_f(\bar{y}) - G(\bar{y}) \right]$$

(2.29)

A coarse space is constructed to obtain discrete approximations of the locally invariant manifolds $G_f$ and $G$ from equation 2.28. The parametrization process to obtain the invariant manifolds is discussed in [Sawant and Acharya, 2005]. This process of parameterization can be computationally exhaustive if the number of coarse variables are large. Also in order to form the discretized coarse space, the lower and upper limits of the coarse variables needs to be known a priori. The WATMUS method does not involve a parameterization process and hence advantageous over this method.
2.3 Wavelet transformation based multi-time scale method for first order ODEs

The WATMUS method is developed to decouple the oscillatory response of variables whose evolution is governed by 1\textsuperscript{st} order rate equations shown in equation 2.9. An example of such an evolution obtained from the 1-d viscoplastic model subjected to cyclic strain is shown in figure 2.5. As can be observed from the figure, the evolution of $y^\varepsilon$ has a low frequency component that evolves with coarse time or cycles as shown in figure 2.5(d) and a high frequency component that shows large fluctuations within a cycle as shown in figures 2.5(b) and 2.5(c). Due to the dual-time behavior of $y^\varepsilon$, temporal variables $N$ and $\tau$ are associated with the cyclic evolution (coarse scale) and rapid oscillatory response within a cycle (fine scale) respectively.

Decoupling is achieved through transformation of the temporally evolving variables over each cycle to a space spanned by orthogonal basis functions as follows:

$$y^\varepsilon(t) = y(N, \tau) = \sum_{k=1}^{n} y_k(N)\psi_k(\tau) \quad \text{where} \quad \tau \in [NT, (N+1)T] \quad (2.30a)$$

$$y_k(N) = \frac{1}{T} \int_{NT}^{(N+1)T} y(N, \tau)\psi_k(\tau)d\tau \quad (2.30b)$$

In the above equation, $y_k(N)$ are the coefficients of the orthogonal basis functions which evolve with cycles and forms the coarse scale variables, $\psi_k(\tau)$ are the basis functions capturing the oscillatory fine scale response within the cycle, $n$ is the number of basis functions required for accurate representation of oscillatory response of $y$ within a cycle and $T$ is the time period associated with the fine scale evolution and depends on the frequency of response $y^\varepsilon$ or the external applied signal $v^\varepsilon$. This transformation associates the evolution of $y(N, \tau)$ with the monotonic evolution of the coefficients $y_k(N)$ which are integrated with time steps of cycles to obtain computational benefit. For the 1-d viscoplastic model in section 2.2.1, $y^\varepsilon = \{\epsilon_p^\varepsilon, g^\varepsilon\}$ and $v^\varepsilon = \epsilon^\varepsilon$. 

24
The number of basis functions $n$ are selected from the first few cycles of single time scale integration, after which the cycle scale integration scheme is used. It is assumed that $n$ does not change with subsequent evolution and hence the selection of proper basis functions is essential for accurate, stable and efficient coarse scale integration. Based on these requirements, the chosen family of basis functions should satisfy the following conditions:

- The functions should be orthogonal

$$\frac{1}{T} \int_{0}^{T} \psi_k \psi_l d\tau = \delta_{kl} \quad (2.31)$$

- The functions should represent all possible waveforms to a predefined resolution.

- The number of coefficients that needs to be evolved should be optimally small.

Though the Fourier basis functions are orthogonal, they are infinitely supported and this results in spurious oscillations in the fine scale response when a finite set of coefficients are selected from the infinite series. Moreover the periodic nature of these basis functions make them inappropriate for representing non-periodic fine scale oscillations. The wavelet basis functions are advantageous over Fourier basis representation and hence used in the present work. The advantageous properties of wavelet basis functions are summarized below:

- **Compact Support**: Each wavelet basis spans a finite domain and hence doesn’t exhibit spurious instabilities like Gibb’s phenomenon associated due to truncation of infinite series as in Fourier series representations.

- **Multi-resolution**: At different resolutions the set of basis functions is finite and known a priori unlike Fourier series where this is found by trial and error.

- **Projection in time and frequency domain**: Since wavelet transformation performs projection in both time and frequency domain unlike Fourier transform, it enables
the reduction of the number of coefficients required to be solved to a larger extent than Fourier transform.

- The wavelet basis functions are non-periodic and hence suitable for accurate representation of non-periodic oscillatory response.

In problems involving non-linear rate equations, numerical integrations are performed at discrete fine time points resulting in discrete approximations of continuous functions. Hence a discrete wavelet transformation based on filter banks is used in this method and an overview is given in the following section.

### 2.3.1 Wavelets overview

In the wavelet transformation, the basis functions are obtained from translations and dilations of compactly supported scaling function $\phi(\tau)$ and mother wavelet $\psi(\tau)$ [Strang and Nguyen, 1996, Walker, 1999]. The dilations form the different resolutions and represent the different frequencies whereas the translations in different resolutions maintain the temporal characteristics. A wavelet transformation of square integrable function $y$ is shown

$$
C_{mn} = \int_{-\infty}^{\infty} y(\tau) 2^{-\frac{m}{2}} \phi(2^m \tau - n) d\tau
$$

$$
y(\tau) = \sum_{m=1}^{M_{res}} \sum_{n=1}^{N_{trans}^m} C_{mn} 2^{\frac{m}{2}} \phi(2^m \tau - n) \tag{2.32}
$$

where $M_{res}$ is the number of resolutions (dilations) and $N_{trans}^m$ is the number of translation in each resolution.

The compactly supported scaling functions $\phi(\tau)$ satisfy the refinement condition which relates the scaling functions at a higher resolution to the scaling functions at a lower resolution and is of the form:

$$
\phi(\tau) = \sum_{k=1}^{N_{filter}} h_k \phi(2\tau - k) \tag{2.33}
$$
where the parameters $h_k$ and $N_{filter}$ depends on the family of wavelet that is used. The scaling functions can be used to produce a nested sequence of sub spaces at different resolutions as shown below.

$$0 \subset \ldots \subset V_0 \subset \ldots \subset V_m \subset V_{m+1} \subset \ldots \subset L^2(R) \quad (2.34)$$

The nested sequence of functions $y_m$ obtained by projection at different sub spaces $V_m$ are the approximations to the original function $y$ at different resolution levels. This multi resolution property yields a complimentary space and is the detail space $W_m$. The detail space is the orthogonal difference between two consecutive resolutions $V_m$ and $V_{m+1}$ and is spanned by the wavelet basis functions $\psi(\tau)$. The wavelet basis functions have compact support and satisfy refinement condition similar to the scaling functions as shown below.

$$\psi(\tau) = \sum_{k=1}^{N_{filter}} g_k \phi(2\tau - k) \quad (2.35)$$

Discrete wavelet transformation can be achieved through a recursive projection of the original function into approximate and detail spaces at coarser resolutions

$$y^m(\tau) = \sum_n (y^m, \phi_{m-1,n}) \phi_{m-1,n} + \sum_n (y^m, \psi_{m-1,n}) \psi_{m-1,n}$$

$$= \sum_n d^{m-1,n} \phi_{m-1,n} + \sum_n d^{m-1,n} \psi_{m-1,n}$$

$$= y^{m-1} + \sum_n d^{m-1,n} \psi_{m-1,n} \quad (2.36)$$

where $m$ is the resolution and $n$ is the translation in the corresponding resolution. The function $y^m(\tau)$ is the discrete approximation of the original continuous function $y(\tau)$ and consists of $2^m$ uniformly spaced points where the resolution is determined from the minimum time step that is required to integrate the differential equations dictating the evolution of $y(\tau)$ [Joseph et al., 2010]. The recursive procedure yields approximate coefficients $d^{0,n} \in V_0$ and detail coefficients $d^{l,n} \in W_l$ where $l \in [0, m-1]$ . This multi resolution property of wavelet transformation can be used to retain coefficients where response variations
are high and eliminate coefficients where changes are slow. A wavelet representation of an oscillatory signal is shown in figure 2.6. As can be observed from the figure, higher resolution basis functions are required where changes in the response is large, whereas basis functions at lower resolution captures the slow change.

Discrete wavelet transformation described in equation 2.36 can be performed through matrix operation where the orthogonal transformation matrix $T$ is created from the low pass filters $h_k$ and high pass filters $g_k$ as explained in [Joseph et al., 2010, Strang and Nguyen, 1996, Walker, 1999]. In the discrete wavelet transformation through matrix vector operation

$$\{C\} = [T]\{y\} \quad (2.37)$$

$y$ is a $p$-dimensional vector containing $p$ uniformly spaced points in time and $C$ is a $p$-dimensional vector containing the coefficients. The number of approximate coefficients in $C$ depends on the span of the mother wavelet and scaling function. For example in Daubechies-4 wavelet there are 2 approximate coefficients in $C$, whereas in Haar wavelet there is 1 approximate coefficient. The inverse transform to obtain the $p$ uniformly spaced points from the coefficients is as follows:

$$\{y\} = [T]^T\{C\} \quad (2.38)$$

The filter coefficients arise from the refinement conditions shown in equations 2.33 and 2.35. Since the filter coefficients are finitely spanned, the transformation matrix, created by assembling these filter coefficients is sparse. The sparsity property can be used to expedite the decomposition and reconstruction of responses in a cycle.

**2.3.2 Coarse scale rate equations**

The evolution of $y$ within a cycle is obtained by integrating the first order rate equation

$$y(N, \tau) = y_0(N) + \int_0^\tau f(y, v, N, \tau)d\tau \quad (2.39)$$
where \( f \) is a function, \( y_0(N) = y(N, \tau = 0) \) is the initial value of \( y \) and \( v(N, \tau) \) is the oscillatory external signal, at cycle \( N \). The coefficients \( y_k \) at any cycle are obtained by projecting \( y \) in the wavelet space and hence their cycle scale evolution depend on \( y_0(N) \) and the coefficients \( v_k(N) \) as shown below.

\[
y_k(N) = \frac{1}{T} \int_0^T y(N, \tau) \psi_k d\tau
\]

\[
= y_0(N) \frac{1}{T} \int_0^T \psi_k d\tau + \frac{1}{T} \int_0^T \int_0^\tau f(y, v_k, N, \tau') d\tau' \psi_k d\tau
\]  

(2.40)

The cycle scale evolution of \( y_0 \) depends on the underlying fine scale evolution and hence its evolution rate is defined based on it. From the coarse scale evolution of \( y_0 \), the evolution of the coefficients \( y_k \) can be obtained following equation 2.40.

**Numerical implementation**

The cyclic rate equation of \( y_0 \) is integrated numerically by second order backward difference formula as shown below.

\[
y_0(N + \Delta N) = \beta_1 y_0(N) - \beta_2 y_0(N - \Delta N_p) + \beta_3 \left. \frac{\partial y_0}{\partial N} \right|_{N + \Delta N} \Delta N
\]

where \( \beta_1 = \frac{(r + 1)^2}{(r + 1)^2 - 1} \)

\( \beta_2 = \frac{1}{(r + 1)^2 - 1} \)

\( \beta_3 = \frac{(r + 1)^2 - (r + 1)}{(r + 1)^2 - 1} \)

and \( r = \frac{\Delta N_p}{\Delta N} \)  

(2.41)

Three different forms of coarse scale rate equations of \( y_0 \) are defined and their computational expense and integration error are compared by considering the 1d viscoplastic model described in section 2.2.1. The definition which has minimum error and also computationally viable is used for coarse scale integration. The three different definitions of coarse scale rate equation are as follows:

(i) The rate equation at any cycle \( N \) is defined as:

\[
\frac{\partial y_0}{\partial N} = y_0(N + 1) - y_0(N) = y(N, T) - y_0(N)
\]  

(2.42)
Fine scale integration of the viscoplastic model at cycle $N$ over one time period $T$ is performed to evaluate the coarse scale evolution rate. The backward difference formula shown in equation (2.41) is solved implicitly using Newton-Raphson scheme. For this definition the residual is

$$
r = (1 + \beta_3 \Delta N) y_0(N) - \beta_3 \Delta N y_0(N, T) - \beta_1 y_0(N - \Delta N) + \beta_2 y_0(N - \Delta N - \Delta N_p)$$  (2.43)

and the corresponding linearized equation is

$$\frac{\partial r}{\partial y_0}(N) \Delta y_0 = -r_i$$  where  $$\frac{\partial r}{\partial y_0}(N) = (1 + \beta_3 \Delta N) - \beta_3 \Delta N \frac{\partial y_0(N, T)}{\partial y_0}$$  (2.44)

(ii) The rate equation at any cycle $N$ is defined as:

$$\frac{\partial y_0}{\partial N} = y_0(N) - y_0(N - 1)$$  (2.45)

Similar to the first definition, fine scale integration is performed for one time period $T$. For this definition the residual is shown below.

$$r = (1 - \beta_3 \Delta N) y_0(N) + \beta_3 \Delta N y_0(N - 1) - \beta_1 y_0(N - \Delta N) + \beta_2 y_0(N - \Delta N - \Delta N_p)$$  (2.46)

The corresponding linearized equation is

$$\frac{\partial r}{\partial y_0(N - 1)} \Delta y_0(N - 1) = -r_i$$  where  $$\frac{\partial r}{\partial y_0(N - 1)} = (1 - \beta_3 \Delta N) \frac{\partial y_0(N)}{\partial y_0(N - 1)} + \beta_3 \Delta N$$

and  $$y_0(N) = y_0(N - 1) + \int_0^T f(y, v_k, N - 1, \tau) d\tau$$  (2.47)

(iii) The rate equation is derived from the condition that when $\Delta N = 1$ and $\Delta N_p = 1$, equation (2.41) is satisfied exactly and the error in the numerical integration is only
due to truncation of the Taylor series to a second order approximation. The rate
equation thus obtained at any cycle $N$ is as follows:

$$\frac{\partial y_0}{\partial N} = \frac{3}{2}y_0(N) - 2y_0(N-1) + \frac{1}{2}y_0(N-2) \tag{2.48}$$

This definition involves fine scale integration over two consecutive cycles. The resid-
ual for this definition is

$$r = (1 - \frac{3}{2}\beta_3\Delta N)y_0(N) + 2\beta_3\Delta Ny_0(N-1)$$

$$- \frac{1}{2}\beta_3\Delta Ny_0(N-2) - \beta_1y_0(N - \Delta N) + \beta_2y_0(N - \Delta N - \Delta N_p) \tag{2.49}$$

and the corresponding linearized equation is

$$\frac{\partial r}{\partial y_0(N-2)}|_{\Delta y_0(N-2)} = -r_i$$

where

$$\frac{\partial r}{\partial y_0(N-2)} = (1 - \frac{3}{2}\beta_3\Delta N) \frac{\partial y_0(N)}{\partial y_0(N-2)}$$

$$+ 2\beta_3\Delta N \frac{\partial y_0(N-1)}{\partial y_0(N-2)} - \frac{1}{2}\beta_3\Delta N ,$$

$$y_0(N) = y_0(N-2) + \int_0^{2T} f(y, v, k, N-2, \tau) d\tau$$

and

$$y_0(N-1) = y_0(N-2) + \int_0^{T} f(y, v, k, N-2, \tau) d\tau \tag{2.50}$$

Backward Euler scheme is used to perform fine scale integration in any cycle. A time
step $\Delta \tau = 0.0078125$ is used for the fine time scale integration. This time step is converged
and results in a resolution $M_{res} = 7$. The integration of the coarse variables using a Newton-
Raphson scheme requires the evaluation of the variation in response of variable $y(N, \tau)$ with
respect to the initial value $y_0(N)$ as shown in equations 2.44, 2.47 and 2.50. In the backward

Euler scheme used for fine scale integration, the variation of response at increment $n+1$ with respect to its previous increment $n$ can be obtained as follows:

$$y|_{n+1} = y|_n + f|_{n+1} \Delta \tau_{n+1}$$

$$\delta y_{n+1} = \left[ 1 - \left( \frac{\partial f}{\partial y} \right)_{n+1} \Delta \tau_{n+1} \right]^{-1} \delta y_n = A_{n+1} \delta y_n$$

$$A_{n+1} = \frac{\partial y_{n+1}}{\partial y_n}$$  \hspace{1cm} (2.51)

A product of $A_k$ from the first increment in the fine scale integration of any cycle to the increment $n$ gives the variation of $y$ at that increment with respect to the coarse variable $y_0$ and is shown below.

$$\frac{\partial y}{\partial y_0}|_n = \prod_{k=1}^n A_k$$  \hspace{1cm} (2.52)

In the 1-d viscoplastic model described in section 2.2.1, $y$ is vector of internal variables $\dot{e}^p$ and $g$ for which coarse scale equations are derived. In the incremental integration, $f$ is a rank 2 vector valued function and $A$ is a $2 \times 2$ matrix as shown below.

$$f = \begin{bmatrix} \dot{e}^p \\ \dot{g} \end{bmatrix} = \begin{bmatrix} \dot{\mathcal{E}}^2 \\ h|\dot{\mathcal{E}}^p| \end{bmatrix} \begin{bmatrix} \frac{\partial \mathcal{E}}{\partial \mathcal{E}} & \text{sign}(\sigma) \\ 0 & \frac{\partial \mathcal{E}}{\partial \mathcal{E}} \end{bmatrix} \begin{bmatrix} 1 \\ h|\dot{\mathcal{E}}^p| \end{bmatrix}$$

$$A = \begin{bmatrix} 1 + \frac{BE}{\sigma} & \frac{BE}{\sigma} \\ h\Delta \tau \text{sign}(\Delta \mathcal{E}^p) & 1 \end{bmatrix}^{-1} \begin{bmatrix} 1 & 0 \\ -h\Delta \tau \text{sign}(\Delta \mathcal{E}^p) & 1 \end{bmatrix}$$

where $B = \frac{\dot{\mathcal{E}}}{m} (\frac{\sigma}{2})^{\frac{1}{2}} \Delta \tau$ and $\Delta \mathcal{E}^p = \mathcal{E}^p - \mathcal{E}^p|_n$  \hspace{1cm} (2.53)

The error in the coarse scale integration occurs due to approximation of the coarse scale rate $\partial y_0/\partial N$ and due to truncation of the series to second order as follows.

$$e = \left\| y_0 - y_0^{exact} \right\| \leq \beta_3 \Delta N \left\| \frac{\partial y_0}{\partial N} - \frac{\partial y_0}{\partial N}^{exact} \right\| + \left\| O(\Delta N^3) \right\|$$  \hspace{1cm} (2.54)
Two different error measures are considered to compare the different coarse scale rate definitions. The first definition compares the difference between $\epsilon_0^p$ as obtained from the coarse scale and single time scale integration schemes and is as follows:

$$\epsilon_0 = \frac{\left| \epsilon_0^p - \epsilon_0^p \right|_{\text{exact}}}{\left| \epsilon_0^p \right|_{\text{exact}}}$$  \hfill (2.55)

The second definition compares the difference of $\epsilon^p$ over a cycle obtained from coarse scale and single time scale integration schemes and is as follows:

$$\epsilon_{\text{char}} = \frac{\left[ \sum_{k=1}^{m} \left( \frac{\epsilon^p(N,\tau_k) - \epsilon^p(N,\tau_k)}{\text{exact}} \right)^2 \right]^{1/2}}{\left[ \sum_{k=1}^{m} \left( \epsilon^p(N,\tau_k) \right)_{\text{exact}}^2 \right]^{1/2}}$$  \hfill (2.56)

where $m$ is the number of discrete time points in a cycle. In both the error measures, the response obtained from single time scale integration is considered as the exact solution. These error measures are evaluated for different $\Delta N$ and $\Delta N_p = 2$ as shown in figure 2.7. As can be observed from figure 2.7, all the definitions of coarse scale rate has approximately the same error for large cycle jumps where truncation error is the dominant contributor to the total error in $y_0$. However for lower cycle jumps definition (iii) has the least error due to the higher order approximation of the coarse scale rate. However definition (iii) involves fine scale integration for two consecutive time periods which reduces the computational efficiency of the method. Definition (i) has less error than definition (ii) and is computationally more efficient than definition (iii) and hence used in the current work.

The local and global integration error of definition (i) is further investigated. To obtain the local error, coarse scale simulations of the 1-d viscoplastic model is performed with different $\Delta N$ and $r = 1$. The initial condition for the coarse variable $\epsilon_0^p$ and $g_0$ are obtained from the single time scale solution. Relative error in $\epsilon_0^p$ as obtained from coarse and fine scale simulations consistent with equation 2.55 are compared and is shown in figure 2.8. The error in $\epsilon_0^p$ is a combination of the coarse scale rate definition and truncation of Taylor
series as shown in equation 2.54. Since the error due to approximation of coarse scale
evolution rate is almost comparable for the same definition, the total error is dominated by
the truncation error. The figure shows that the total local error increases with ΔN and for
better accuracy reduced time steps are desired. However some discrepancy is observed at
ΔN = 16 and 32 because of the two errors getting canceled and resulting in a lower error
for this problem.

To obtain the global error, coarse scale integration is performed for 1000 cycles with
different ΔN and r = 1. The evolution of ϵ₀ with cycles and the reconstructed ϵ at a cycle
is shown in figure 2.9. Equation 2.55 is used to evaluate the error in ϵ₀ at two different
cycles and is shown in figure 2.10. The global error in integration captures the effect of
propagation of integration errors from the previous increments as shown below.

\[
\begin{align*}
\begin{bmatrix}
\delta y_0(N+2\Delta N) \\
\delta y_0(N+\Delta N)
\end{bmatrix} &= \left[ I - \begin{pmatrix} A_{N+2\Delta N} & \beta_1 \\ 0 & A_{N+\Delta N} \end{pmatrix} \right]^{-1} \begin{bmatrix} \beta_2 \\ \beta_1 \end{bmatrix} \begin{bmatrix}
\delta y_0(N) \\
\delta y_0(N-\Delta N)
\end{bmatrix} \\
&+ \begin{bmatrix}
\delta e(N+2\Delta N) \\
\delta e(N+\Delta N)
\end{bmatrix}
\end{align*}
\]

and
\[
A_N = \frac{\partial}{\partial y_0} \left[ \frac{\partial y_0}{\partial N} \right]_N \beta_3 \Delta N
\] (2.57)

where \( \delta y_0 \) is the total integration error, \( \beta_1, \beta_2 \) and \( \beta_3 \) are coefficients defined in equation
2.41 and \( \delta e \) is the local integration error. As can be observed from figure 2.10, error in-
creases uniformly for ΔN = 2, 4, 8 and 64. However, for ΔN = 16 and 32 there is a reduction
in the global error as the problem progresses. This may be due to the cancellation of errors
as explained before.
2.4 Wavelet transformation based multi-time scale method for initial boundary value problems involving damage

In finite element method to solve initial boundary value problems involving damage, the physical domain is spatially discretized and equilibrated in a weak sense [Belytschko et al., 2000]. The kinematically admissible displacement field is obtained by solving the semi-discrete system of equations obtained from out of balance forces at discrete nodal points

\[
R_\alpha^i(t) = R_\alpha^i(N, \tau) = \sum_e \int_{V_e} \frac{\partial P^\alpha}{\partial x_j} \sigma_{ji} dV_e - \sum_S \int_S P^\alpha t dS = 0 \tag{2.58}
\]

where \( P^\alpha \) are the polynomial shape functions, \( S_T \) are the surfaces on which tractions are applied and \( \alpha \) are the nodes of the discretized domain. Body forces and inertia effects are neglected in equation 2.58. For systems to be in equilibrium, equation 2.58 needs to be satisfied at all times \( t \) during the loading process. In the wavelet space this would imply that the wavelet coefficients of out of balance forces at nodes in the spatially discretized domain is zero at all cycles (coarse time) as shown.

\[
R_\alpha^i \bigg|_{\tau_0}^{\tau_1} = \frac{1}{T} \int_{0}^{T} \tilde{R}_\alpha^i (N, \tau) \psi_k d\tau
\]

\[
= \sum_e \int_{V_{0,e}} \frac{1}{T} \int_{0}^{T} B^\alpha_{ji} \sigma_{ji} \psi_k d\tau dV_{0,e} - \sum_{S_{0}} \frac{1}{T} \int_{0}^{T} \int_{S_{0}} P^\alpha t J_A \psi_k d\tau dS_{0} = 0 \tag{2.59}
\]

Numerical methods are employed in conventional finite element method to obtain the evolution of nodal displacements \( u^\alpha_\beta \), in which equation 2.58 is linearized and iteratively solved at discrete fine time points.

\[
R_\alpha^i \bigg|_{p}^{p+1} (t_n) = R_\alpha^i \bigg|_{p} \bigg( t_n \bigg) + \frac{\partial R_\alpha^i}{\partial u^\beta_j} \bigg|_p \Delta u_j^\beta = 0
\]

\[
u_j^\beta \bigg|_{p}^{p+1} (t_n) = u_j^\beta \bigg|_{p} \bigg( t_n \bigg) + \Delta u_j^\beta \tag{2.60}
\]
A similar procedure is followed for the coarse scale problem, whereby the coefficients of nodal displacements \( C_{\alpha i k} \) are solved at discrete cyclic increment as shown below.

\[
R_{i k|p+1}^\alpha (N) = R_{i k|p}^\alpha (N) + \frac{\partial R_{i k}^\alpha}{\partial C_{\beta j l}^\beta} \Delta C_{\beta j l}^\beta = 0
\]

\[
C_{\beta j l|p+1}^\beta (N) = C_{\beta j l|p}^\beta (N) + \Delta C_{\beta j l}^\beta
\]

(2.61)

In dissipative systems modeled by viscoplastic or crystal plasticity based evolution laws, the stress \( \sigma_{ij} \) at a material point depends on the local strain \( \epsilon_{ij} \) or deformation gradient \( F_{ij} \) and the internal variables \( y^z \).

\[
\sigma^z(X, t) = \hat{\sigma}(X, F, y^z, t)
\]

(2.62)

The internal variables capture the irreversible and history dependent behavior of dissipative materials undergoing damage whose evolution is of the form

\[
\dot{y}^z(X, t) = f(y^z, F, X, t), \quad y(t=0) = y^0
\]

(2.63)

In the coarse scale framework, the fine scale stresses \( \sigma(X, N, \tau) \) at any cycle is obtained from

\[
\sigma(X, N, \tau) = \hat{\sigma}(X, F_k, y_k, N, \tau)
\]

(2.64)

where \( F_{ij}^k(X, N) \) are the coefficients of deformation gradient and \( y_k(X, N) \) are the coefficients of internal variables. The coefficients of deformation gradient \( F_{ij}^k(X, N) \) at any material point in the spatially discretized domain can be obtained from the coefficients of nodal displacements \( C_{\alpha i k}^\alpha \) as shown.

\[
F_{ij}^k(X, N) = \delta_{ij} \frac{1}{T} \int_0^T \psi_k d\tau + \frac{\partial P_{\alpha j}^\alpha}{\partial X_j} C_{\alpha i k}^\alpha (N)
\]

(2.65)

The coarse scale internal variables \( y_k(X, N) \) at a cycle are obtained by solving the coarse scale rate equations obtained from their respective single time scale rate equations. The
most accurate and computationally efficient coarse scale rate definition in section 2.3.2 is used to perform the coarse scale integration of internal variables at a material point

\[
\frac{\partial y_0}{\partial N}(X, N + \Delta N) = y(X, N + \Delta N, T) - y_0(X, N + \Delta N)
\]

\[
y_0(X, N + \Delta N) = \beta_1 y_0(X, N) - \beta_2 y_0(X, N - \Delta N_p) + \beta_3 \frac{\partial y_0}{\partial N} \bigg|_{N+\Delta N} \Delta N \tag{2.66}
\]

where \( y_0 \) is the set of all coarse internal variables which are integrated. A Newton-Raphson scheme similar to equation 2.43 is used to solve the implicit second order backward difference formula.

\[
r = (1 + \beta_3 \Delta N)y_0(N) - \beta_3 \Delta N y(N, T) - \beta_1 y_0(N - \Delta N) + \beta_2 y_0(N - \Delta N - \Delta N_p)
\]

\[
\frac{\partial r}{\partial y_0} \bigg|_{\Delta y_0} = -r_i \quad \text{where} \quad \frac{\partial r}{\partial y_0} = (1 + \beta_3 \Delta N) - \beta_3 \Delta N \frac{\partial y(N, T)}{\partial y_0} \tag{2.67}
\]

The Jacobian in the Newton-Raphson procedure is a \( n \times n \) matrix, where \( n \) is the number of coarse scale internal variables in \( y_0 \).

A basis representation of the spatial field variables characterizes their cyclic variation and facilitates the use of implicit schemes to integrate these variables in the cycle scale. However cyclic representation of the variables increase the size of the FE model to be solved by the number of coefficients \( n_{wav} \) required to characterize the waveform. An adaptive criterion is developed to solve only the evolving coefficients to reduce the size of the FE model and is described in section 2.4.1. The compact support property of the wavelet basis functions facilitates an accurate representation with reduced set of coefficients and is compared with the Fourier basis representation in section 2.4.2. A Quasi-Newton method with approximate Jacobian is used to improve the efficiency to solve the linearized system shown in equation 2.61 and is described in section 2.4.3. Automatic fine time stepping is used to accelerate the fine scale integration of internal variables in any cycle. However it causes a non-uniform distribution of time points for wavelet transformation. A procedure is developed to perform discrete wavelet transformation for the non-uniformly spaced
time points and is described in section 2.4.4. An adaptive criterion is developed to predict
the cycle jumps for the coarse scale integration based on truncation error of the 2\textsuperscript{nd} order
backward difference scheme and is described in section 2.4.5.

2.4.1 Selection of evolving coefficients

To reduce the number of equations to be solved in the linearized system, only the evolving
coefficients are considered in the global set of equations. However the displacement
waveform can change shape as the problem progresses. Hence the use of a fixed set of
displacement coefficients from the start of the simulation can cause instability and inaccuracy
in the solution. Adaptive criteria are developed to add the evolving coefficients and
remove the non-evolving coefficients. The use of adaptive criteria at the start of each cyclic
increment keeps the optimal number of degrees of freedom that is solved. In this adaptive
criterion, the total set of wavelet coefficients of any nodal displacement degree of freedom
$I = \{C_k|k = 1..n_{\text{wav}}\}$, where $n_{\text{wav}}$ is the total number of coefficients, is divided into a set of
evolving $I^{\text{evol}}$ and non-evolving $I^{\text{non-evol}}$ coefficients, i.e. $I = I^{\text{evol}} \cup I^{\text{non-evol}}$. The set
of evolving coefficients at each cyclic increment is selected from the wavelet space by

$$I^{\text{evol}} = \{C_k|C_{k+1} - 2C_k + C_{k-1} > \eta C_{\text{tol}}^k, k = 1..n_{\text{wav}}\}$$

$$= \{\hat{C}_k, k = 1..n_{\text{evol}}\} \quad (2.68)$$

where the coefficient $C_{\text{tol}}^k = \max_{2^{(\log_2 k)} < j < 2^{(\log_2 k)} + 1} (C_{j+1} - 2C_j + C_{j-1})$ is the maximum value of
all coefficients at each resolution and $\eta$ is a tolerance. The set of non-evolving coefficients
is obtained from

$$I^{\text{non-evol}} = I - I^{\text{evol}} \quad (2.69)$$
2.4.2 Representation using reduced set of coefficients and comparison of accuracy between discrete wavelet and Fourier transforms

In the transformed space spanned by orthogonal basis functions, the evolution of coefficients captures the cyclic evolution of the waveform. Depending on the characteristics of the external signal, the functional form of the fine scale rate equations and different parameters in the model, a subset of these coefficients evolve. The number of evolving coefficients that needs to be considered to accurately capture the cyclic evolution depends on the family of basis function that is used. An 8 element CPFE model is used to compare the accuracy of representation based on reduced number of coefficients between the Daubechies-4 wavelet and Fourier basis functions. The variation of one of the nodal displacement degrees of freedom \( u \) at cycles 10 and 8000 is shown in figure 2.11.

Uniform time steps are used to perform the single time scale integration resulting in 128 uniformly spaced points to represent the waveform in each cycle. For the discrete wavelet transform, the 128 coefficients in the 10\(^{th}\) cycle is shown in figure 2.12. The arrangement of the set of coefficients based on the dilations and translations is as follows:

\[
C = \begin{bmatrix}
a_1^{-2} & d_1^{-2} & d_2^{-4} & d_3^{-8} & d_4^{-16} & d_5^{-32} & d_6^{-64}
\end{bmatrix}^T
\]

(2.70)

where \( a \) and \( d \) are the approximate and detail coefficients as described in equation 2.36 respectively. The criterion in equation 2.68 selects different number of evolving coefficients for different values of \( \eta \) and is shown in figure 2.13. The coefficients selected from equation 2.68 only evolves and the non-evolving coefficients retain their values at the start of the coarse scale integration. Reconstruction of the waveform is performed at 8000\(^{th}\) cycle based on exact values of evolving coefficients obtained from transformation of single time scale solution at 8000\(^{th}\) cycle and values of non-evolving coefficients from 10\(^{th}\) cycle.
as shown below.

\[
\begin{align*}
  u(N_0, \tau) &= \sum_{k=1}^{n} C_k(N_0) \psi_k(\tau) = \sum_{k=1}^{n_{evol}} C_k(N_0) \psi_k(\tau) + \sum_{k=n_{mod-evol}}^{n_{non-evol}} C_k(N_0) \psi_k(\tau) \\
  u(N, \tau) &= \sum_{k=1}^{n} C_k(N) \psi_k(\tau) \\
  \tilde{u}(N, \tau) &= \sum_{k=1}^{n_{evol}} C_k(N) \psi_k(\tau) + \sum_{k=n_{mod-evol}}^{n_{non-evol}} C_k(N_0) \psi_k(\tau)
\end{align*}
\] (2.71)

where \( n \) is the total number of coefficients, \( n_{evol} \) is selected from 10\(^{th} \) cycle based on criterion described in section 2.4.1, \( N_0 = 10 \) and \( N = 8000 \). The reconstructed waveform at 8000\(^{th} \) cycle for \( n_{evol} = 43 \) and \( n_{evol} = 65 \) are shown in figures 2.14(a) and 2.14(b) respectively.

A similar procedure is followed for the discrete Fourier transform where the absolute values of the coefficients are used in equation 2.68. Since Fourier transform has no multi-resolution property, all the 128 coefficients are considered to exist in a single resolution in equation 2.68. The 128 coefficients in the 10\(^{th} \) cycle is shown in figure 2.15 and the number of evolving coefficients for different values of \( \eta \) is shown in figure 2.16. Reconstruction of the waveform is performed at 8000\(^{th} \) cycle similar to the discrete wavelet transform and the corresponding reconstructed waveform for \( n_{evol}=49 \) and \( n_{evol}=87 \) are shown in figures 2.17(a) and 2.17(b) respectively.

In figure 2.18, the relative error in the reconstruction for different evolving set of coefficients for the discrete wavelet and Fourier transform are compared. Discrete wavelet transform shows less error than discrete Fourier transform for lower number of evolving coefficients. This is can be attributed to the compact support and multi-resolution property of the wavelet basis functions which prevent the error to propagate through out the waveform. Adding the necessary evolving coefficients locally corrects the fluctuations in the reconstructed response. As can be observed from figure 2.18, discrete Fourier transform requires \( n_{evol} > 120 \) for accurate reconstruction.
2.4.3 Quasi-Newton Method

The wavelet coefficients of nodal displacements $C_{i,k}^\alpha$ are the primary degrees of freedom in the modified finite element model and are solved iteratively at every cyclic increment using a Quasi-Newton method. An approximate stiffness matrix $K$ is formed and factorized once in first increment and used in the subsequent increments. Reformation of the stiffness matrix is done in an increment only when convergence is not achieved within a desired number of iterations. A Broyden rank one update scheme is used to iteratively update the inverse of stiffness matrix and corresponding increments of wavelet coefficients of nodal displacements $\Delta C_{i,k}^\alpha$ as shown below.

$$\Delta C_{i+1} = K_{i+1}^{-1} R_{i+1}$$

$$K_{i+1}^{-1} = K_i^{-1} + \frac{\Delta C_i - K_i^{-1} \Delta R_i}{\Delta R^T \Delta R_i} \Delta R^T$$

$$\Delta R_{i+1} = R_{i+1} - R_i$$ \hspace{1cm} (2.72)

The cyclic representation of the nodal displacements in terms of the wavelet coefficients increases the number of equations to be solved at every iteration from $n_{dof}$ to $n_{wav} \times n_{dof}$, where $n_{dof}$ is the number of degrees of freedom of the conventional FE model and $n_{wav}$ is the number of wavelet coefficients required to capture the cyclic variation. The corresponding increase in the size of the stiffness matrix is $n_{wav}^2$ and number of operations for factorization is $n_{wav}^3$. To overcome this computational bottleneck, the approximate stiffness matrix is formed by $n_{wav}$ repetitions of the $n_{dof} \times n_{dof}$ stiffness matrix evaluated at $\tau_p = 0$ and is shown in equation (2.73).

$$K_{i,j,k,l}^{\alpha \beta} = \delta_{kl} \frac{\partial R_i^\alpha}{\partial u_j^\beta}(\tau_p = 0) = \bar{K}_{i,j}^{\alpha \beta}$$ \hspace{1cm} (2.73)

This approximation reduces the size of the stiffness matrix and the number of operations for factorization. As can be observed from equation (2.72), the iterative update of coefficients of nodal displacements involves backward substitution of the factorized stiffness matrix.
The block diagonal structure of the approximate stiffness matrix reduces this operation to $n_{\text{wav}}$ backward substitutions of the $n_{\text{dof}} \times n_{\text{dof}}$ matrix $\tilde{K}_{ij}^{\alpha \beta}$ as shown below.

$$\Delta C_{i,k}^\alpha = - \left[ \tilde{K}_{ij}^{\alpha \beta} \right]^{-1} R_{j,k}^\beta \quad \text{for} \quad k = 1...n_{\text{wav}}$$ (2.74)

### 2.4.4 Non-uniform discrete wavelet transform

The discrete wavelet transform described in the previous section considers an uniform distribution of points which implies uniform time increments $\tau$ to perform fine scale integration of non-linear evolution laws. However when large time periods are involved, the use of uniform time stepping to perform fine scale integration can prove computationally ineffectve. An automatic time stepping algorithm based on integration error of internal variables is employed to alleviate this problem. However this results in a set of non-uniform data points that needs to be transformed to the wavelet space. An interpolation scheme is developed to map the non-uniform data set to an uniform distribution of points for wavelet transformation. Moreover the maximum resolution of wavelet space is dictated by the minimum time increment. Such fine time steps may not be required through out the loading cycle and can be estimated a priori, hence the total time period can be segmented with different maximum resolution to reduce the total number of coefficients that needs to be stored. The split of the total time period with different maximum resolutions which are inversely proportional to the minimum time steps in each segment is as follows:

$$I = \bigcup_{j=1}^{N_{\text{seg}}} I_{\text{seg}}^j$$ (2.75)

where $N_{\text{seg}}$ is the total number of segments. The different segments are decided based on the load characteristics. For example, in crystal plasticity based finite element models subjected to triangular loads with $R = 0$, the initial portion of loading and trailing portion of unloading have a dominant elastic response and hence a coarser resolution can be used.
While near the peak of loading and unloading much finer resolution is required for accuracy and convergence of the fine scale integration. The division of the time period into different segments with different maximum resolutions reduces the total number of wavelet coefficients and improves the efficiency of the method.

Automatic time steps based on evolution of internal variables are used to accelerate fine scale integration within each segment as shown below.

\[
y(X, N, \tau_{p+1}) = y(X, N, \tau_p) + f(X, y_{p+1}, F_{p+1}, N, \tau_{p+1})\Delta\tau_{p+1}
\]

where \( \Delta\tau_{\min,\text{seg}} \leq \Delta\tau_{p+1} \leq \Delta\tau_{\max,\text{seg}} \) (2.76)

However the use of variable time steps generates non-uniformly spaced data points which are then interpolated to \(2^n\) uniformly spaced data points to perform a discrete wavelet transform.

\[
y(X, N, \tau_w) = (1 - \zeta)y(X, N, \tau_p) + \zeta y(X, N, \tau_{p+1}) \quad \text{where} \quad \zeta = \frac{\tau_w - \tau_p}{\tau_{p+1} - \tau_p} \quad (2.77)
\]

where \(\tau_p\) are the integration time points and \(\tau_w\) are the uniformly spaced time points for discrete wavelet transform. If the time points \(\tau_p\) are arbitrary and are not in multiples of 2, the discrete wavelet transform of their interpolated values have error which can result in convergence problems. Hence it is ensured that the time increments as predicted from the evolution of variables is also a multiple of 2 as shown.

\[
\Delta\tau_{p,i} = \frac{T_i}{2^{m+1}} \quad \text{when} \quad \frac{T_i}{2^{m+1}} \leq \Delta\tilde{\tau}_{p,i} = c \leq \frac{T_i}{2^m}
\]

where \(i \equiv I_{\text{seg}}\) and \(m_{i\min} \leq m \leq m_{i\max}\) (2.78)

where \(T_i\) is the time of the \(i^\text{th}\) segment, \(m_{i\min}\) and \(m_{i\max}\) are the minimum and maximum resolution of the \(i^\text{th}\) segment and \(c\) is a criterion based on which fine scale time increments are predicted. For the finite element model, internal \(F_{el}^{\text{int}}(N, \tau_p)\) and external \(F_{el}^{\text{ext}}(N, \tau_p)\) forces for each of the elements at any cycle are evaluated at \(\tau_p\). The interpolation method in
equation 2.77 followed by discrete wavelet transform is performed to obtain the coefficients of local residual vector

\[ \hat{R}_i^a(N, \tau_w) = (1 - \zeta) \hat{R}_i^a(N, \tau_p) + \zeta \hat{R}_i^a(N, \tau_{p+1}) \]

\[ \hat{R}_{i,k}^a(N) = T_{kw} \hat{R}_i^a(N, \tau_w) \]  

(2.79)

where \( T_{kw} \) is the wavelet transformation matrix. The transformed local residual vectors for each element are then assembled to obtain the global residual vector \( R_{i,k}^a(N) \).

### 2.4.5 Automatic selection of cycle jumps

An automatic coarse scale time stepping criterion is developed to estimate the number of cycles traversed in each increment of the numerical integration scheme. The optimal step size is estimated from the truncation error of the coarse scale internal variable \( y_0 \) in conjunction with the residual of the weak form in equation 2.59. For the implicit second order backward difference scheme, the truncation error is derived as follows:

\[ \delta y_0 = \frac{1}{6} \left| \frac{d^3 y_0 (r + 1)^2 - (r + 1)^3}{dN^3 (r + 1)^2 - 1} \right| \Delta N^3 \]  

(2.80)

The effect of the local constitutive level integration error on the global equilibrium equations in the coarse scale problem is shown below.

\[ \delta f_{err} = \sum_{el} \frac{1}{6} \left| \int_{\Omega_{el}} B^T \frac{\partial \sigma}{\partial y_0} (r + 1)^2 \left( \frac{r + 1)^3}{(r + 1)^2 - 1} \frac{d^3 y_0}{dN^3} \right) \, d\Omega_{el} \right| \Delta N^3 \]  

(2.81)

For the error to be bounded by a prescribed relative tolerance \( \eta \), the maximum allowed cycle step jump \( \Delta N \) is obtained as

\[ \Delta N \leq \left( \frac{6\eta f_{err}}{\delta f_{err}} \right)^{\frac{1}{3}} \text{ where } f_{err} = \sum_{el} \left| \int_{\Omega_{el}} B^T \sigma \, d\Omega_{el} \right| \]  

(2.82)
2.5 Conclusions

In this chapter, the WATMUS method for non-linear ODEs and initial boundary value problems, is discussed. Orthogonal wavelet basis functions with compact support and multi-resolution properties are advantageous over other basis representation and hence used for transformation. The method is advantageous over the existing multi-time scale methods since it has no assumption of periodicity or almost periodicity of response and there is no calibration process involved. It also provides an implicit framework to perform coarse scale integration and hence does not exhibit stability issues. To extend the applicability of the WATMUS method to larger problems, automatic time stepping for fine scale integration of internal variables and non-uniform discrete wavelet transformation is developed. Approximate stiffness matrix is used to solve the coefficients of displacements for the spatially discretized domain to improve the performance of the method. Adaptive criteria to reduce the number of evolving coefficients and to determine cycle jumps are developed to enhance the computational efficiency and accuracy of the multi-time scale method.
Figure 2.5: Evolution of viscoplastic variable subjected to cyclic strain: (a) Single time scale response (b) Magnified view of response over few cycles (c) High frequency fine time scale response over one load period (d) Coarse time/Cycle scale evolution corresponding to the value at start of cycle.
Figure 2.6: Wavelet transformation of an oscillatory signal. High and low resolution basis functions capture the fast and slow change of the signal.
Figure 2.7: Relative error $\epsilon$ in log scale as described in equations 2.55 and 2.56, of coarse scale integration for the viscoplastic model using different coarse scale rate equations defined in section 2.3.2 with varying $\Delta N$ and $\Delta N_p=2$: (a) $\epsilon_0^p$ (b) $\epsilon_p$ over a cycle
Figure 2.8: Comparison of local error in $\varepsilon_0$ obtained from coarse scale integration using rate equation (i) defined in section 2.3.2 with different $\Delta N$ and $r = 1$. 

\[
\log_2(\varepsilon_0) \quad \log_2(\Delta N)
\]
Figure 2.9: Comparison of coarse scale evolution for different $\Delta N$ and $r = 1$ using coarse scale rate equation (i) defined in section 2.3.2: (a) $\epsilon_0^p$ with cycles (b) Reconstructed $\epsilon^p$ at cycle 963 from coarse variables.
Figure 2.10: Comparison of global error in $\epsilon_0$ at cycles 259 and 963 obtained from coarse scale integration with different $\Delta N$ and $r = 1$ using coarse scale rate equation (i) defined in section 2.3.2.
Figure 2.11: Evolution of a nodal displacement degree of freedom within cycle: (a) 10 (b) 8000.
Figure 2.12: Coefficients from discrete wavelet transform at 10\textsuperscript{th} cycle.

Figure 2.13: Number of evolving coefficients based on different values of $\eta$. 

53
Figure 2.14: Comparison of reconstructed and exact response at 8000$^{th}$ cycle for different set of evolving coefficients: (a) $n_{evol}=43$ (b) $n_{evol}=65$. 

54
Figure 2.15: Coefficients from discrete Fourier transform at $10^{th}$ cycle.

Figure 2.16: Number of evolving coefficients based on different values of $\eta$. 

55
Figure 2.17: Comparison of reconstructed and exact response at 8000\(^{th}\) cycle for different set of evolving coefficients: (a) \(n_{evol}=49\) (b) \(n_{evol}=87\).
Figure 2.18: Comparison of error $e = \frac{|y(N,\tau)-\hat{y}(N,\tau)|}{|y(N,\tau)|}$ in reconstruction for different set of evolving coefficients between discrete wavelet and Fourier transform.
CHAPTER 3
NUMERICAL EXAMPLES

The WATMUS method provides an implicit framework to perform coarse scale simulations of initial boundary value problems where temporal evolutions are governed by first order rate equations. The wavelet coefficients form the coarse variables and are solved numerically at discrete cyclic increments. The fine scale response at any cycle can be reconstructed from the corresponding wavelet coefficients. Four different numerical examples are presented in this chapter to provide a quantitative estimate of accuracy and computational efficiency of the proposed multi-time scale method. In the first example described in section 3.1, the WATMUS method is used to decouple the evolution of volume fraction of one of the variants of martensite in a plate subjected to biaxial loading and is taken from the work of [Acharya and Sawant, 2006]. Though the development of the WATMUS method is motivated from viscoplastic and crystal plasticity based finite element models, it can be extended to other systems as can be seen from this example. In the second example, a 1d viscoplastic model with heterogeneous properties is considered and is shown in section 3.2. A completely reversible displacement loading \((u_{\text{min}}/u_{\text{max}} = -1)\) is applied which results in a stress ratio \(R = \sigma_{\text{min}}/\sigma_{\text{max}} \to -1\). The ability of the method to work under completely reversible loading condition is demonstrated through this example. The adaptive criteria proposed in sections 2.4.1 and 2.4.5 are applied to improve the efficiency of coarse scale integration scheme. The ability of the criteria to select evolving coefficients and predict cycle jumps based on accuracy requirements is also demonstrated through this
example. In the third and fourth example, 3d CPFE problem is solved using the proposed multi-time scale method. In the third example described in section 3.3, an experimentally validated size and rate dependent CPFE model for Ti-6242 is solved using the WATMUS method. In the fourth example described in section 3.4, CPFE model for nickel based super alloys is solved using the proposed methodology. The cycle scale response and oscillatory evolutions within a cycle, obtained from the WATMUS and single time scale simulations are compared to demonstrate the accuracy of the method. Computational efficiency of the method is also reported.

### 3.1 Kinetics of phase transforming material

This example is originally from the work of [Abeyaratne et al., 1996] in which evolution equation of one of the variants of martensite in a plate subjected to biaxial loading is developed. The evolution laws are modified in [Acharya and Sawant, 2006] to obtain an autonomous fine system

\[
\dot{\lambda} = -\mu \frac{\partial W}{\partial \lambda}(\lambda, \sigma_1, \sigma_2), \quad \lambda(0) = \lambda^0 \tag{3.1}
\]

where \(\lambda\) is the volume fraction of martensitic phase, \(\sigma_1\) and \(\sigma_2\) are the uniform tractions, and \(W\) is the total energy of the specimen. The total energy is comprised of 3 terms

\[
W = W_{\text{load}} + W_{\text{trans,layer}} + W_{\text{pert}}
\]

\[
W_{\text{load}} = -\left\{ \frac{\lambda^2(\sigma_1^2 + \sigma_2^2)(\alpha^2 - \gamma^2)^2}{(\alpha^2 + \gamma^2)} + 2\lambda(\sigma_1^2\gamma^2 - \sigma_2^2\alpha^2)(\alpha^2 - \gamma^2)/(\alpha^2 + \gamma^2) + (\sigma_1\gamma + \sigma_2\alpha) \right\}^{\frac{1}{2}}
\]

\[
W_{\text{trans,layer}} = c_1\lambda^2 + c_2(1 - \lambda)^2
\]

\[
W_{\text{pert}} = a\epsilon \cos\left(\frac{\lambda}{\epsilon}\right); \quad \epsilon \rightarrow 0 \tag{3.2}
\]

where \(\alpha, \gamma, c_1, c_2, a, \epsilon\) are parameters. The values of the different parameters are as follows: \(\alpha = 1.0619, \gamma = 1.0231, c_1 = 0.017 \text{ MPa}, c_2 = 0.0255 \text{ MPa}, a = 0.025 \text{ MPa}, \mu =\)
5.4 MPa$^{-1}$s$^{-1}$ and $\epsilon = 0.005$. In equation 3.2, though the term $W_{\text{pert}}$ is a perturbation to the total energy, its contribution to the driving force is finite and sufficient to cause changes to the evolution of volume fraction $\lambda$. Two different loading situations are considered. In the first case, constant stresses with magnitude $\sigma_1 = 7.0$ MPa and $\sigma_2 = 6.09$ MPa are applied. In the second case, a cyclic stress with $\sigma_1 = 5.81 + \cos(2\pi t/T)$ MPa and a constant stress $\sigma_2 = 5.85$ MPa is applied. The time period $T$ of the applied stress is 20 sec. A backward Euler integration scheme is used to obtain the single time scale solution. The initial value of volume fraction at a cycle, $\lambda(N, \tau = 0) = \lambda_0$, is considered as the coarse scale variable for the WATMUS method. A second order backward difference formula is used to perform the coarse scale integration. Equation 2.42 is used to define the coarse scale evolution rate and is shown below.

\[
\frac{d\lambda_0}{dN}(N) = \lambda(N, T) - \lambda_0(N) \\
\lambda_0(N + \Delta N) = \beta_1\lambda_0(N) - \beta_2\lambda_0(N - \Delta N_p) + \beta_3 \left. \frac{d\lambda_0}{dN} \right|_{N+\Delta N} \Delta N
\]  

(3.3)

where $\beta_1$, $\beta_2$ and $\beta_3$ are defined in equation 2.41. The coarse and single time scale simulation results for both the loading situations are compared below.

### 3.1.1 Case 1: Constant load

The coarse and single time scale solution obtained in [Acharya and Sawant, 2006] for different initial conditions $\lambda(t = 0) = \lambda^0$ is shown in figure 3.1. As can be observed from figure 3.1, the response varies with changes in the initial condition. The perturbations in the response is due to $W_{\text{pert}}$ in the total energy of the system as shown in equation 3.2. For the WATMUS simulations one of the initial condition $\lambda(t = 0) = 0.12$ is considered. The response has no clearly defined time period, hence 2 different time periods of 0.5 and 1 sec are considered. The single time simulations and fine scale integration with a cycle in the WATMUS method, are performed with time increment 0.0078125 sec. The comparisons
Figure 3.1: Evolution of volume fraction $\lambda$ under constant applied stresses as obtained from single time scale and method of parameterized invariant manifold [Acharya and Sawant, 2006].
of the coarse scale solutions obtained by solving using the WATMUS method and that obtained from single time scale solution are shown in figure 3.2.

3.1.2 Case 2: Cyclic load

The single time scale solution under cyclic applied stresses is shown in figure 3.3. As can be observed from figure 3.3 the response has 2 oscillatory component. One is due to the periodic applied stresses and the other due to the non-periodic perturbation energy. The coarse scale variable $\lambda_0$ is evolved based on time period of 0.5 sec and the comparison with single time scale simulations are shown in figure 3.4.
Figure 3.2: Comparison of evolution of coarse scale variable $\lambda_0$ obtained from WATMUS methodology and single time scale solution for 2 different time period: (a) $T=0.5$ sec (b) $T=1$ sec.
Figure 3.3: Evolution of volume fraction $\lambda$ under cyclic applied stresses.

Figure 3.4: Comparison of evolution of coarse scale variable $\lambda_0$ obtained from WATMUS methodology and single time scale solution.
3.2 1d viscoplastic model with heterogeneous properties

A 1-d viscoplastic finite element model with 2 elements is considered in this example and is shown in figure 3.5. The plastic evolution laws are shown in equation 2.5. The 2 elements are assigned different initial hardness values of 320 MPa and 600 MPa. The other parameters are kept the same as in section 2.2.1.

![1-d viscoplastic finite element model with 2 elements](image)

Figure 3.5: 1-d viscoplastic finite element model with 2 elements.

Displacement boundary conditions are applied on both the ends with \( u(x = 0, t) = 0 \) and \( u(x = 2L, t) = 0.006 \sin(2\omega t) \) as shown in figure 3.5. The time period \( T \) of applied cyclic displacement is 1 sec. Single time scale finite element simulations are performed for 2000 cycles. Due to a high hardness value, element 2 behaves elastically. Under the applied displacement, element 1 undergoes plastic deformation and the evolution of plastic strain \( \epsilon_p \) is shown in figure 3.6. In the WATMUS algorithm, integration of cycle scale variables \( \epsilon_0^p \) and \( g_0 \) in each element is performed by following the procedure described in 2.3.2. The wavelet coefficients of strain \( \epsilon_k \) in each element is obtained from the nodal displacement.
coefficients $C_k$, which are solved from the coarse scale weak form by using an iterative Newton-Raphson scheme as shown below.

$$R_k^{(2)}(N) = \sigma_k^{e_1}(N) - \sigma_k^{e_2}(N)$$

$$C_k^{(2)}(N)_{i+1} = C_k^{(2)}(N)_i + \Delta C_k^{(2)}(N)_i$$

$$\Delta C_k^{(2)}(N)_i = - \left[ \frac{\partial R_l}{\partial C_k} \right]^{-1} R_l^{(2)}(N)_i$$

(3.4)

In the Newton Raphson scheme, the exact jacobian is evaluated at each iteration following

$$\frac{\partial R_l}{\partial C_k} = \frac{\partial \sigma_j^{e_1}}{\partial C_k} - \frac{\partial \sigma_j^{e_2}}{\partial C_k}$$

$$\frac{\partial \sigma_j^{e_1}}{\partial C_k} = (-1)^{j-1} T_{km} \left\{ \frac{\partial \sigma}{\partial \epsilon}(\tau_m) + \frac{\partial \sigma}{\partial \epsilon}(\tau_m) \frac{\partial \epsilon_0}{\partial \epsilon}(\tau_m) \frac{\partial \epsilon_0}{\partial \epsilon}(\tau_m) \right\}$$

(3.5)

where $j = 1$ or 2 for element 1 or 2 respectively, $T$ is the discrete wavelet transformation matrix, $L$ is the length of the bar and $\tau$ are the discrete time points in the fine scale integration.

The initial values of the coarse scale internal variables and initial guess of nodal displacement coefficients are obtained from the first few cycles of single time scale integration. An uniform time step $\tau = 0.0078125$ sec is used for fine scale integration. This gives a total number of 128 displacement coefficients to be solved in the cycle scale finite element framework. In order to reduce the number of evolving coefficients to be solved, the criterion described in section 2.4.1 is used. The initial set of coefficients are selected based on $\eta = 10^{-3}$ and coefficients are added or removed based on the criterion as the simulation progresses. Appropriate number of coefficients must be selected at the starting cycle to attain convergence.

A cycle jump of $\Delta N = 2$ is used to start the coarse simulation. As the simulation progresses, cycle jumps are predicted based on the criterion described in section 2.4.5. The truncation error in the second order backward difference formula of $\epsilon_0^p$ and the corresponding error in the residual is used for predicting the cycle jumps. The WATMUS simulation is
performed for 2000 cycles and the results are compared with the single time scale solution. Figure 3.7 compares the evolution of the coarse scale internal variable $e_0^p$ with cycles, obtained from the coarse scale simulation and single time scale simulation. From the wavelet coefficients of the variables at any cycle, the corresponding fine scale response can be reconstructed. A comparison of the reconstructed fine scale response at 2000th cycle with the single time scale solution is shown in figure 3.8. The evolution of number of coefficients with cycles based on the criterion 2.4.1 is shown in figure 3.9. As can be observed from figure 3.7, between $N = 300$ and 800, the change in the rate of evolution of coarse plastic variables is large. Hence the set of evolving coefficients required and the change in the number of evolving coefficients in the set, to attain convergence within a certain accuracy, is large. However, once stability in response is achieved, the change in the number of evolving coefficients reduces and is fairly constant as can be seen in figure 3.9. Also the cycle jumps are large after stabilized response is obtained as can be observed in figure 3.7.
Figure 3.6: Evolution of $\epsilon^p$ of element 1 from 1d viscoplastic finite element model: (a) Single time scale response for 2000 cycles (b) Response in 800$^{th}$ cycle.
Figure 3.7: Comparison of evolution of $\varepsilon_p^0$ with cycles in the 1\textsuperscript{st} element.

Figure 3.8: Comparison of $\varepsilon^p$ in the 1\textsuperscript{st} element at 2000\textsuperscript{th} cycle.
Figure 3.9: Variation of number of evolving coefficients solved in the modified cycle scale FE method with cycles.
3.3 Crystal plasticity based FE model for Ti-alloys

In crystal plasticity theory, the plastic deformation in polycrystalline alloys happens through slip on different slip systems [Kalidindi et al., 1992, Anand and Kothari, 1996, Balasubramanian, 1998]. The number of slip systems and their strength depends on the morphological and crystallographical characteristics of the micro-structure. Hence the micro-structural effect on the deformation of polycrystalline material is captured through crystal plasticity based models. The micro-structure of Ti-alloys (Ti-6Al, Ti-6242) is composed of primary α grains and transformed α + β colonies. The primary α grains have a hexagonal close packed (hcp) crystal lattice structure and is strongly anisotropic [Hasija et al., 2003]. The transformed α + β colonies consists of alternate lathe of hcp lattice (α phase) and symmetric body centered cubic (bcc) lattice (β phase) [Deka et al., 2006] as shown in figure 3.10.

![Figure 3.10: Microstructure of forged Ti-6242 alloy: (a) SEM image (b) Schematic of the lathe structure in the α + β colonies.](image)

The hcp crystal structure consists of 3 ⟨a⟩ basal slip systems {0001}\(\langle 11\bar{2}0\rangle\), 3 ⟨a⟩ prismatic slip systems \{10\(\bar{1}0\))\(\langle 11\bar{2}0\rangle\), 6 ⟨a⟩ pyramidal slip systems \{10\(\bar{1}1\))\(\langle 11\bar{2}0\rangle\), 12 ⟨c + a⟩
first order pyramidal slip systems \(\{10\bar{1}1\} \langle 11\bar{2}3 \rangle\) and 6 \(\langle c + a \rangle\) second order pyramidal slip systems \(\{11\bar{2}2\} \langle 11\bar{2}3 \rangle\). The strongly anisotropic and orientation dependent plastic behavior of the \(\alpha\) phase is due to the vastly different slip system resistances. The basal and prismatic \(\langle a \rangle\) slip systems have the lowest resistance and are most favorable for slip activity, whereas the pyramidal \(\langle c + a \rangle\) slip systems have the highest resistance showing no slip activity at room temperature. A transversely isotropic elastic tensor, with 5 independent constants, is used to model the elastic behavior of the \(\alpha\) phase in these alloys. The \(\beta\) phase in these alloys have a cubic symmetry requiring 3 independent constants to model the elastic response and 48 slip systems divided into 3 families, \{110\}\langle111\rangle, \{110\}\langle112\rangle and \{110\}\langle123\rangle, to model the plastic response.

In crystal plasticity model, the total deformation gradient at a material point is multiplicatively split into an elastic and plastic part [Kalidindi et al., 1992, Anand and Kothari, 1996, Balasubramanian, 1998].

\[
F = F^e F^p
\] (3.6)

The elastic part of the deformation gradient \(F^e\) captures the stretching and rotation of the lattice. Plastic deformation happens through crystallographic slip on different slip systems and is obtained from

\[
\dot{F}^p F^{-1} = \sum_{\alpha} \dot{\gamma}^\alpha S_0^\alpha
\] (3.7)

where \(\dot{\gamma}^\alpha\) is the slip rate on different slip systems and \(S_0^\alpha\) is the Schmid tensor. The Schmid tensor is formed from the slip direction \(\mathbf{m}_0^\alpha\) and slip plane normal \(\mathbf{n}_0^\alpha\) in the intermediate configuration such that \(S_0^\alpha = \mathbf{m}_0^\alpha \otimes \mathbf{n}_0^\alpha\). A power law is used to model slip rate on different slip systems as shown below.

\[
\dot{\gamma}^\alpha = \dot{\alpha} \left| \frac{\tau^\alpha - \chi^\alpha}{g^\alpha} \right|^\beta \text{sign}(\tau^\alpha - \chi^\alpha)
\] (3.8)
where \( \dot{a} \) is the reference slip rate, \( \tau^\alpha \) is the resolved shear stress on the slip system, \( \chi^\alpha \) is the back stress, \( g^\alpha \) is the slip system resistance and \( m \) is the power law exponent. The resolved shear stress on a slip system is obtained from

\[
\tau^\alpha = F^e T^* : \frac{1}{2} \left( S_0^\alpha + S_0^{\alpha T} \right)
\]  

(3.9)

where \( T^* \) is the 2nd Piola-Kirchoff (PK2) stress. A hyper-elastic law is used to obtain the PK2 stress from the work conjugate Lagrange-Green strain tensor

\[
T^* = C : F^e \text{ where } F^e = \frac{1}{2} (F^e T^e - I)
\]  

(3.10)

The evolution of slip system hardness is obtained from

\[
\dot{g}^\alpha = \sum_\beta q^{\alpha \beta} h^\beta \left| \dot{\gamma}^\beta \right|
\]  

(3.11)

where \( h^\beta \) is the self hardening parameter and \( q^{\alpha \beta} \) is a matrix describing latent hardening.

The evolution of back stress on a slip system is as follows:

\[
\dot{\chi}^\alpha = c \dot{\gamma}^\alpha - d \chi^\alpha \left| \dot{\gamma}^\alpha \right|
\]  

(3.12)

where \( c \) and \( d \) are the direct hardening and dynamic recovery coefficients respectively [Morrissey et al., 2001]. Different self hardening relationships are used for the \( \alpha \) and \( \beta \) phases. The evolution of self hardening for the \( \alpha \) phase is

\[
h^\alpha = h_0^\alpha \left| 1 - \frac{g^\alpha}{g_s^\alpha} \right|^r \text{sign} \left( 1 - \frac{g^\alpha}{g_s^\alpha} \right)
\]

\[
g_s^\alpha = \tilde{g} \left| \dot{\gamma}^\alpha \right|
\]  

(3.13)

where \( h_0^\alpha \) is the reference value of self hardening and \( g_s^\alpha \) is the saturation value of slip system resistance. The evolution of self hardening of the \( \beta \) phase is

\[
h^\beta = h_s^\beta + sech^2 \left( \frac{h_0^\beta - h_s^\beta}{\tau_s^\beta - \tau_0^\beta} \gamma_{acc} \right) \left( h_0^\beta - h_s^\beta \right)
\]

\[
\gamma_{acc} = \int_0^t \sum_\alpha \left| \dot{\gamma}^\alpha \right| dt
\]  

(3.14)
where $\gamma^{acc}$ is the accumulated plastic slip.

The explicit modeling of the alternate lathe structure of the transformed $\alpha + \beta$ colonies for finite element simulations is computationally exhaustive. An equivalent homogenized model is developed in [Deka et al., 2006] based on mixture rule for the colonies in which the individual phases at a material point experiences the same deformation field but have independent evolution for the plastic variables and stresses. The stress at the material point is the weighted sum of the stresses in the individual phases in the colony

$$\sigma = w_\alpha \sigma_\alpha + w_\beta \sigma_\beta$$

(3.15)

where the weights $w_\alpha$ and $w_\beta$ correspond to the volume fractions of individual phases and depend on the chemical composition and processing conditions of these alloys.

The effect of grain size and lath thickness on the slip system resistance is also considered in the crystal plasticity model [Venkataramani et al., 2007]. A Hall Petch type relation is used to modify the initial slip system resistances to capture the size effect and is shown below.

$$g^\alpha = g_0^\alpha + \frac{K^\alpha}{\sqrt{D^\alpha}}$$

(3.16)

where $D^\alpha$ is a characteristic length parameter. For the globular $\alpha$ grains, the grain boundaries prevent transmission of dislocations to adjacent grains and resist further dislocation motion in these grains. Based on this observation, the grain diameter is considered as the characteristic length for the globular $\alpha$ grains in equation 3.16. For the transformed $\alpha + \beta$ colonies, depending on the burgers relation between the $\alpha$ and $\beta$ lathe, dislocation motions can either be impeded by colony boundaries or lathe boundaries. Hence for the colonies, either the colony size or the lathe thickness is used in equation 3.16 to modify the initial slip system resistances. The different parameters in the modified crystal plasticity model are calibrated from experiments and finite element simulations of single crystal Ti-6Al and Ti-6242 [Hasija et al., 2003, Deka et al., 2006, Venkataramani et al., 2007].
In the WATMUS method for CPFE model of Ti-alloys, the coarse scale internal variables are \( F_{p0}^0 \), \( g_{0}^{\alpha} \), \( \chi_{0}^{\alpha} \) and \( \gamma_{0}^{acc} \). The evolution of the coarse variables are determined from definition (i) described in section 2.3.2 and is shown below.

\[
\begin{align*}
\frac{\partial F_{ij0}}{\partial N}(X,N) &= F_{ij}^p(X,N,T) - F_{ij0}^p(X,N) \\
\frac{\partial g_{0}^{\alpha}}{\partial N}(X,N) &= g_{\alpha}(X,N,T) - g_{0}^{\alpha}(X,N) \\
\frac{\partial \chi_{0}^{\alpha}}{\partial N}(X,N) &= \chi_{\alpha}(X,N,T) - \chi_{0}^{\alpha}(X,N) \\
\frac{\partial \gamma_{0}^{acc}}{\partial N}(X,N) &= \gamma(X,N,T) - \gamma_{0}^{acc}(X,N)
\end{align*}
\]  

(3.17)

At any cycle, fine scale integration over one time period of loading is performed to obtain the coarse scale evolution rate. A backward Euler scheme is used to numerically integrate the fine scale rate equations at discrete fine time points in the cycle. Automatic time stepping is employed to expedite the fine scale integration. A time step \( \Delta \tau_n \) in the \( n^{th} \) increment is selected based on

\[
\max_{\alpha} \left| \Delta \gamma_{\alpha}(\tau_n) \right| = \max_{\alpha} \left| \dot{\gamma}_{\alpha}(\tau_n) \right| \Delta \tau_n \leq 0.1 \dot{\alpha}
\]  

(3.18)

where \( \dot{\alpha} \) is the reference slip rate. If the maximum incremental slip exceeds the tolerance, the time step is halved. The use of automatic time stepping results in non-uniformly distributed set of points. Hence the non-uniform discrete wavelet transform described in section 2.4.4 is used to obtain the coefficients of the field variables.

A second order backward difference scheme shown in equation 2.41 is used to integrate the coarse variables. Two set of coarse scale internal variables \( Y_0 \) are chosen separately for the hcp and bcc phases. For the hcp phase \( Y_0 \) is a vector consisting of 9 components of \( F_{p0}^0 \), 30 slip system resistances \( g_{0}^{\alpha} \) and 30 slip system back stresses \( \chi_{0}^{\alpha} \). For the bcc phase \( Y_0 \) consists of 9 components of \( F_{p0}^0 \), 48 slip system resistances \( g_{0}^{\alpha} \), 48 slip system back stresses \( \chi_{0}^{\alpha} \) and \( \gamma_{0}^{acc} \). At any cycle, the coarse variables are obtained iteratively by employing a Newton Raphson scheme as shown in equations 2.51 and 2.52. The size of the Jacobian
matrix $A$ for the crystal plasticity model is $69 \times 69$ for the hcp phase and $106 \times 106$ for the bcc phase. Due to the large size of the matrix $A$, successive inversion and product operations are expensive. To improve the efficiency of the coarse scale integration scheme, a two level procedure is used. In this iterative process, $F^p_0$, $g_0^\alpha$ and $\gamma^{acc}_0$ are updated using the Newton-Raphson iterative scheme followed by an implicit update of the back stresses $\chi^\alpha_0$ as shown below.

$$\chi^\alpha_0(N) = \beta_1 \chi^\alpha_0(N - \Delta N) - \beta_2 \chi^\alpha_0(N - \Delta N - \Delta N_p) + \beta_3 (\chi^\alpha(N, T) - \chi^\alpha_0(N)) \Delta N$$  \hspace{1cm} (3.19)

The nested procedure is continued till convergence is achieved by all the coarse scale internal variables.

To reduce the number of iterations to integrate the coarse scale internal variables, the initial guess for these variables are obtained from

$$y_0(N + \Delta N) = \frac{r^2 - 1}{r^2} y_0(N) - \frac{1}{r^2} y_0(N - \Delta N_p) + \frac{r + 1}{r} \frac{\partial y_0}{\partial N} \bigg|_N \Delta N$$ \hspace{1cm} (3.20)

The initial guess for the coefficients of nodal displacements are also extrapolated based on

$$C^\alpha_{i,k}(N) = (1 + a_1 + a_2) C^\alpha_{i,k}(N - \Delta N_1) - a_1 C^\alpha_{i,k}(N - \Delta N_1 - \Delta N_2)$$

$$- a_2 C^\alpha_{i,k}(N - \Delta N_1 - \Delta N_2 - \Delta N_3)$$

where $a_1 = c_{11} \Delta N_1 + \frac{1}{2} c_{21} \Delta N_1^2$, $a_2 = c_{12} \Delta N_1 + \frac{1}{2} c_{22} \Delta N_1^2$,

$$\begin{bmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \end{bmatrix} = \begin{bmatrix} \Delta N_2 & -\frac{1}{2} r_p \Delta N_2^2 \\ (r_p + 1) \Delta N_2 & -\frac{1}{2} ((r_p + 1) \Delta N_2)^2 \end{bmatrix}^{-1}$$ and $r_p = \frac{\Delta N_3}{\Delta N_2}$  \hspace{1cm} (3.21)

The single time scale and modified coarse scale finite element models are implemented in a parallel message passing interface (MPI) environment to solve statistically equivalent microstructures consisting of thousands of grains. In the parallel framework, a domain decomposition is performed based on balancing the number of elements and nodal displacement degrees of freedom to be solved in each processor. A parallel direct sparse solver (Super LU) is employed to factorize the global stiffness matrix [Xiaoye, 2005].
the single time scale simulations, a Quasi-Newton method is employed where the global stiffness matrix is formed and factorized at the first increment. Subsequent reformations are done based on convergence of iterations at any increment. A modified Quasi-Newton scheme, described in section 2.4.3 is used for the coarse scale simulations. Since factorization of the global stiffness matrix involves communication between processors, this adaptation significantly improves the performance of the method.

A statistically equivalent microstructure of Ti-6242 consisting of 955 grains is used to evaluate the accuracy and computational advantage of the multi-time scale method. For this alloy, the volume fraction of $\alpha$ and $\beta$ phases in the colonies are 0.88 and 0.12 respectively. The c-axis orientation distribution of the grains is shown in figure 3.11.

![Figure 3.11: Microstructural distribution of c-axis orientation.](image-url)
A representative volume of 65\(\mu m\times 65\mu m\times 65\mu m\) is constructed from the orientation, misorientation, size and micro-texture distributions of the grains and is spatially discretized using 4 noded tetrahedral elements. The spatial discretization results in 78540 elements and 16045 nodes and is shown in figure 3.12(a). The microstructure is subjected to a triangular follower load on the y-face with \(S_{\text{max}} = 869\) MPa and \(S_{\text{min}} = 0\) MPa and minimum displacement boundary conditions are applied to constrain the rigid body modes as shown in figure 3.12(b). The response from first few cycles of single time scale simulation is used to obtain the initial values for the coarse scale problem. Since the single time scale simulations are computationally exhaustive, the response over 215 cycles are obtained to compare with the evolution from the WATMUS method. The evolution of one of the components of \(F_{0}^p\) and one of the slip systems \(g_0^\alpha\) at a material point is compared in figure 3.13.

As can be observed from the figure the evolutions are almost identical. Fine scale evolution at any cycle can be reconstructed from the wavelet coefficients of nodal displacements and coarse internal variables in that cycle. The relative error in the fine scale evolution of one of the components of \(F^p\), \(\sigma\) and one of the slip systems \(g^\alpha\) at 211\(^{th}\) cycle at a material point as obtained from the WATMUS method and single time scale solution is shown in figure 3.14. A comparison of the distribution of \(\sigma_{22}\) and \(F_{22}^p\) in the microstructure at \(\tau = 1\) sec and \(N = 211\) cycle, as reconstructed from WATMUS method and obtained from single time scale simulation are shown in figure 3.15 and 3.16(b) respectively. The results are in very good agreement as can be observed from the figures. A material line is considered in the microstructure and \(\sigma_{22}\) along that line at \(\tau = 1\) sec and \(N = 211\) cycle is compared and shown in figure 3.17(a). The relative error in \(\sigma_{22}\) along the material line from the WATMUS and single time scale simulations is shown in figure 3.17(b) where the error is defined as

\[
e(X,N,\tau) = \frac{|\tilde{y}(X,N,\tau) - y_{\text{exact}}(X,N,\tau)|}{|y_{\text{exact}}(X,N,\tau)|} \quad (3.22)
\]

The coarse scale simulation is continued for 300,000 cycles and the evolution of one of
Figure 3.12: FE model of statistically equivalent microstructure of Ti-6242: (a) Mesh (b) Boundary conditions.
the components of $\mathbf{F}_0^p$ and one of the slip systems $g_0^\alpha$ at a material point is shown in figure 3.18. As the number of cycles of loading increases, the response tends to saturate and coarse scale integration with larger cycle jumps can be performed. The automatic coarse scale time stepping criterion discussed in section 2.4.5 is used to predict the cycle jump at any cycle. The truncation error in the coarse scale integration of $\mathbf{F}_0^p$ is used to determine the coarse scale time step.

$$\delta \mathbf{F}_0^p = \frac{1}{6} \left| \frac{d^3 \mathbf{F}_0^p}{dN^3} \frac{(r+1)^2 - (r+1)^3}{(r+1)^2 - 1} \right| \Delta N^3$$

To evaluate the computational benefit from the WATMUS method to perform 300,000 cycles of CPFE simulation, an estimate of the time required for single time scale simulation is obtained by extrapolating the time required for 215 cycles of simulation. An advantage of $\sim 100$ times is obtained for this case. The oscillatory $F_{22}^p$ and $g^\alpha$ at 300,000th cycle at a material point reconstructed from the coarse variables is shown in figure 3.19. The evolution of oscillatory stress $\sigma_{22}$ response with cycles at material point is shown in figure 3.20.
Figure 3.13: Comparison of evolution of coarse internal variables: (a) $F_{0,22}^p$ (b) $g_0^\alpha$.  

81
Figure 3.14: Relative error $e(N, \tau) = \frac{\|\tilde{y}(N, \tau) - y(N, \tau)\|}{\|y(N, \tau)\|}$ of fine scale evolution of internal variables at 211$^{th}$ cycle reconstructed from coarse scale variables ($\tilde{y}(N, \tau)$) and single time scale solution ($y(N, \tau)$): (a) $F_{22}^{p}$ (b) $g^a$ (c) $\sigma_{22}$.
Figure 3.15: Comparison of distribution of $\sigma_{22}$ (MPa) in the microstructure at $N = 211$ and $\tau = 1$ sec as obtained from WATMUS and single time scale simulation (a) WATMUS (b) Single time scale.
Figure 3.16: Comparison of distribution of $F_{22}^P$ in the microstructure at $N = 211$ and $\tau = 1$ sec as obtained from WATMUS and single time scale simulation (a) WATMUS (b) Single time scale.
Figure 3.17: Comparison of stress distribution in the microstructure along a material line at $N = 211$ and $\tau = 1$ sec as obtained from WATMUS and single time scale simulation: (a) $\sigma_{22}$ (b) relative error in $\sigma_{22}$. 
Figure 3.18: Evolution of coarse internal variables from WATMUS CPFE simulation: (a) $F_{0.22}^p$ (b) $g_0^\alpha$. 
The $\alpha$ phase in the alloy has a hcp crystal structure and is strongly anisotropic in its plastic behavior. Depending on the orientation of a $\alpha$ grain or the $\alpha$ lathe in a $\alpha + \beta$ colony with respect to the loading axis it can have drastically different plastic deformation. The unfavorably oriented grains have little or no plasticity and are called hard grains whereas the favorably oriented grains have large plastic deformation. This orientation dependent inhomogeneous plastic flow in the microstructure causes high stresses in hard grains surrounded by soft grains and this phenomenon is known as load shedding [Venkatramani et al., 2006, Venkataramani et al., 2007]. In figure 3.21, the $\sigma_{22}$ along a material line is shown for cycles $N = 211, \tau = 1$ sec and $N = 300,000, \tau = 1$ sec. As can be observed from the figure, the maximum stresses has increased and the effect of load shedding is more severe with advancing load cycles.
Figure 3.20: Evolution of oscillatory stress $\sigma_{22}$ with cycle at a material point.

Figure 3.21: Evolution of $\sigma_{22}$ along a material line in the microstructure with cycles.
3.4 Crystal plasticity based FE model for nickel based superalloys

The microstructure of nickel based superalloys consists of a matrix phase having a face centered cubic crystal structure (γ phase) and precipitates having an ordered L12 crystal structure (γ′ phase) ([Karthikeyan et al., 2006, Viswanathan et al., 2005, Kovarik et al., 2009, Ardakani et al., 1999]) as shown in figure 3.22. The size, shape and distribution of the precipitates depends on the cooling rate and internal stresses experienced by these alloys during the casting and heat treatment processes [Sabol and Stickler, 1969, Durand-Charre, 1997]. The ordered γ′ precipitates impede the motion of dislocations and increases the strength and creep resistance in the superalloys. Depending on the orientation of the grains in the polycrystalline alloy, the stress level, temperature and the morphology of the precipitates, different mechanisms dominate the inelastic deformation behavior in the superalloys [Karthikeyan et al., 2006, Unocic et al., 2011, Sondhi et al., 2004, Jiao et al., 1996, Torster et al., 1997, Hong et al., 2009, Knobloch et al., 1997, Soula et al., 2009, Chatterjee et al., 2010, Cormier et al., 2007, Milhet et al., 2010]. Since the inelastic deformation strongly depends on the crystallographical and morphological features, nickel based superalloys exhibit tension compression asymmetry in creep [Kakehi, 1999, Knowles and Gunturi, 2002, Hopgood and Martin, 1986, Sondhi et al., 2004, Jiao et al., 1996].

Anti-phase boundary (APB) shearing and microtwinning are considered as dominant mechanisms in the crystal plasticity based model developed for polycrystalline Ni based superalloys. In APB shearing, the paired a/2 < 110> dislocations in the matrix couples together with an anti-phase boundary in the secondary γ′ precipitates and shears through them causing inelastic deformation [Kovarik et al., 2009, Kozar et al., 2009, Sun and Hazzledine, 1988]. In microtwinning, the a/2 < 110> dislocations in the matrix dissociate into leading and trailing partials in the secondary γ′ phase. As the partials traverse with different velocities, faults happen in the secondary γ′ precipitates. A thermally activated diffusive
rate limiting reordering process restores the ordered L12 crystal structure in the precipitates and cause formation of twins with thickness of few (4-50) atomic layers [Viswanathan et al., 2005, Kolbe, 2001, Kovarik et al., 2009, Unocic et al., 2011, Karthikeyan et al., 2006].

In the crystal plasticity model, the $\gamma$ and $\gamma'$ phases are not distinguished morphologically, but their effect on the deformation behavior is captured through the different parameters. The plastic velocity gradient in the intermediate configuration ($L_0^p$) shown in equation 3.7 is assumed to evolve due to APB shearing or microtwin formation and is shown below.

$$\dot{F}^p F_0^{-1} = (1 - f) \left( \sum_\alpha \dot{\gamma}_{APB} S^\alpha_{0,APB} \right) + f \left( \sum_\alpha \dot{\gamma}_{twin} S^\alpha_{0,twin} \right)$$

(3.24)

where $f$ is 0 or 1 if inelastic deformation is due to APB shearing or microtwin formation respectively. $S^\alpha_{0,APB}$ are the Schmid factors corresponding to the 12 \{111\} <110> slip systems and $S^\alpha_{0,twin}$ are the Schmid factors corresponding to the 12 systems of the partial dislocations. The different slip and twin systems are listed in table 3.1 and 3.2 respectively.

An activation energy based law [Balasubramanian, 1998, Xie et al., 2004] is used to
Table 3.1: Slip plane normal $n^\alpha$ and direction $m^\alpha$ for APB shearing

<table>
<thead>
<tr>
<th>$\alpha$</th>
<th>$n^\alpha$</th>
<th>$m^\alpha$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$\frac{1}{\sqrt{3}} \frac{1}{\sqrt{3}} \frac{1}{\sqrt{3}}$</td>
<td>$-\frac{1}{\sqrt{2}} 0 \frac{1}{\sqrt{2}}$</td>
</tr>
<tr>
<td>2</td>
<td>$\frac{1}{\sqrt{3}} \frac{1}{\sqrt{3}} \frac{1}{\sqrt{3}}$</td>
<td>$0 \frac{1}{\sqrt{2}} -\frac{1}{\sqrt{2}}$</td>
</tr>
<tr>
<td>3</td>
<td>$-\frac{1}{\sqrt{3}} \frac{1}{\sqrt{3}} \frac{1}{\sqrt{3}}$</td>
<td>$\frac{1}{\sqrt{2}} \frac{1}{\sqrt{2}} 0$</td>
</tr>
<tr>
<td>4</td>
<td>$-\frac{1}{\sqrt{3}} \frac{1}{\sqrt{3}} \frac{1}{\sqrt{3}}$</td>
<td>$0 \frac{1}{\sqrt{2}} -\frac{1}{\sqrt{2}}$</td>
</tr>
<tr>
<td>5</td>
<td>$-\frac{1}{\sqrt{3}} \frac{1}{\sqrt{3}} \frac{1}{\sqrt{3}}$</td>
<td>$\frac{1}{\sqrt{2}} \frac{1}{\sqrt{2}} 0$</td>
</tr>
<tr>
<td>6</td>
<td>$-\frac{1}{\sqrt{3}} \frac{1}{\sqrt{3}} \frac{1}{\sqrt{3}}$</td>
<td>$-\frac{1}{\sqrt{2}} -\frac{1}{\sqrt{2}} 0$</td>
</tr>
<tr>
<td>7</td>
<td>$-\frac{1}{\sqrt{3}} \frac{1}{\sqrt{3}} \frac{1}{\sqrt{3}}$</td>
<td>$0 \frac{1}{\sqrt{2}} \frac{1}{\sqrt{2}}$</td>
</tr>
<tr>
<td>8</td>
<td>$-\frac{1}{\sqrt{3}} \frac{1}{\sqrt{3}} \frac{1}{\sqrt{3}}$</td>
<td>$0 \frac{1}{\sqrt{2}} \frac{1}{\sqrt{2}}$</td>
</tr>
<tr>
<td>9</td>
<td>$-\frac{1}{\sqrt{3}} \frac{1}{\sqrt{3}} \frac{1}{\sqrt{3}}$</td>
<td>$-\frac{1}{\sqrt{2}} \frac{1}{\sqrt{2}} 0$</td>
</tr>
<tr>
<td>10</td>
<td>$\frac{1}{\sqrt{3}} \frac{1}{\sqrt{3}} \frac{1}{\sqrt{3}}$</td>
<td>$0 -\frac{1}{\sqrt{2}} \frac{1}{\sqrt{2}}$</td>
</tr>
<tr>
<td>11</td>
<td>$\frac{1}{\sqrt{3}} \frac{1}{\sqrt{3}} \frac{1}{\sqrt{3}}$</td>
<td>$-\frac{1}{\sqrt{2}} 0 \frac{1}{\sqrt{2}}$</td>
</tr>
<tr>
<td>12</td>
<td>$\frac{1}{\sqrt{3}} \frac{1}{\sqrt{3}} \frac{1}{\sqrt{3}}$</td>
<td>$-\frac{1}{\sqrt{2}} \frac{1}{\sqrt{2}} 0$</td>
</tr>
</tbody>
</table>
Table 3.2: Twin plane normal $n^\alpha$ and direction $m^\alpha$ for microtwinning

<table>
<thead>
<tr>
<th>$\alpha$</th>
<th>$n^\alpha$</th>
<th>$m^\alpha$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$\frac{1}{\sqrt{3}} \ - \frac{1}{\sqrt{3}} \ \frac{1}{\sqrt{3}}$</td>
<td>$\frac{2}{\sqrt{6}} \ - \frac{1}{\sqrt{6}} \ \frac{1}{\sqrt{6}}$</td>
</tr>
<tr>
<td>2</td>
<td>$\frac{1}{\sqrt{3}} \ - \frac{1}{\sqrt{3}} \ \frac{1}{\sqrt{3}}$</td>
<td>$\frac{1}{\sqrt{6}} \ - \frac{2}{\sqrt{6}} \ \frac{1}{\sqrt{6}}$</td>
</tr>
<tr>
<td>3</td>
<td>$\frac{1}{\sqrt{3}} \ - \frac{1}{\sqrt{3}} \ \frac{1}{\sqrt{3}}$</td>
<td>$\frac{1}{\sqrt{6}} \ - \frac{1}{\sqrt{6}} \ \frac{2}{\sqrt{6}}$</td>
</tr>
<tr>
<td>4</td>
<td>$\frac{1}{\sqrt{3}} \ - \frac{1}{\sqrt{3}} \ \frac{1}{\sqrt{3}}$</td>
<td>$\frac{2}{\sqrt{6}} \ - \frac{1}{\sqrt{6}} \ \frac{1}{\sqrt{6}}$</td>
</tr>
<tr>
<td>5</td>
<td>$\frac{1}{\sqrt{3}} \ - \frac{1}{\sqrt{3}} \ \frac{1}{\sqrt{3}}$</td>
<td>$\frac{1}{\sqrt{6}} \ - \frac{2}{\sqrt{6}} \ \frac{1}{\sqrt{6}}$</td>
</tr>
<tr>
<td>6</td>
<td>$\frac{1}{\sqrt{3}} \ - \frac{1}{\sqrt{3}} \ \frac{1}{\sqrt{3}}$</td>
<td>$\frac{1}{\sqrt{6}} \ - \frac{1}{\sqrt{6}} \ \frac{2}{\sqrt{6}}$</td>
</tr>
<tr>
<td>7</td>
<td>$\frac{1}{\sqrt{3}} \ - \frac{1}{\sqrt{3}} \ \frac{1}{\sqrt{3}}$</td>
<td>$\frac{2}{\sqrt{6}} \ - \frac{1}{\sqrt{6}} \ \frac{1}{\sqrt{6}}$</td>
</tr>
<tr>
<td>8</td>
<td>$\frac{1}{\sqrt{3}} \ - \frac{1}{\sqrt{3}} \ \frac{1}{\sqrt{3}}$</td>
<td>$\frac{1}{\sqrt{6}} \ - \frac{2}{\sqrt{6}} \ \frac{1}{\sqrt{6}}$</td>
</tr>
<tr>
<td>9</td>
<td>$\frac{1}{\sqrt{3}} \ - \frac{1}{\sqrt{3}} \ \frac{1}{\sqrt{3}}$</td>
<td>$\frac{1}{\sqrt{6}} \ - \frac{1}{\sqrt{6}} \ \frac{2}{\sqrt{6}}$</td>
</tr>
<tr>
<td>10</td>
<td>$\frac{1}{\sqrt{3}} \ - \frac{1}{\sqrt{3}} \ \frac{1}{\sqrt{3}}$</td>
<td>$\frac{2}{\sqrt{6}} \ - \frac{1}{\sqrt{6}} \ \frac{2}{\sqrt{6}}$</td>
</tr>
<tr>
<td>11</td>
<td>$\frac{1}{\sqrt{3}} \ - \frac{1}{\sqrt{3}} \ \frac{1}{\sqrt{3}}$</td>
<td>$\frac{1}{\sqrt{6}} \ - \frac{2}{\sqrt{6}} \ \frac{1}{\sqrt{6}}$</td>
</tr>
<tr>
<td>12</td>
<td>$\frac{1}{\sqrt{3}} \ - \frac{1}{\sqrt{3}} \ \frac{1}{\sqrt{3}}$</td>
<td>$\frac{1}{\sqrt{6}} \ - \frac{1}{\sqrt{6}} \ \frac{2}{\sqrt{6}}$</td>
</tr>
</tbody>
</table>
define the slip and twin rate at any material point and has the following form:

\[
\dot{\gamma}_\alpha = \begin{cases} 
\dot{\gamma}_0 \exp\left(-\frac{Q}{K_B \theta}\right) \left[1 - \frac{\left|\tau_{eff} - s^\alpha_a\right|}{s^\alpha_a}\right] \sign\left(\tau_{eff} - s^\alpha_a\right) & \text{when } 0 < \frac{\left|\tau_{eff} - s^\alpha_a\right|}{s^\alpha_a} \leq 1 \\
0 & \text{otherwise}
\end{cases}
\]

where \( \tau_{eff} = \tau^\alpha - \chi^\alpha \) (3.25)

In the above equation, \( \tau^\alpha \) is the resolved shear stress, \( \chi^\alpha \) is the back stress, \( s^\alpha_a \) and \( s^\alpha_a \) are the athermal and thermal resistances to slip or twin, \( Q \) is the activation energy, \( K_B \) is the Boltzmann constant and \( \theta \) is the absolute temperature. The thermal and athermal slip system resistances evolve with advancing inelastic deformation as shown below.

\[
s^\alpha = \sum_\beta q^{\alpha\beta} h^\beta \dot{\gamma}^\beta \\
h^\alpha = h^\alpha_0 \left[1 - \frac{s^\alpha}{s^\alpha_{sat}}\right]^r \sign\left(1 - \frac{s^\alpha}{s^\alpha_{sat}}\right) \text{ and } s^\alpha_{sat} = \tilde{s}_{sat} \left|\frac{\dot{\gamma}_0}{\dot{\gamma}_0}\right|^c
\]

(3.26)

The evolution of back stress is determined from equation 3.12. Different values of parameters \( \dot{\gamma}_0, p, q, \tilde{s}_{sat}, h_0, r, c \) and initial values of athermal \( (s^\alpha_a(t = 0)) \) and thermal \( (s^\alpha_a(t = 0)) \) resistances are chosen for APB shearing and microtwinning. The latent hardening matrix \( q^{\alpha\beta} \) for APB shearing is adopted from [Ma et al., 2006, Alcala et al., 2011] and is shown in table 3.3. The latent hardening matrix for microtwinning is adopted from [Balasubramanian, 1998, Anand and Kothari, 1996] and is as follows.

\[
q^{\alpha\beta} = (1 - \delta^{\alpha\beta}) q_L + q_0
\]

where \( q_L = 0.4 \) and \( q_0 = 1.0 \) (3.27)

The two mechanisms are considered to be competing and cannot be active simultaneously at a material point. A criterion based on in plane stresses and critical stresses on partials.
Table 3.3: The values of latent hardening matrix $q^{\alpha\beta}$ based on interactions between different systems

<table>
<thead>
<tr>
<th>Interaction product</th>
<th>$q^{\alpha\beta}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Self-interaction</td>
<td>1.0</td>
</tr>
<tr>
<td>Coplanar</td>
<td>2.2</td>
</tr>
<tr>
<td>Cross-slip</td>
<td>3.0</td>
</tr>
<tr>
<td>Glissile junction</td>
<td>3.8</td>
</tr>
<tr>
<td>Hirth lock</td>
<td>1.6</td>
</tr>
<tr>
<td>Lomer-Cotrell lock</td>
<td>4.5</td>
</tr>
</tbody>
</table>

for dissociation is used to determine the dominant mechanism at a material point

$$f = 1 \quad \text{when} \quad \begin{cases} 
\tau_{inplane} > \tau_{lead}^{cr} \quad \text{and} \quad \tau_{inplane} < \tau_{trail}^{cr} \\
\tau_{inplane} > \tau_{trail}^{cr} \quad \text{and} \quad \tau_{trail}^{cr} - \tau_{lead}^{cr} > \tau_{cut} 
\end{cases}$$

$$f = 0 \quad \text{otherwise} \quad (3.28)$$

where $\tau_{inplane}$ is the resolved shear stress on slip planes evaluated from the Cauchy stress as shown below.

$$\tau_{inplane}^\text{inplane} = \sigma n - (\sigma : n \otimes n)n \quad \tau_{inplane} = |\tau_{inplane}|$$

$$v_{inplane}^\text{inplane} = \frac{\tau_{inplane}}{|\tau_{inplane}|} \quad \theta_s = \cos^{-1}(v_s, v_s) \quad (3.29)$$

where $n$ is the normal to a slip plane and $v_s$ is the slip direction of the partials. $\tau_{lead}^{cr}$ and $\tau_{trail}^{cr}$ are the critical leading and trailing shear stresses as developed in [Unocic et al., 2011]
Table 3.4: Parameters for APB shearing based inelastic deformation in activation energy based model

<table>
<thead>
<tr>
<th>( \dot{\gamma}_0 ) (sec(^{-1} ))</th>
<th>Q (J)</th>
<th>( \sigma_a^\alpha ) (MPa)</th>
<th>( \sigma_s^\alpha ) (MPa)</th>
<th>( h_0 ) (MPa)</th>
<th>( \bar{s}_{sat} ) (MPa)</th>
<th>p</th>
<th>q</th>
<th>r</th>
</tr>
</thead>
<tbody>
<tr>
<td>5e(^6 )</td>
<td>6.5e(^{-19} )</td>
<td>150.0</td>
<td>480.0</td>
<td>1500.0</td>
<td>300.0</td>
<td>0.78</td>
<td>1.15</td>
<td>1.115</td>
</tr>
</tbody>
</table>

Table 3.5: Parameters for microtwinning based inelastic deformation in activation energy based model

<table>
<thead>
<tr>
<th>( \dot{\gamma}_0 ) (sec(^{-1} ))</th>
<th>Q (J)</th>
<th>( \sigma_a^\alpha ) (MPa)</th>
<th>( \sigma_s^\alpha ) (MPa)</th>
<th>( h_0 ) (MPa)</th>
<th>( \bar{s}_{sat} ) (MPa)</th>
<th>p</th>
<th>q</th>
<th>r</th>
</tr>
</thead>
<tbody>
<tr>
<td>1e(^6 )</td>
<td>6.5e(^{-19} )</td>
<td>100.0</td>
<td>1020.0</td>
<td>700.0</td>
<td>10.0</td>
<td>0.78</td>
<td>1.15</td>
<td>1.115</td>
</tr>
</tbody>
</table>

and is as follows.

\[
\tau_{cr}^{lead} = \frac{2\tau_f}{\cos(\theta_l) + \cos(\theta_t)} + \frac{\alpha \mu b}{\lambda \cos(\theta_l)} \quad \text{for} \quad \cos(\theta_l) > \cos(\theta_t)
\]

\[
\tau_{cr}^{lead} = \frac{2}{\cos(\theta_l) + \cos(\theta_t)} \left( \frac{\alpha \mu b}{\lambda} + \tau_f \right) \quad \text{for} \quad \cos(\theta_l) \leq \cos(\theta_t)
\]

\[
\tau_{cr}^{trail} = \frac{1}{2 \cos(\theta_l)} \left( \frac{\alpha \mu b}{\lambda} + \tau_f + \frac{\mu b}{2\pi \lambda (1 - \nu)} - \frac{2Q_{ISF}}{b} \right)
\]

\[
\left( \frac{\alpha \mu b}{\lambda} + \tau_f + \frac{\mu b}{2\pi \lambda (1 - \nu)} - \frac{2Q_{ISF}}{b} \right)^2 - 4 \times \left( \frac{Q_{ISF}}{b} \left( \frac{Q_{ISF}}{b} - \tau_f \right) - \frac{\mu b}{2\pi \lambda (1 - \nu)} \left( \frac{Q_{ISF}}{b} - \tau_f \right) - \frac{\alpha \mu Q_{ISF}}{\lambda} \right)^{0.5}
\]

(3.30)

where \( \tau_f \) is the friction stress, \( \alpha \) is a factor, \( \mu \) is the shear modulus, \( b \) is the burger’s vector, \( \lambda \) is the channel width and \( Q_{ISF} \) is the activation energy of intrinsic stacking faults. \( \tau_{cut} \) in equation 3.28 is a reference stress value. The crystal plasticity model parameters are obtained from single crystal tension and compression experiments from [Knowles and Gunturi, 2002] and are listed in tables 3.4, 3.5 and 3.6.
Table 3.6: Parameters for microtwin nucleation model

<table>
<thead>
<tr>
<th></th>
<th>( \tau_f )</th>
<th>b</th>
<th>( Q_{ISF} )</th>
<th>( \mu )</th>
<th>( \lambda )</th>
<th>( \alpha )</th>
<th>( \nu )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(MPa)</td>
<td>(m)</td>
<td>(J)</td>
<td>(MPa)</td>
<td>(m)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>100.0</td>
<td>1.44e(-10)</td>
<td>1e(-8)</td>
<td>6.74e(4)</td>
<td>1.1e(-7)</td>
<td>2.0</td>
<td>0.33</td>
<td></td>
</tr>
</tbody>
</table>

In the WATMUS method, the coarse scale internal variables \( y_0 \) at a material point are \( F^p_0, s^\alpha_{at,APB,0}, s^\alpha_{at,tw,0}, \chi_0^\alpha \) and are integrated using a 2\(^{nd}\) order backward difference formula 2.41. In single time scale integration, the thermal slip system resistance \( s^\alpha \) is not evolved and hence not considered in the set of evolving coarse scale internal variable \( y_0 \). Though at any instant of time either APB shearing or microtwinning can be active, transition of mechanisms can happen within a cycle and \( s^\alpha_{at} \) associated with both APB shearing and microtwinning can evolve within a cycle. Hence the cycle scale variables \( s^\alpha_{at,APB,0} \) and \( s^\alpha_{at,tw,0} \) are solved simultaneously. A two step iterative algorithm as described in section 3.3 is used where \( F^p_0, s^\alpha_{at,APB,0} \) and \( s^\alpha_{at,tw,0} \) are solved by Newton-Raphson followed by an implicit update of \( \chi_0^\alpha \). A coarse variable \( f_0 \) is associated with \( f \) in equation 3.24 and is assigned the value of \( f \) at end of a cycle as shown below.

\[
f_0(X, N) = f(X, N, \tau = T)
\] (3.31)

A cube consisting of 216 grains is considered to demonstrate the accuracy and efficiency of the WATMUS method for nickel based superalloys. The corresponding FE mesh and Euler angle distributions are shown in figure 3.24(a) and 3.24(b) respectively. The polycrystalline microstructure is subjected to a dwell load of 750 MPa along the y direction, with a loading and unloading time of 1 sec each and a hold time of 120 sec. A schematic of dwell load is shown in figure 3.23.

Single time scale simulations are performed for 700 cycles and the evolution of variables are compared with WATMUS simulations. In figure 3.25(a) the evolution of coarse
internal variable $F_{0,22}^p$ at a material point is compared with $F_{22}^p(N, \tau = 0)$ as obtained from single time scale simulation. A similar comparison is made for the initial value of athermal slip system resistance $s_{at,0}^a$ and is shown in figure 3.25(b). From the figures it can be observed that the coarse scale evolution as obtained from WATMUS method and single time scale solution are almost similar. The fine scale solution at the 700th cycle is reconstructed from the coarse scale variables and is compared with single time scale solution at 700th cycle. The relative error in the fine scale evolution of $F_{22}^p$ and $\sigma_{22}$ at a material point is shown in figures 3.26(a) and 3.26(b) respectively and are within acceptable limits. In figures 3.27 and 3.28, the distribution of $F_{22}^p$ and $\sigma_{22}$ at $N = 700$, $\tau = 121$ sec in the microstructure as obtained from WATMUS and single time scale simulations is shown and they are similar. By using the WATMUS method, a computational benefit of 20 times with sufficient accuracy is achieved for 1000 cycles of coarse scale and single time scale simulation.
3.5 Conclusion

In this chapter, 4 different numerical examples are presented. The first example shows the applicability of the WATMUS method to ODE’s for phase transforming material where the time period of cyclic evolution of the phase is not clearly defined. The coarse scale response is shown to have more accurate results when smaller time periods are considered. This is consistent with the definition of local error which depends on the cyclic evolution and is more for longer time periods. In the second example, WATMUS method is used to solve a 1-d viscoplastic FE problem with 2 elements having largely differing hardness values. A displacement boundary condition is applied that produces a stress ratio $R \to -1$. This example demonstrates the ability of the WATMUS method to solve $R \to -1$ problems where asymptotic expansion based methods fail. The ability of the adaptive criteria to predict cycle jumps and evolving set of coefficients is also demonstrated. In the third and fourth examples, the WATMUS method has been used to perform accelerated cyclic CPFE simulations of Ti-alloys and nickel based superalloys respectively. The CP based material model for the two alloys are different and separate set of coarse scale internal variables are integrated in the coarse scale framework. The evolution of CPFE variables as obtained from the WATMUS and single time scale method are compared in the two examples to demonstrate the accuracy and efficiency of the method to perform accelerated cyclic CPFE simulations for large number of cycles.
Figure 3.24: FE model to demonstrate the accuracy of WATMUS method for nickel based super alloys: (a) FE mesh (b) Euler angle distribution.
Figure 3.25: Comparison of coarse scale evolution of internal variables at a material point:
(a) $F_{0,22}^p$ (b) $s_0^\alpha$.
Figure 3.26: Relative error in the reconstructed response at a material point: (a) $F_{22}^p$ (b) $\sigma_{22}$. 
Figure 3.27: Distribution of $P_{22}^p$ in the microstructure at $N = 700$ and $\tau = 121$ sec: (a) Single time scale simulation (b) WATMUS simulation.
Figure 3.28: Distribution of $\sigma_{22}$ in the microstructure at $N = 700$ and $\tau = 121$ sec: (a) Single time scale simulation (b) WATMUS simulation.
CHAPTER 4
MICROSTRUCTURAL SENSITIVITY OF CRACK INITIATION IN TI-6242

Fatigue life in \( \alpha \) or near \( \alpha \) Ti-alloys shows large variation with load characteristics at temperatures where diffusion mediated deformation mechanisms are absent and is due to the strong influence of the underlying microstructure on the fatigue behavior in these alloys [Bache, 2003, Bache et al., 1997, Sinha et al., 2004, Williams, 2006, Lutjering and Williams, 2007]. Since 80 – 90\% of the total life in these alloys is spent to initiate a crack, accurate prediction of fatigue crack nucleation is one of the primary interest of the research community [Hall, 1997, Biavant et al., 2002, Lykins et al., 2001, Lykins et al., 2000]. To accurately predict the number of cycles to crack initiation, the influence of the underlying microstructure on the local deformation behavior in these alloys should be addressed. Crystal plasticity based finite element models have been used widely to capture this effect [Dunne et al., 2007, Sackett et al., 2007, Venkatramani et al., 2006, Sinha and Ghosh, 2006, Goh et al., 2001, Bridiera et al., 2009, Zhang et al., 2007, Harder, 1999, Bate, 1999]. A physically motivated non-local crack nucleation model based on the crystal plasticity variables developed in [Anahid et al., 2011] has been used to study the microstructure and load sensitive behavior of crack nucleation in Ti-6242.

The strong orientation dependent inelastic behavior of \( \alpha \) phase, having \( hcp \) crystal structure, results in inhomogeneous plastic flow in the microstructure. This inhomogeneous plastic deformation causes stress concentration and plastic strain accumulation at
boundaries of grain pairs where one has large plastic deformation (soft grain) and the other has little or no plasticity (hard grain). Such grain boundaries are considered susceptible to crack nucleation in these alloys. CPFE model of statistically equivalent microstructure of Ti-alloys can capture this plastic strain accumulation and stress concentration accurately. Based on the variables obtained from CPFE simulations, a physically motivated crack nucleation law is developed. The law is non-local since it considers the effect of dislocation pile up and stress concentration at the interface of hard and soft grains to determine crack initiation. Due to the consideration of effect of microstructural features on deformation behavior through CPFE simulations and physical mechanism behind crack formation, the proposed model is effective in capturing the microstructural sensitivity to crack nucleation.

In this chapter the non-local crack nucleation model based on crystal plasticity variables is presented. In section 4.1 a detailed description of the model and the drawbacks of some existing models to predict cycles to crack nucleation in α and near α Ti-alloys is presented. The model parameters are calibrated and validated from experiments performed on Ti-6242 and is described in section 4.2. The sensitivity of fatigue crack initiation to the microstructural features is presented in section 4.3. The dependency of cycles to crack nucleation on the load characteristics like load-form, frequency and maximum applied stress is presented in section 4.4. The chapter is concluded in section 4.5.

4.1 Non-local crack initiation model

The proposed crack nucleation model is developed for α or near α Ti-alloys [Anahid et al., 2011], where the β phase is absent or present in low volume fraction and is motivated by experimental studies performed on samples of Ti-6242 [Sinha et al., 2004, Sinha et al., 2006a, Sinha et al., 2006b]. In the experiments, the samples are subjected to fatigue and creep loads at 90 – 95% of yield strength and failure sites are analyzed using electron
backscattered diffraction technique (EBSD) and tilt fractography in scanning electron microscope (SEM). From the experiments it is observed that the fracture surfaces are faceted and are formed on or near the basal plane. A detailed crystallographical study is performed in [Sinha et al., 2006b] to characterize the microstructure at the crack initiation site. The c-axis orientation of grains with the loading axis ($\theta_c$) at the initiation site is found to be small ($\sim 0^\circ - 30^\circ$). Furthermore, low prism and basal activities with Schmid factors (SF) $\sim 0.1$ and $\sim 0.3 - 0.45$ respectively, are observed at the nucleation site. The region surrounding the failure site shows high prismatic and basal activity with SF $\sim 0.5$.

These observations suggest that crack nucleation happens at regions with little or no plasticity (hard grain) surrounded by grains with large plastic deformation (soft grain). A crack nucleation model based on dislocation pile up is proposed in [Stroh, 1954] and provides a possible explanation of crack initiation at such locations. According to the model, basal slip within a favorably orientated grain (soft grain) causes dislocation pile up at its boundary with an unfavorably orientated grain (hard grain). This pile up induces shear stress in the hard grain and initiates the formation of slip bands. This slip bands are acted upon by long range cyclic stresses and local tensile stresses causing them to open up and form the nucleus of fatigue crack. However this model considers only one slip system and ignores effect of interaction of different slip systems on crack nucleation. Moreover the combination of multi-axial stresses are not considered in this model. An alternative theory is proposed in [Bache, 2003] to explain the weakening of a hard grain adjacent to a soft grain based on a simplified two grain model. In this model, under the application of a fixed stress inhomogeneous plastic deformation between adjacent hard and soft grain results in stress rise in the hard grain to satisfy the strain compatibility conditions. This stress rise cause the eventual failure in hard grains. Though the simplistic model is able to explain the cause of stress rise in hard soft grain pairs, its extension to capture such
effects in real microstructures involve large scale mechanistic calculations of representative polycrystalline aggregates.

Crystal plasticity based model described in section 3.3, capture the size and orientation dependent plastic behavior of Ti-alloys. Finite element simulations of representative microstructures using this model successfully capture the stress rise in hard grains surrounded by soft grains [Deka et al., 2006, Venkataramani et al., 2007]. This phenomenon of stress rise due to anisotropic plastic deformation is referred to as *load shedding*. To accurately capture such local deformation behavior from CPFE simulations, statistical quantification of crystallographical and morphological features of the microstructure is essential. The features considered to generate statistically equivalent microstructures are the orientation distribution, misorientation distribution, size distribution and microtexture of grains. Serial sectioning via focused ion-beam scanning electron microscope (FIB-SEM) followed by electron backscatter diffraction (EBSD) is used to collect the crystallographical and morphological distributions in 3D [Groeber et al., 2008a]. From the distribution functions, a statistically equivalent microstructure and corresponding finite element mesh is generated as shown in figure 3.12(a) and is discussed in detail in [Groeber et al., 2008b].

For the microstructure shown in figure 3.12(a), fatigue simulation under normal cyclic loading condition by using the WATMUS method is performed and the stress distribution $\sigma_{22}$ along a material line in the microstructure is shown in figure 4.1(a). The corresponding SF distribution is shown in figure 4.1(b). The maximum value of the basal and prismatic SFs is considered in figure 4.1(b). The SF value gives a measure of the amount of plastic deformation in a grain. High and low SF values indicate soft and hard grains respectively. As can be observed from the figures, high stresses develop in grains with low SF values (region A and C) or hard grains and which are adjacent to grains with high SF values (regions B and D) or soft grains. Also the peak stresses increase with cycles, which increases the propensity of such regions to nucleate a crack. Based on CPFE simulations, a purely
stress based crack nucleation law has been proposed in [Kirane and Ghosh, 2008] where crack initiation is assumed to happen when the effective traction on the basal plane exceeds a critical value. However the evolution of peak stresses in the microstructure under fatigue simulations saturate early and hence the model shows error in its prediction. The model also does not consider the underlying physical mechanism of formation of micro cracks at the interface and its propagation to form macroscopic crack nucleation sites.

Plastic deformation in the soft grain happens through dislocation motion. At the interface of a hard and soft grain, the motion of dislocations are inhibited and they pile up. Since the dislocations are of similar sign, they don’t annihilate but results in the formation of micro defects at the interface and is shown in figure 4.2. At a material point in the interface, the length of the micro-crack due to closure failure is of order of burgers vector (n-m) whereas the local stresses act on areas which are fractions of grain size (µ-m). Since a scale difference exists between the micro-cracks and the regions on which the local stresses act, the micro defects can be assumed as preexisting cracks acted upon by macroscopic stresses. Similar to linear elastic fracture mechanics, a stress intensity factor $K$ is defined for the growth of micro-cracks

$$K = T_{eff} \sqrt{\pi c}$$

where $T_{eff} = \sqrt{< T_n >^2 + \beta T_t^2}$ \hspace{1cm} (4.1)

Both shear and normal stresses are considered in defining the stress intensity factor. In the above equation $T_n$ and $T_t$ are the normal and shear component of traction on the crack plane in a hard grain and $c$ is the micro-crack length obtained from dislocation pile up in the adjacent soft grain at the interface. Crack opening only happens for tensile nature of $T_n$ and hence a Macaulay bracket is used implying $< T_n > = 0$ when $T_n < 0$.

There are two formulas that relates the crack opening displacement with the dislocation pile up length [Anahid et al., 2011] and has been used in the crack nucleation model. In
the first formula, a 90° intercept definition proposed in [Rice, 1968] is used to relate the micro-crack length \( c \) and dislocation pileup length \( B \)

\[
c = B/2
\]  

(4.2)

In the second formula proposed in [Stroh, 1954], the equilibrated wedge shaped micro-crack length \( c \) is related the dislocation pile up length \( B \), shear modulus \( G \) and surface energy \( \gamma_s \)

\[
c = \frac{G}{8\pi(1-\nu)\gamma_s}B^2
\]  

(4.3)

The dislocation pile up happens due to inhomogeneous plastic deformation in the microstructure causing closure failure around any burgers circuit and is related to the curl of plastic deformation gradient \( \mathbf{F}^p \) [Dai, 1997] as shown below.

\[
\mathbf{B} = \oint_{\mathbf{\Gamma}} d\mathbf{\bar{x}} = \oint_{\mathbf{\Gamma}} \mathbf{F}^p d\mathbf{X} = \int_{\Omega} \mathbf{\Lambda} \mathbf{n} d\Omega
\]

where \( \mathbf{\Lambda} = \nabla^T \times \mathbf{F}^p \)  

(4.4)

In the above equation, \( \mathbf{n} \) is the normal to the surface \( \Omega \) and \( \mathbf{\Lambda} \) is the Nye’s dislocation tensor. The Nye’s dislocation tensor is non-local since it depends on the spatial gradient of \( \mathbf{F}^p \) at a point. The crystal plasticity model in section 3.3 is local where \( \mathbf{F}^p \) evolves at gauss points in an element following the first order rate equation shown in equation 3.7 and is only influenced by local variables at gauss points. To calculate the non-local variable \( \mathbf{\Lambda} \) at a gauss point, the variable \( \mathbf{F}^p \) is first evaluated at nodal points \( \alpha \)

\[
y_{\alpha} = \sum_{i=1}^{N^g} \frac{w_{i}^\alpha y_i}{\sum_{i=1}^{N^g} w_{i}^\alpha} 
\]

\[
w_{i}^\alpha = \exp \left( -\frac{1}{2} \left( \frac{\|X_{\alpha} - X_i\|}{d} \right)^2 \right) V_i
\]  

(4.5)

where \( y \) is any gauss point variable whose nodal values needs to be obtained, \( N^g \) is the total number of gauss points in the grain containing the nodal point \( \alpha \), \( V_i \) is the volume
associated with the gauss point, \( \mathbf{X}_\alpha \) and \( \mathbf{X}_i \) are the position vectors of the nodal point \( \alpha \) and gauss point \( i \) respectively and \( d \) is a length parameter based on the node density of the finite element mesh. For nodes at grain interfaces, multiple instances of node belonging to each grain is considered, to evaluate nodal \( \mathbf{F}^p \). Once the nodal values of \( \mathbf{F}^p \) are obtained, the elemental shape functions are used to calculate the Nye’s tensor \( \mathbf{A} \) at every gauss point. For a given normal \( \mathbf{n} \), the closure failure per unit area at any material point can be obtained from equation 4.4.

To evaluate the stress intensity factor, nodes on grain interfaces are considered. A node \( \alpha \) at an interface between a pair of grains has 2 instances, \( \alpha_I \) and \( \alpha_{II} \). The stress tensor \( \mathbf{\sigma} \) and the Nye’s tensor \( \mathbf{A} \) can be obtained for the both the instances by using the methodology described above. The normal and shear component of traction on the basal plane for \( \alpha_I \) and \( \alpha_{II} \) can be obtained from \( \mathbf{\sigma} \) and the orientation of the grain to which they belong and is shown below.

\[
\mathbf{T} = \mathbf{\sigma n}_b \quad T_n = \mathbf{T} \cdot \mathbf{n}_b \quad T_t = ||\mathbf{T} - T_n \mathbf{n}_b||_2
\]  
(4.6)

where \( \mathbf{n}_b \) is the basal plane normal that can be obtained from

\[
\mathbf{n}_b = [\sin \theta \sin \phi \quad -\sin \theta \cos \phi \quad \cos \theta]^T
\]  
(4.7)

where \( \phi, \theta \) and \( \psi \) are the Euler angles of the grain. Among both the instances of node \( \alpha \), the one with higher value of effective traction on basal plane \( T_{\text{eff}} \) is considered as node in the hard grain (\( \alpha_h \)) and the other instance is considered as node in the soft grain (\( \alpha_s \)). It is assumed that the micro-crack happens on the basal plane of the hard grain and the direction of the closure failure per unit area in the soft grain is collinear to the basal plane normal \( \mathbf{n}_{bh} \). Hence the closure failure per unit area at \( \alpha_s \) in the soft grain is evaluated from

\[
\mathbf{n}_s^B = \frac{\mathbf{A}^{-1} \mathbf{n}_{bh}^b}{||\mathbf{A}^{-1} \mathbf{n}_{bh}^b||}, \quad \mathbf{B} = \mathbf{A} \mathbf{n}_s^B \quad \text{and} \quad B = ||\mathbf{B}||
\]  
(4.8)
where $\mathbf{n}_B^s$ is the normal to the plane of closure failure in the soft grain and $\mathbf{n}_B^h$ is the basal plane normal in the hard grain. The micro-crack length $c$ can then be obtained from equation 4.2 or 4.3. The stress intensity factor is evaluated at each node at the interface based on equation 4.1 and is shown below.

$$R = K / \sqrt{\pi} = T_{h}^{\text{eff}} \sqrt{c_s}$$

(4.9)

The stress intensity factor $R$ evolves with the state in the microstructure. Crack nucleation is assumed to happen when $R$ exceeds the critical stress intensity factor $R_c$ and the micro-crack becomes unstable. The critical stress intensity factor $R_c$ is a material constant for a given alloy and is calibrated from experiments.

### 4.2 Calibration and validation of critical stress intensity factor $R_c$

The material constant $R_c$ is calibrated and validated based on experiments performed on samples of Ti-6242 [Rokhlin et al., 2005, Williams, 2006]. The samples are subjected to dwell load with a maximum stress of 869 MPa, which is 95% of the macroscopic yield stress and a minimum stress of zero. Each dwell cycle consists of loading for 1 sec, hold at maximum stress for 2 min, followed by unloading for 1 sec and is shown in figure 3.23. The crack growth is monitored through micro-radiographic images obtained by interrupting the experiment after every 15 cycles and the number of cycles to crack nucleation is obtained by extrapolating back the macroscopic crack growth to zero [Anahid et al., 2011]. The calibration and validation of $R_c$ is performed by using two different microstructures (MS1 and MS2) and is discussed in the sections below.
4.2.1 Calibration

The 1\textsuperscript{st} microstructure (MS1) is considered for calibrating \( R_c \). A statistically equivalent representative volume of the microstructure is constructed from the orientation, misorientation distributions and micro-texture of the sample. The representative volume consists of 955 grains and is spatially discretized using 4-noded tetrahedral elements. The corresponding finite element mesh of the representative volume is shown in figure 3.12(a). The crystal plasticity material model and the corresponding parameters described in section 3.3 is used to perform the finite element simulations. A constant strain rate simulation is performed to determine the yield stress of the statistically equivalent microstructure. As can be observed from figure 4.3, the yield stress of the reconstructed microstructure of MS1 is 915 MPa.

Cyclic simulation under dwell load using the WATMUS method is performed with a maximum applied stress of 869 MPa (95\% of yield stress) and a stress ratio \( \sigma_R = 0 \). The evolution of \( R \) at every node at the interfaces of grains is evaluated at \( \tau = 121 \text{ s} \) in each cycle and crack initiation is considered to happen when \( R(N, \tau = 121) \) at any node at the interfaces of grains exceeds \( R_c \). The total number of cycles to failure (\( N_f \)) of MS1 from dwell fatigue experiment is 352 cycles and crack nucleation happens at 80 – 85\% of total life. Based on this observation, the maximum \( R \) value from the nodes at the interfaces of grains at \( N = 282 \) (80\% of \( N_f \)) and at \( N = 300 \) (85\% of \( N_f \)) are considered as the lower and upper limits of \( R_c \) and is shown below.

\[
R_c(80\%) = \max_{\alpha} R^{\alpha}(N = 282, \tau = 121 \text{ sec}) = 6.54 \text{ MPa} \sqrt{\mu m}
\]
\[
R_c(85\%) = \max_{\alpha} R^{\alpha}(N = 300, \tau = 121 \text{ sec}) = 6.80 \text{ MPa} \sqrt{\mu m}
\]

(4.10)

where \( \alpha \) are the nodes at the grain interfaces and \( R^{\alpha} \) are the corresponding \( R \) values. The evolution of \( R \) having the maximum value at 282\textsuperscript{nd} and 300\textsuperscript{th} cycle is shown in figure 4.4.
4.2.2 Validation

The 2\textsuperscript{nd} microstructure (MS2) is considered for validation. The number of cycles to crack initiation for this sample is 530 and has been obtained from interrupted dwell fatigue test under maximum applied stress of 869 MPa and stress ratio $\sigma_R = 0$ [Rokhlin et al., 2005]. To perform the CPFE simulations, statistically equivalent microstructure is constructed from the orientation, misorientation distributions and micro-texture of the sample. An yield stress of 915 MPa is obtained from constant strain rate CPFE simulation of the reconstructed microstructure and is shown in figure 4.5.

WATMUS method is used to perform the dwell fatigue simulation with the same maximum stress and stress ratio as MS1. The stress intensity factor $R$ is evaluated at all nodes at the interfaces of grains. The number of cycles to crack initiation is evaluated based on calibrated $R_c$ values at 80 and 85\% of total life as shown below.

\begin{align*}
N_c(80\%) : \max_{\alpha} R^\alpha(N_c(80\%), \tau = 121 \text{ sec}) = R_c(80\%) \Rightarrow N_c(80\%) = 620 \\
N_c(85\%) : \max_{\alpha} R^\alpha(N_c(85\%), \tau = 121 \text{ sec}) = R_c(85\%) \Rightarrow N_c(85\%) = 694
\end{align*}

The evolution of $R$ at the node with maximum value of $R$ at $N_c(80\%)$ and $N_c(85\%)$ cycle is shown in figure 4.6. The prediction of cycles to crack nucleation for MS2 based on calibrated $R_c$ from MS1 and the associated error in prediction is summarized in table 4.1. The microstructural features at the crack nucleation site predicted from the model for MS1 and MS2 is compared with experimentally observed characteristics and is shown in table 4.2.
4.3 Microstructural sensitivity of fatigue crack nucleation

The deformation behavior of Ti-alloys is strongly influenced by the underlying microstructural features like orientation and size distributions and can be used to describe the macroscopic properties of the polycrystalline alloy. The orientation of a grain with respect to the loading axis dictates the magnitude of the resolved shear stresses on the slip planes causing plastic flow and the size of grains governs the resistance to slip activity through the Hall-Petch type relation described in section 3.3. Hence a microstructural descriptor (softness...
index) is defined based on the orientation and size distributions to characterize macroscopic yield strength of the microstructure.

\[
SI = \max_\alpha \left( \frac{T : S_0^\alpha}{g_0^\alpha} \right)
\]  

(4.12)

where SI is the softness index, \( T \) is some applied load, \( S_0^\alpha \) is the Schmid factor of slip systems in a grain which depends on the grain orientation and \( g_0^\alpha \) is the grain size dependent initial hardness of the slip systems. The SI distribution of MS1 and MS2 is shown in figure 4.7. It can be observed from figure 4.7 that the two microstructures have approximately the same volume fraction of grains with softness index values in the range \( 1.1 \leq SI < 1.2 \) and this seems to drive the yield strength of the 2 microstructure. To validate this observation, a 3\(^{rd}\) representative microstructure (MS3) is constructed by randomly assigning orientations to the grains of the spatially discretized FE model of MS1. The softness index distribution and stress-strain evolution obtained from constant strain rate simulation of MS3 is compared with MS1 and is shown in figure 4.8. The volume fraction of grains in MS3 with softness index \( 1.1 \leq SI < 1.2 \) is less than MS1 as shown in figure 4.8(a) and hence have a higher yield strength of 940 MPa as can be seen in figure 4.8(b).

Macroscopic properties of the microstructure, like yield strength, can be characterized through descriptors like softness index which provides a measure of degree of plastic deformation in the microstructure. However such descriptors are unable to capture the local variations in the microstructure and hence not suitable to characterize fatigue behavior of polycrystalline alloys. From fatigue experiments on Ti-6242 it has been observed that crack initiation sites have grains with low c-axis orientation and are surrounded by grains having large plastic deformation. Based on these observations, a local microstructural variable is constructed that considers the surface area fraction of soft grains surrounding a hard grain. A grain is labeled as hard when its c-axis orientation (\( \theta_c \)) is between 0 and 40° and soft otherwise. The distribution of this microstructural variable for MS1, MS2 and MS3 is shown in figure 4.9. The number of cycles to crack initiation at a point in the microstructure de-
Table 4.3: Microstructural features at crack initiation site as predicted from the model for MS3.

<table>
<thead>
<tr>
<th>Microstructural parameters</th>
<th>Experiments</th>
<th>MS3</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \theta_c )</td>
<td>0 – 30°</td>
<td>5.6</td>
</tr>
<tr>
<td>Prismatic Schmid factor</td>
<td>0.0 – 0.1</td>
<td>0.005</td>
</tr>
<tr>
<td>Basal Schmid factor</td>
<td>0.3 – 0.45</td>
<td>0.01</td>
</tr>
</tbody>
</table>

pends on the extreme of the distribution shown in figure 4.9 implying that a microstructure with a higher volume fraction of hard grains with high surface area fraction of surrounding soft grains is likely to fail earlier. Hence it can be concluded from figure 4.9 that MS2 should have the longest life and MS3 should have the shortest life. This observation is validated for MS1 and MS2 from the dwell fatigue simulations and experiments. To further validate this observation, dwell fatigue simulations are performed for MS3. Since the macroscopic yield stress of MS3 is 940 MPa, a maximum stress of 894 MPa (95% of yield stress) is applied. Similar to MS1 and MS2, the stress intensity factor \( R \) is evaluated at all nodes at the grain interfaces in every cycle (N) at \( \tau = 121 \) sec. Crack initiation is considered to happen at a cycle when \( R(N, \tau = 121 \) sec) at any node exceeds the calibrated critical stress intensity factor \( R_c \). Corresponding to \( R_c(80\%) \) and \( R_c(85\%) \) the predicted number of cycles to crack initiation are \( N_c(80\%) = 167 \) and \( N_c(85\%) = 177 \) respectively. The evolution of \( R \) at the node where crack initiation happens for the 3 different microstructures is shown in figure 4.10. From the dwell fatigue simulations of MS1, MS2 and MS3, the ability of the local microstructural variable to qualitatively capture the variation in life to crack nucleation for Ti-6242 is verified. The microstructural features at the crack nucleation site for MS3 is shown in table 4.3.
4.4 Sensitivity of crack nucleation to load characteristics

Ti-alloys experience premature failure under dwell load as compared to normal cyclic load and is due to the influence of underlying microstructure on fatigue behavior of these alloys [Bache, 2003, Sinha et al., 2004]. The proposed crack nucleation model, based on micro-crack growth due to dislocation pile up in soft grain acted upon by mixed mode stress from the adjacent hard grain, effectively captures the microstructural sensitivity to fatigue life behavior. The model is calibrated and validated from dwell fatigue simulations and experiments performed on samples of Ti-6242. In this section, the sensitivity of cycles to crack initiation to the characteristics of applied load is investigated. The 1st microstructure (MS1) is considered for this sensitivity study and is subjected to 4 different types of load as shown below:

- Case A: \( \sigma_{\text{max}} = 869 \text{ MPa}, \sigma_r = 0, T_{\text{load}} = T_{\text{unload}} = 1 \text{ sec} \) and \( T_{\text{hold}} = 120 \text{ sec} \)
- Case B: \( \sigma_{\text{max}} = 825 \text{ MPa}, \sigma_r = 0, T_{\text{load}} = T_{\text{unload}} = 1 \text{ sec} \) and \( T_{\text{hold}} = 120 \text{ sec} \)
- Case C: \( \sigma_{\text{max}} = 869 \text{ MPa}, \sigma_r = 0, T_{\text{load}} = T_{\text{unload}} = 61 \text{ sec} \) and \( T_{\text{hold}} = 0 \text{ sec} \)
- Case D: \( \sigma_{\text{max}} = 869 \text{ MPa}, \sigma_r = 0, T_{\text{load}} = T_{\text{unload}} = 1 \text{ sec} \) and \( T_{\text{hold}} = 0 \text{ sec} \)

The maximum applied stress (\( \sigma_{\text{max}} \)) is 95% of the yield strength in cases A, C and D and is 90% of the yield strength in case B. Dwell load with 2 min hold is applied in cases A and B. Triangular load with time periods \( T = 122 \text{ sec} \) and \( T = 2 \text{ sec} \) is applied in cases C and D respectively. The WATMUS method is used to perform the cyclic CPFE simulations and the stress intensity factor \( R \) is evaluated at nodes situated at grain interfaces. In a cycle, \( R \) is evaluated at the start of unloading and corresponds to \( \tau = 121 \text{ sec} \) in cases A and B, \( \tau = 61 \text{ sec} \) in case C and \( \tau = 1 \text{ sec} \) in case D. The evolution of maximum nodal \( R \) at \( N = 10^4 \) for cases B and C and \( N = 3 \times 10^5 \) for case D is shown in figure 4.11. As can be observed from the figure, the microstructure has a shorter life when subjected to dwell load (A and
B) as compared to normal cyclic loading (C and D). In the normal cyclic loading cases, the
decrease in frequency of the load detoriates the life of the microstructure as can observed
from case C and D.

The number of cycles to crack nucleation for dwell (case A) and normal fatigue (case
d) at 95% of yield strength shows the same trend as observed experimentally [Bache,
2003,Bache et al., 1997,Sinha et al., 2004]. In every cycle of dwell load, the microstructure
is held at the maximum stress level for a longer period of time than normal cyclic load.
This results in a larger inelastic deformation and strain accumulation in the microstructure
within each dwell cycle as compared to a normal cycle. Similar observations are made
from experiments on Ti-6242 [Sinha et al., 2004] and Timetal 685 [Bache, 2003]. Hence
the stress concentration and micro crack growth at the hard soft grain interface is more
severe in every cycle of dwell load as compared to normal cyclic load. This explains the
significant reduction in life to crack nucleation under dwell load (case A) as compared
to normal cyclic load (case D). A reduction in the maximum applied stress in the dwell
load (case B) reduces the cyclic strain accumulation and stress rise and hence shows a
longer life than case A. When the frequency of normal cyclic loading is reduced (case C),
the ramping to the maximum applied stress in every cycle happens slowly and results in
increased plastic strain accumulation and stress rise as compared to a higher frequency
(case D). Hence a reduction in frequency at same maximum stress level decreases the life
of the microstructure.

The number of cycles to crack nucleation for MS1 under different dwell loads at \( \sigma_{max}=869 \) MPa and \( \sigma_{min}=0 \) MPa is also compared. Different hold times at the maximum applied
stress is considered. The WATMUS based CPFE simulations are performed for three dif-
f erent load cases shown below:

- Case E: \( T_{load} = T_{unload} = 16 \text{ sec} \) and \( T_{hold} = 90 \text{ sec} \)
- Case F: \( T_{load} = T_{unload} = 31 \text{ sec} \) and \( T_{hold} = 60 \text{ sec} \)
• Case G: $T_{load} = T_{unload} = 1 \text{ sec}$ and $T_{hold} = 30 \text{ sec}$

The number of cycles to initiate a crack is evaluated from the non-local crack nucleation model. The evolution of maximum $R$ at $\tau=106 \text{ sec}$, $91 \text{ sec}$ and $31 \text{ sec}$ at cyclic increments is shown in figure 4.12.

4.5 Conclusion

Cycles to crack nucleation in Ti-alloys is strongly influenced by their underlying microstructure and the lifing models developed for these alloys should consider this effect. The non-local crack nucleation model based on micro-crack growth under the influence of local stresses at hard soft grain interfaces is effective in capturing the microstructural influence. Cyclic simulations of CPFE models are performed to obtain the stress and plastic strain distribution in polycrystalline aggregates of Ti-alloys. A local stress intensity factor at hard soft grain interfaces is defined based on the stress in the hard grains and dislocation pile up in the soft grains and is evaluated from evolving variables of cyclic CPFE simulations. Crack initiation is considered to happen when the local stress intensity factor at any material point at hard soft grain interfaces exceeds the critical value which is a material parameter for the given alloy. The model is calibrated and validated from dwell fatigue experiments performed on samples of Ti-6242. A local microstructural variable is defined based on the neighborhood of hard grains, as observed in experiments, to relate the sensitivity of cycles to crack initiation to its underlying microstructure. WATMUS method is used to perform dwell fatigue simulations of 3 representative microstructures and the cycles to crack nucleation is predicted based on the non-local model. The local microstructural variable is able to qualitatively capture the sensitivity of cycles to crack nucleation to the underlying microstructure. One of the microstructure is subjected to different cyclic load
patterns and cycles to crack nucleation is predicted from the proposed model. The predictions suggest that the fatigue life of Ti-alloys is strongly dependent on load characteristics and comply with experimental observations.
Figure 4.1: Stress variation along a material line in the microstructure. A and C are the hard regions, B and D are the soft regions. (a) $\sigma_{22}$ distribution and its evolution with cycles (b) Schmid factor (SF) distribution along the material line.
Figure 4.2: Schematic of micro crack formation due to dislocation pile up at a hard soft grain interface [Anahid et al., 2011].

Figure 4.3: Volume averaged stress-strain plot of statistically equivalent microstructure 1 (MS1) obtained from constant strain rate CPFE simulations.
Figure 4.4: Evolution of maximum nodal R evaluated in every cycle (N) at $\tau = 121$ sec of MS1.

Figure 4.5: Volume averaged stress-strain plot of statistically equivalent microstructure 2 (MS2) obtained from constant strain rate CPFE simulations.
Figure 4.6: Evolution of maximum nodal R evaluated in every cycle (N) at $\tau = 121$ sec of MS2.

Figure 4.7: Softness index (SI) distribution for MS1 and MS2.
Figure 4.8: Comparison of softness index distribution and yield strength of MS1 and MS3:
(a) Softness index (SI) distribution (b) Volume averaged stress-strain obtained from constant strain rate FE simulations.
Figure 4.9: Distribution of volume fraction of hard grains and corresponding surface area fractions of neighboring soft grains in MS1, MS2 and MS3.

Figure 4.10: Comparison of evolution of $R$ at the crack nucleation site for MS1, MS2 and MS3.
Figure 4.11: Evolution of $R$ with Cycles for 4 different fatigue load cases A, B, C and D described in section 4.4.

Figure 4.12: Evolution of $R$ with Cycles for 4 different fatigue load cases A, E, F and G described in section 4.4.
CHAPTER 5
CONCLUSIONS AND FUTURE WORK

In the present work, crystal plasticity based finite element (CPFE) simulations of statistically equivalent microstructures under cyclic loading conditions have been used to capture microstructurally dependent deformation behavior of polycrystalline alloys. The experimentally validated crystal plasticity model captures the orientation dependent inelastic behavior of individual grains in the polycrystalline alloy and the equivalent microstructure includes the key microstructural features that influence the deformation behavior of the alloy. Though CPFE simulations of polycrystalline alloys are accurate, the use of conventional integration schemes reduce their applicability to perform fatigue analysis for large number of cycles. A wavelet transformation based multi-time scale method (WATMUS) has been developed to mitigate this computational drawback. In the WATMUS method, wavelet basis functions are used to decompose the oscillatory response of variables. The basis functions capture the high frequency oscillations within each cycle. The coefficients evolve monotonically and are integrated with time steps in orders of cycles to obtain computational benefit. The advantage of the WATMUS algorithm over the existing methods is demonstrated. An accurate representation of the waveform with optimally minimum number of coefficients is necessary for the accuracy, efficiency and stability of the multi-time scale method. The multi-resolution and compact support property of wavelets make them an ideal selection over Fourier basis functions and is shown through examples. Adaptive
criteria to reduce the coefficients that are evolved and predict cycle jumps based on accuracy of integration, has been developed to enhance the efficiency and accuracy of the algorithm. WATMUS based CPFE simulations of Ti-6242 has been performed and compared with single time scale simulations to obtain a quantitative estimate of the accuracy and efficiency of the method.

The sensitivity of fatigue crack nucleation to the underlying microstructure in Ti-6242 has been studied using the WATMUS based CPFE simulations of representative microstructures and a physically motivated crack nucleation law. The crack nucleation model parameters are calibrated and validated with experiments. A variable based on experimentally observed local orientation distributions at crack initiation site, has been defined to relate the fatigue crack nucleation life to the underlying microstructural features. From the WATMUS based CPFE simulations of different microstructures, a correlation between the microstructural variable and cycles to nucleate a crack has been observed. The WATMUS based CPFE simulations of a microstructure under different load characteristics is performed to demonstrate the load sensitive crack nucleation of Ti-6242. The required number of cycles to initiate a crack as predicted from the model agrees with the experimentally observed trends.

The ability of the WATMUS based method to perform CPFE simulations of statistically equivalent microstructures has been demonstrated. As a future work, the method can be extended to perform fatigue simulations in other class of alloys. In the present work, a qualitative correlation between a local microstructural variable and fatigue crack nucleation has been obtained for Ti-6242. Such a correlation can be helpful to obtain the scatter in crack nucleation in Ti-6242 by permutating the orientations and sizes of grains in the statistically equivalent microstructure to match a given orientation and size distribution but creating different local textures. The local microstructural variable can then be used to estimate the number of cycles to nucleate a crack. However a quantitative measure of
the local microstructural variable and the number of cycles to nucleate a crack should be obtained before.


