Abstract

ELKHODARY, KHALIL IBRAHIM. Modeling the Dynamic Deformation and Failure Modes in High Strength and Damage Tolerant Aluminum Alloys. (Under the direction of Professor Mohammed A. Zikry.)

The major objective of this work has been to develop, within a continuum framework, a microstructurally-based computational approach to investigate dynamic shear strain localization and failure in alloys with heterogeneous microstructures, spanning length scales from the nano to the micron, with specific application to high strength and damage tolerant Al-Cu-Mg-Ag alloys.

Dominant secondary phases, such as dispersoids and precipitates, were identified, and their physical scales and crystallographic orientations were determined. A new crystallographic orientation scheme based on the rational orientation of Ω and θ′ precipitates, was formulated. High strain-rate microstructurally-based finite-element analyses were undertaken, which incorporated a rate-dependent dislocation density-based crystalline plasticity framework that explicitly accounts for the behavior of precipitates, dispersoids, and grain-sizes. These analyses delineated how the nano-sized Ω and θ′ precipitates and the micron-sized Mn-bearing dispersoids affect dynamic shear-strain localization and failure in crystalline materials. The computational predictions, which are consistent with experimental observations, indicate that the Ω and θ′ precipitates result in both the homogenous strengthening and toughening of the alloy. This homogenous deformation inhibits the formation of localized shear bands, as compared with an alloy that would have only Mn-bearing dispersoids. The
computational predictions also indicate that the experimentally observed step-ladder deformation of the Ω precipitates could be the direct consequence of a preferred propagation of dislocation densities along the Al/Ω interface, resulting in the uniform deformation of the precipitate along its entire length, instead of localizing within a segment of the precipitate, and this collective behavior enhances the homogenous deformation and toughening of the aluminum alloy.

To model the nucleation and propagation of failure at the microstructural scale, under large deformations and dynamic loading conditions, the general finite-deformation theory, related to the decomposition of the deformation gradient, can be tailored to account for displacement incompatibilities and fracture in crystalline solids. Based on this proposed decomposition, a general fracture criterion for finitely deforming crystals, using the integral law of incompatibility, is developed. With this new criterion, computational analyses of single crystals, polycrystals, and microstructural constituents, such as precipitates and dispersoids, were conducted to elucidate the mechanisms of dynamic crack nucleation and growth in Al-Cu-Mg-Ag alloys. The analyses indicate that the newly proposed fracture criterion accurately predicts ductile and brittle failure modes, and intergranular and transgranular fracture modes in polycrystals. It also accounts for the microstructural effects due to dispersoids and precipitates, and their roles in crack branching and arrest. Coarse precipitates promoted the overall dynamic strengthening of the microstructure and improved the uniformity of deformation. They, however, accelerated catastrophic crack propagation, an effect which is amplified by the presence of a pre-crack. On the other
hand, large Mn-bearing particles decrease the overall toughness and strain-to-failure, while improving microstructural damage tolerance under dynamic loading, especially in the presence of a pre-crack, in comparison with an alloy that has only precipitates and/or no pre-crack.

As part of the new finite-deformation formulation for crystalline solids, subproblems related to twinning and geometrically necessary dislocation (GND) densities can also be formulated. In this study, the role of GND densities in crack behavior was investigated for single crystals. GND densities were shown to form in loops that are associated with stationary crack tips, but not propagating cracks. GND density loops were also shown to form and annihilate in crack-free single crystals under transient loads, which result in homogenous deformations.

The computational predictions clearly indicate that microstructural effects and mechanisms due to the presence of dispersoids and precipitates have a dominant effect on the dynamic deformation and failure of high strength and damage tolerant alloys. This behavior could only be understood and quantified with the appropriate crystalline descriptions, computational framework, and fracture criterion.
Modeling the Dynamic Deformation and Failure Modes of High Strength and Damage Tolerant Aluminum Alloys

by

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A dissertation submitted to the Graduate Faculty of North Carolina State University In partial fulfillment of the requirements for the Degree of Doctor of Philosophy

Mechanical Engineering

Raleigh, North Carolina

2010

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Dedication

To the reader.
Biography

Khalil I. Elkhodary was born in Rome, Italy in 1981 to Egyptian parents: Ibrahim Elkhodary, a translator for the United Nations, and Gamalat Maghraby, a political analyst for the Egyptian Radio and Television Union, where they lived for nine years. His first years in education were spent at the schools of St. Francis and Ambrit in Rome. In 1990, his family moved to Montreal, Quebec, where he studied at Sylwen House for a year. They then moved to Cairo, Egypt for two years, where he studies at the schools of Thebes and Manor House. They subsequently moved to Nairobi, Kenya for five years, where he studied at St. Austin’s Academy, and earned his IGCSE and AS degrees. He then returned to Egypt, where he studied mechanical engineering at the American University in Cairo (AUC) for five years, earning his Baccalaureate in 2003. The Air Defense Forces then conscripted him for a year, after which he worked at OMNI oil technologies as design engineer in the Cairo R&D office for a year. In 2006, he completed a master's degree in mechanical engineering from AUC, and then came to the US in pursuit of a PhD in computational mechanics at North Carolina State University. After four years, he completed his degree, also earning a master's in applied mathematics. Next, he will pursue his post-doctoral research in theoretical and applied mechanics at Northwestern University in Evanston, Illinois.
Acknowledgements

It is indeed my pleasant duty to record my heart-felt gratitude to the many people who have contributed to the shaping of my life. But even were I to blacken reams with their names, I could not exhaust the ever-growing list. It is not, however, my intention to embark on such an elusive task. I will limit my mention, therefore, to those who, by virtue of their involvement in my PhD, are at the forefront of my vision.

I would like to begin by thanking my advisor, Dr. Mohammed Zikry, especially so for a number of things. First, for giving me plenty of rope in doing my research…eventually, I learned how it is done. Second, for letting me pursue my interest in mathematics, at times slowing our research, and thankfully culminating in my master’s degree. Third, for putting together such a congenial team of researchers, I felt at home in every sense during my stay. Finally, not to infect the reader, for his allowing me every leave I asked for!

Next, I would like to thank my treasured friends and colleagues in the research team: William Lee, Pratheek Shanthraj, Tarek Hatem, Omid Rezvanian, James Pearson, and Siqi Xu. I am particularly grateful for all the insightful discussions and exchanges we’ve had over the years, many of which have matured into invaluable contributions to my research, for which I am deeply indebted.

I am also especially indebted to Dr. Gary Howell at the High Performance Computing (HPC) center for his unabated technical support; in particular for his constant help with the difficulties that faced me interfacing my FORTRAN codes with
ABAQUS in a Linux environment, and running them in parallel. Without his support, many of the simulations contained in this dissertation would not have materialized.

I would also like to thank all my professors at NC State, with special thanks to my committee members: Dr. Donald Brenner, Dr. Kara Peters and Dr. Lawrence Silverberg, for kindly participating in my dissertation, offering invaluable remarks and recommendations.

The support we received for this research from the Army Research Office is likewise gratefully acknowledged.

I will conclude by expressing my most profound gratitude to all those ‘behind the scenes’: my parents, for their inestimable patience, untiring support and much-needed prayers; my brother and sister, for managing all affairs in my absence, freeing me from any distracting attachment; finally, and above all, God, for setting all causes in motion, giving us minds to unveil their workings, and hearts to witness the Majesty at which they point.
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Chapter 1

Introduction

1.1 Overview

Understanding and predicting the mechanical behavior of metals and alloys under dynamic loading conditions is essential for the optimal design of a variety of civilian and defense applications. For example, metal forming processes and ballistic applications require a detailed understanding of the dynamic behavior of alloys under large deformations and extreme loading conditions at different temporal and spatial scales. To obtain such an understanding, experiments are needed to characterize the mechanical properties of interest for each alloy, such as tensile strength, ductility, toughness, and strain-rate sensitivity. However, many other properties are difficult, if not impossible, to quantify experimentally, such as subsurface damage and local deformation modes. Microstructural modeling can offer insights into such difficult-to-measure phenomena by elucidating how they evolve at their corresponding scales.

In metals and alloys, the microstructure is generally composed of crystals (Hull and Bacon (2006)) arising from an ordered arrangement of their atoms. However, due to the large scale of engineering and scientific applications, it is not usually feasible to retain an atomic description of crystals; instead, a continuum approach is needed. Thus,
the theory of crystalline plasticity (Rice and Asaro (1977)) has been developed, offering unique theoretical insight into the microstructural mechanisms governing the mechanical behavior of metals and alloys.

In applications involving large deformations and extreme loading conditions, crystalline plasticity can shed light on microstructural phenomena that are as of yet poorly understood, and difficult to experimentally quantify, such as dynamic localization, crack nucleation and propagation, and adiabatic heating. In particular, the prediction of dynamic localization and crack growth at the microstructural scale is critical in determining the dynamic toughness and damage tolerance of alloys, especially for high strain-rate applications that require extensive plastic deformation. The design of alloys to resist these different deformation and failure modes could greatly benefit from microstructurally-based computational modeling and fracture methodologies.

For example, metallurgists have long known that adding certain alloying elements can result in secondary phases in an alloy's microstructure, which can greatly enhance its strength, toughness or ductility. Moreover, by controlling the steps in the production of the alloy, it is possible to produce different alloy properties for the same alloy composition. The most typical case is age hardening of alloys, charted by different time-temperature-transformation curves (Reed-Hill (1973)), for aluminum and steel alloys.

For instance, 2024-Al and 2048-Al have been specifically tailored for use in
applications that require high fracture toughness and crack propagation resistance, such as aircraft structures, automotive applications, armored vehicles, and electronic packaging devices. These alloys do not, however, perform well at high temperatures. Therefore, heat resistant alloys, such as 2219-Al and 2618-Al have been developed for applications that require high specific strength and high temperature capability. These heat resistant Al-Cu-Mg alloys, however, have limited fracture strength and damage tolerance (Eschbach, et al. (1999)). Nonetheless, the addition of small amounts of Ag to Al-Cu-Mg alloys, with high Cu to Mg ratios can significantly improve the age hardening response by the nucleation of thermally stable, plate-like Ω precipitates on {111} planes in the aluminum matrix (Polmear and Couper (1988)). Moreover, Al-Cu-Mg-Ag alloys have less grain boundary (GB) precipitation, and therefore retain most of their toughness after age hardening, and are less susceptible to intergranular fracture (Hono, et al. (1993), Howe and Basile (1988)). Therefore, Al-Cu-Mg-Ag alloys currently being developed can potentially have relatively high strength, temperature resistance, toughness, and damage tolerance. For example, the alloy 2139-T8, with Mn additions (Cho and Bes (2006)), has precipitates, dispersoids and constituents spanning multiple length scales, and thus exhibits significantly improved fatigue life and fracture toughness in comparison to currently used alloys in the aerospace industry. The ballistic performance of 2139-Al has also been shown to be superior to that of Al-2519, which is used in armored vehicles (Cho and Bes (2006)).

The potential use of such Al-Cu-Mg-Ag alloys for different applications is
therefore predicated on understanding, identifying, and optimizing the material mechanisms related to increased strength and toughness. Specifically, if these alloys are to be tailored for the desired ballistic applications, optimal trade-offs between competing requirements on strength and toughness have to be controlled.

1.2 Research Objectives

The main objective of this work has been to develop, within a continuum framework, a descriptive microstructurally-based numerical approach to investigate dynamic localization and failure in alloys with heterogeneous microstructures, and spanning multiple length scales, with particular application to Al-Cu-Mg-Ag alloys.

The secondary phases in the Al-Cu-Mg-Ag microstructure were first identified, and their length scales quantified. Then, a new crystallographic orientation scheme that accounts for rationally oriented secondary phases in the microstructure was devised. Using this new scheme, various dynamic finite-element studies of the microstructure were conducted, incorporating rate-dependent dislocation-density based crystalline plasticity, and accounting for the multiple length scales of the secondary phases. The aim of these studies was primarily to identify and distinguish the role of nano-sized precipitates and micron-sized dispersed particles in the localization of deformation in dynamically loaded microstructures.

To model the nucleation and propagation of failure at the microstructural scale, under large deformations and dynamic loading conditions, we subsequently tailor finite
deformation theory, by introducing a decomposition of the deformation gradient, as an alternative to the Kroner-Lee decomposition, which is specific to crystalline solids. We then propose a general fracture criterion for finitely deforming crystals, based on the integral law of incompatibility. With this new criterion, finite element studies of single crystals, polycrystals and secondary phases were conducted to elucidate the mechanisms of dynamic fracture in Al-Cu-Mg-Ag alloys.

1.3 Outline of the Dissertation

The outline of this dissertation is as follows. In Chapter 2, we introduce the microstructure of an Al-Cu-Mg-Ag alloy to be investigated in this study, and subsequently formulate the theory of dislocation-density based crystalline plasticity, which is fundamental to our microstructural modeling. We then propose a new rational orientation scheme, necessary for the representation of precipitates in the Al-Cu-Mg-Ag alloy. In Chapter 3, we propose a new theory for the large deformation and dynamic fracture of crystalline solids, based on the integral law of incompatibility. The results of the proposed formulations of Chapters 2 & 3 are then presented and discussed. We present our results in the following order: in Chapters 4-6 we investigate shear strain localization, and in Chapters 7-9 we investigate the dynamic fracture of crystalline solids. Specifically, in Chapter 4, we investigate, by dynamic finite element modeling, and by incorporating the rational orientation scheme, the effects of $\Omega$ and $\theta'$.
precipitates on the shear strain localization of polycrystalline aggregates. In Chapter 5, we focus on a single $\Omega$ precipitate to investigate how interfacial dislocation density evolution affects precipitate deformation. In Chapter 6 we consider how different microstructural length scales, such as those associated with nano-sized precipitates and micron-sized dispersed particles, characterize dynamic localization. In Chapter 7, we apply the proposed fracture theory of Chapter 3 to brittle and ductile single crystals, and validate these predictions. We conclude the chapter with results for geometrically necessary dislocation (GND) density evolution and interaction with stationary and moving cracks. In Chapter 8, we apply the proposed fracture theory to polycrystals, and investigate their intergranular and transgranular failure modes. In Chapter 9, we apply the proposed theory to microstructures with coarse precipitates and dispersed particles, and conduct a detailed investigation of crack nucleation, propagation, and interaction with these coarse secondary phases. Finally, in Chapter 10 recommendations for future research are given.
Chapter 2

Microstructure: Description & Modeling

2.1 Overview of the Microstructure

The crystalline plasticity constitutive formulation requires the identification of the specific crystal structures, slip systems and material properties. We consider in this study Al–Cu–Mg–Ag (Mn, Fe) alloys, which have multiple secondary phases, spanning multiple length scales, as summarized in Fig. 2.1 for a 2139-T8 Al plate. Fig. 2.1 (a) shows the dark-field TEM image of nano-sized Al$_2$Cu precipitate platelets, $\Omega$ and $\theta'$ that are interspersed in the grains of the alloy. Fig. 2.1 (b) shows a bright-field image of micron sized Mn-bearing dispersoids (T-phase) and coarser Mn-bearing inclusions, also found in the microstructure. For more details on the characterization of microstructure see Lee and Zikry (2010). Fig. 2.1 (c) summarizes by schematic the different secondary phases and their associated length scales.

The different phases identified in Fig. 2.1 have different crystallographic properties. For an accurate description of their roles in the deformation of the microstructure, it is paramount to account for these differences, as shown in Fig. 2.2. The $\theta'$ crystal has a tetragonal structure, $\bar{I}4m2$, with $a=0.404$ nm, $c=0.58$ nm (Silcock, et al. (1955)) and whose slip systems have been determined by considering the densest
planes and shortest burgers vectors, six of which are listed in Fig. 2.2. The Ω phase, on the other hand, has been proposed as monoclinic (Auld (1972), Auld (1986)), hexagonal (Kerry and Scott (1984)) and tetragonal distorted θ phase (Garg and Howe (1991)). The accepted structure for the Ω phase is the orthorhombic structure (Fmmm) proposed in Knowles and Stobbs (1988), with a=0.496 nm, b=0.858 nm and c=0.848 nm. In this study, however, the Ω phase has been modeled by the alternative I4/mcm structure (Garg and Howe (1991), Ringer and Hono (2000)), which is only a slight perturbation of Fmmm, but is essentially identical to the θ crystal, with a=0.607 nm and c=0.487 nm (Wang and Starink (2005)), and whose slip systems have been identified experimentally (Bonnet and Loubradou (2002), Ignat and Durand (1976)) six of which are listed in Fig. 2.2. Then Mn-bearing dispersoid has been identified as orthorhombic, with a Bbmm structure (Robinson (1952), Wang, et al. (1989)) or, differing by a rotation of the reference frame, as a Cmcm structure (Mandolfo (1976)). In this study we select the latter, and assign to the dispersoids the slip systems determined experimentally for Cmcm crystals (Hildyard, et al. (2009)), which are listed in Fig. 2.2.

2.2 Rate-dependent Crystalline Plasticity

Constitutive formulations for rate-dependent multiple-slip crystal plasticity, which are coupled to evolutionary equations for dislocation-densities, have been used.

In that formulation, the velocity gradient is decomposed into a symmetric deformation rate tensor $D_{ij}$ and an anti-symmetric spin tensor $W_{ij}$. $D_{ij}$ and $W_{ij}$ are then additively decomposed into elastic and plastic components as

$$D_{ij} = D_{ij}^s + D_{ij}^p, \quad W_{ij} = W_{ij}^s + W_{ij}^p$$

(2.2.1)

The inelastic parts are defined in terms of the crystallographic slip-rates as

$$D_{ij}^p = P_{ij}^{\alpha^s} \dot{\gamma}^\alpha, \quad W_{ij}^p = \omega_{ij}^{\alpha^s} \dot{\gamma}^\alpha$$

(2.2.2)

where $\alpha$ is summed over all slip-systems, $P_{ij}^{\alpha}$ and $\omega_{ij}^{\alpha}$ are the symmetric and anti-symmetric parts of the Schmid tensor, defined with respect to the material frame.

The rate-dependent constitutive description on each slip system can be characterized by a power-law relation as

$$\dot{\gamma}_{(\alpha)} = \dot{\gamma}_{ref} \left( \tau_{(\alpha)}^{\alpha^s} / \tau_{ref}^{\alpha^s} \right) \left( \tau_{(\alpha)}^{\alpha^s} / \tau_{ref}^{\alpha^s} \right)^{1/m-1}$$

(2.2.3)
where \( \dot{\gamma}_{r}^{(\alpha)} \) is the reference shear slip-rate which corresponds to a reference shear stress \( \tau_{ref}^{(\alpha)} \), and \( m \) is the rate sensitivity parameter. The shear stress \( \tau^{(\alpha)} \) is determined from a numerical integration (see Zikry (1994)) of its material rate, given as:

\[
\dot{\tau}^{(\alpha)} = \dot{n}^{(\alpha)} \cdot \mathbf{S}^{(\alpha)} + \dot{n}^{(\alpha)} \cdot \mathbf{S}^{(\alpha)} + \dot{n}^{(\alpha)} \cdot \mathbf{S}^{(\alpha)} + \dot{n}^{(\alpha)} \cdot \mathbf{S}^{(\alpha)}
\]

\[
\dot{\tau}^{(\alpha)} = n^{(\alpha)} \left[ 2 \mu \left( D_{dev} - D^{p} \right) + W^{p} \sigma_{dev} - \sigma_{dev} W^{p} \right] \cdot \mathbf{S}^{(\alpha)}
\]  

(2.2.4)

where we have assumed the Jaumann rate of the deviatoric Cauchy stress (\( \sigma_{dev}^{\alpha} \)) to obtain the final form. The reference stress (\( \tau_{ref}^{(\alpha)} \)) that is used here is a modification of widely used classical forms (Mughrabi (1987)) that relate the reference stress to a square-root dependence on the dislocation-density (\( \rho_{im} \)) as:

\[
\tau_{ref}^{(\alpha)} = \left( \tau_{y}^{(\alpha)} + \mu \sum_{\beta} a_{\alpha\beta} b^{(\beta)} \sqrt{\rho_{im}} \right) \left( \frac{T}{T_{0}} \right)^{-\xi}
\]  

(2.2.5)

where \( \tau_{y}^{(\alpha)} \) is the static yield stress on slip system (\( \alpha \)), \( \mu \) is the shear modulus, \( b^{(\beta)} \) is the magnitude of the Burgers vector for slip system (\( \beta \)), and the coefficients \( a_{\alpha\beta} \) are slip-system interaction coefficients of order 1, which we specify using the formula

\[
a_{\alpha\beta} = 2 \left| P_{ij}^{\alpha} P_{ij}^{\beta} \right|, \text{ such that orthogonal systems do not interact, while aligned systems fully}
\]
interact. $T$ is the temperature, $T_0$ is the reference temperature, and $\xi$ is the thermal softening exponent.

For a given deformed state of the material, the dislocation structure, of total dislocation-density $\rho^{(\alpha)}$, is additively decomposed into a mobile and an immobile dislocation-density, $\rho_m^{(\alpha)}$ and $\rho_{im}^{(\alpha)}$ respectively, as

$$\rho^{(\alpha)} = \rho_m^{(\alpha)} + \rho_{im}^{(\alpha)} \quad (2.2.6)$$

It is assumed that during an increment of strain, there ensues a change in the dislocation structure. The balance between generation and annihilation of dislocation densities as a function of strain is thus taken as a basis for the following equations, which describe the evolution of mobile and immobile dislocation densities

$$\dot{\rho}_m = \dot{\gamma}^{(\alpha)} \left( \frac{g_{sour}}{b_{(\alpha)}} \cdot \rho_{im}^{(\alpha)} - \frac{g_{minter}}{b_{(\alpha)}} \cdot \rho_m^{(\alpha)} \cdot e^{-\frac{\Delta H(T)}{kT}} - \frac{g_{immob}}{b_{(\alpha)}} \sqrt{\rho_{im}^{(\alpha)}} \right)$$

$$\dot{\rho}_{im} = \dot{\gamma}^{(\alpha)} \left( -\frac{g_{recov}}{b_{(\alpha)}} \cdot \rho_{im}^{(\alpha)} \cdot e^{-\frac{\Delta H(T)}{kT}} + \frac{g_{minter}}{b_{(\alpha)}} \cdot \rho_m^{(\alpha)} \cdot e^{-\frac{\Delta H(T)}{kT}} + \frac{g_{immob}}{b_{(\alpha)}} \sqrt{\rho_{im}^{(\alpha)}} \right) \quad (2.2.7)$$

where $g_{sour}$, $g_{minter}$, $g_{recov}$, and $g_{immob}$ are coefficients for: generation of mobile dislocation-densities, trapping of mobile dislocations by dislocation-dislocation interactions, rearrangement and annihilation of immobile dislocations by recovery, and
immobilization of mobile dislocations respectively. For a determination of these coefficients see Kameda and Zikry (1996). \( \Delta H(T) \) is the temperature dependent enthalpy of activation of plastic deformation, and \( k \) is the Boltzmann constant.

2.3 Rational Orientation of Crystals

It is known that the \( \Omega \) and \( \theta' \) crystals nucleate and grow along rational habit planes in the matrix, which results in a predetermined relationship between slip systems in these precipitates and the matrix. Hence, to impart the rational orientations of \( \Omega \) and \( \theta' \) with respect to the matrix crystal, as determined in Wang and Starink (2005), and subsequently with respect to the finite element frame of reference, the following transformation scheme was devised, and is summarized in Fig. 2.3.

The slip directions and planes for the matrix and precipitates are defined in fractional coordinates (Fig. 2.3 (a)). Since the precipitates are non-cubic, the vectors defining slip-plane normals are not equivalent to their miller indices, and normals must be obtained by a reciprocal lattice construct (Kelly, et al. (2000)). The slip vectors are then mapped from the precipitate space to the matrix space (Fig. 2.3 (b)). This is achieved by the transformation sequence \([M_{\text{cart}}^{\alpha*}][M_{\Omega}^{\text{cart}}]\), where \([M_{\Omega}^{\text{cart}}]\) transforms a slip vector in the precipitate (e.g. \( \Omega \)) to a vector in a Cartesian frame, and \([M_{\text{cart}}^{\alpha*}]\) takes the transformed vector from the Cartesian frame to the matrix crystal. The form of \([M]\) is adapted from (Giacovazzo, et al. (2002)). We then identify the rational vectors defining
the orientation relations between the precipitates and the matrix (see Wang and Starink (2005)). These rational vectors define the transformation \([T^{\alpha}_{\alpha*}]\) to be applied to the slip vectors (Fig. 2.3 (c)), in order to properly align them with respect to the matrix frame. Subsequently, Fig. 2.3 (d), another transformation \([M^\alpha_{\alpha}]\) may be needed to take the slip vectors from the matrix space to a Cartesian space, if the matrix crystal is non-cubic. Random Euler angles are then assigned to every grain to align crystals with respect to the polycrystalline aggregate axes. This transformation, defined as \([T^{Poly}_{\text{car}}]\), is adapted from Randle (1993). Finally, Fig. 2.3 (e), the polycrystalline aggregate axes are then aligned with the element frame (initially, the drawing plane) using \([T^{\text{elem}}_{\text{Poly}}]\).

2.4 Non-dimensionalization of Constitutive Properties

The material properties used in this study are summarized in Tables 2.1 and 2.2. For non-dimensionalization, the following characteristic quantities were used: Young’s modulus of the matrix \((E)\), the elastic dilatational wave speed in the matrix \((c)\), burgers vector in the matrix \((b_v)\), and room temperature \((T_{\text{ref}})\). The non-dimensionalized quantities are listed in Table 2.3.
2.5 Tables & Figures

Table 2.1: Material properties of Ω, θ', Mn-Dispersoids and Al-Matrix

<table>
<thead>
<tr>
<th>Property</th>
<th>Description</th>
<th>Value</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Al matrix</td>
<td>Ω, θ', Mn-Disp</td>
</tr>
<tr>
<td>E (GPa)</td>
<td>Young's modulus</td>
<td>69</td>
<td>140</td>
</tr>
<tr>
<td>ν</td>
<td>Poisson's ratio</td>
<td>0.34</td>
<td>0.34</td>
</tr>
<tr>
<td>τs (MPa)</td>
<td>Static yield stress</td>
<td>35</td>
<td>35</td>
</tr>
<tr>
<td>ρ (g/cm³)</td>
<td>Mass density (obtained from unit cell calculations)</td>
<td>2.70</td>
<td>4.36</td>
</tr>
<tr>
<td>Cp (J/kgK)</td>
<td>Specific heat (using the Neumann-Kopp rule for Ω, θ')</td>
<td>902</td>
<td>623</td>
</tr>
<tr>
<td>ΔH/k (K)</td>
<td>Activation enthalpy/ Boltzmann constant (Taking a mass weighted average for Ω, θ')</td>
<td>2500</td>
<td>3100</td>
</tr>
<tr>
<td>υref (s⁻¹)</td>
<td>Reference strain rate</td>
<td>0.001</td>
<td>0.001</td>
</tr>
<tr>
<td>υcritical (s⁻¹)</td>
<td>Critical strain rate</td>
<td>10,000</td>
<td>10,000</td>
</tr>
<tr>
<td>ρimm (m⁻²)</td>
<td>Initial immobile dislocation density</td>
<td>10^{12}</td>
<td>10^{8}</td>
</tr>
<tr>
<td>ρm (m⁻²)</td>
<td>Initial mobile dislocation density</td>
<td>10^{10}</td>
<td>10^{6}</td>
</tr>
<tr>
<td>T₀ (K)</td>
<td>Reference temperature</td>
<td>293</td>
<td>293</td>
</tr>
<tr>
<td>m</td>
<td>Strain rate sensitivity</td>
<td>0.02</td>
<td>0.02</td>
</tr>
<tr>
<td>gsource</td>
<td>Dislocation source coefficient</td>
<td>2.76E-5</td>
<td>2.76E-5</td>
</tr>
<tr>
<td>gimmob</td>
<td>Dislocation immobilization coefficient</td>
<td>0.0127</td>
<td>0.0127</td>
</tr>
<tr>
<td>ginter</td>
<td>Mobile dislocation interaction coefficient</td>
<td>5.53¹</td>
<td>5.53</td>
</tr>
<tr>
<td>grecov</td>
<td>Recovery coefficient</td>
<td>6.69E+5</td>
<td>6.69E+5</td>
</tr>
<tr>
<td>ξ</td>
<td>Thermal softening exponent</td>
<td>0.5</td>
<td>0.5</td>
</tr>
<tr>
<td>χ</td>
<td>Fraction of plastic dissipation to heat</td>
<td>0.9</td>
<td>0.9</td>
</tr>
</tbody>
</table>

¹ The \( g_{\text{minter}} \) coefficient here reflects our usage of the dislocation density evolution equations in Ashmawi & Zikry (2002). The updated equations described in this chapter require a new \( g_{\text{minter}} \) coefficient, as shown in the Table 2.2.
<table>
<thead>
<tr>
<th>Property</th>
<th>Description</th>
<th>Value</th>
<th>Ref</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\nu$</td>
<td>Poisson's ratio</td>
<td>0.34</td>
<td></td>
</tr>
<tr>
<td>$\tau_y$ (MPa)</td>
<td>Static yield stress</td>
<td>35</td>
<td>---</td>
</tr>
<tr>
<td>$\rho$ (g/cm$^3$)</td>
<td>Mass density</td>
<td>2.7</td>
<td>---</td>
</tr>
<tr>
<td>$C_p$ (J/kgK)</td>
<td>Specific heat</td>
<td>902</td>
<td>Smithells (2004)</td>
</tr>
<tr>
<td>$\Delta H/k$ (K)</td>
<td>Activation enthalpy/Boltzmann constant</td>
<td>2500</td>
<td>Ali, <em>et al.</em> (1979)</td>
</tr>
<tr>
<td>$\dot{\gamma}_{ref}$ (s$^{-1}$)</td>
<td>Reference strain rate</td>
<td>0.001</td>
<td>Zikry and Kao (1997)</td>
</tr>
<tr>
<td>$\rho^0_{im}$ (m$^{-2}$)</td>
<td>Initial immobile dislocation density</td>
<td>$10^{12}$</td>
<td>---</td>
</tr>
<tr>
<td>$\rho^0_m$ (m$^{-2}$)</td>
<td>Initial mobile dislocation density</td>
<td>$10^{10}$</td>
<td>---</td>
</tr>
<tr>
<td>$T_0$ (K)</td>
<td>Reference temperature</td>
<td>293</td>
<td>---</td>
</tr>
<tr>
<td>$m$</td>
<td>Strain rate sensitivity</td>
<td>0.02</td>
<td>Zikry (1994)</td>
</tr>
<tr>
<td>$g_{source}$</td>
<td>Dislocation source coefficient</td>
<td>2.76E-5</td>
<td>Zikry and Kao (1997)</td>
</tr>
<tr>
<td>$g_{immob}$</td>
<td>Dislocation immobilization coefficient</td>
<td>0.0127</td>
<td></td>
</tr>
<tr>
<td>$g_{minter}$</td>
<td>Mobile dislocation interaction</td>
<td>5.53E+4</td>
<td></td>
</tr>
<tr>
<td>$g_{recov}$</td>
<td>Recovery coefficient</td>
<td>6.69E+4</td>
<td></td>
</tr>
<tr>
<td>$\xi$</td>
<td>Thermal softening exponent</td>
<td>0.5</td>
<td>Zikry (1994)</td>
</tr>
<tr>
<td>$\chi$</td>
<td>Fraction of plastic dissipation to heat</td>
<td>0.9</td>
<td></td>
</tr>
</tbody>
</table>
### Table 2.3: Non-dimensionalization scheme for dynamic finite element analyses

<table>
<thead>
<tr>
<th>Dimensional Quantity</th>
<th>Non-Dimensional Quantity (*)</th>
<th>Dimensional Quantity</th>
<th>Non-Dimensional Quantity (*)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature (T)</td>
<td>$T^* = \frac{T}{T_0}$</td>
<td>Stresses ($\tau, \sigma$)</td>
<td>$(\tau^<em>, \sigma^</em>) = \left(\frac{\tau}{E}, \frac{\sigma}{E}\right)$</td>
</tr>
<tr>
<td>Length (x)</td>
<td>$x^* = \frac{x}{b_v}$</td>
<td>Strain Rate (\dot{\gamma})</td>
<td>$\dot{\gamma}^* = \dot{\gamma}\frac{b_v}{c}$</td>
</tr>
<tr>
<td>Time (t)</td>
<td>$t^* = \frac{t}{b_v}$</td>
<td>Dislocation Density ($\rho$)</td>
<td>$\dot{\rho}^* = \dot{\rho}\frac{b_v^2}{c^2}$</td>
</tr>
<tr>
<td>Mass Density ($\rho_{mass}$)</td>
<td>$\rho_{mass}^* = \rho_{mass}\frac{c^2}{E}$</td>
<td>Specific Heat Capacity ($C_p$)</td>
<td>$C_p^* = C_p\frac{T}{c^2}$</td>
</tr>
</tbody>
</table>
Figure 2.1: Al-Cu-Mg-Ag microstructure and corresponding length scales
Figure 2.2: Crystal structures and crystallographic properties of secondary phases in Al-Cu-Mg-Ag microstructures
Figure 2.3: Rational orientation transformation sequence
Chapter 3

The Fracture of Finitely-deforming Crystalline Solids

3.1 Decomposing the Deformation Gradient, $F$

3.1.1 Outline of proposed decomposition

We begin by considering a crystalline solid that can be subjected to any general-loading condition as shown in Fig. 3.1. We view the structure of such a solid as a set of volume elements, or lattice blocks. These lattice blocks can be envisioned as material volumes delineated by planes along which glide, or material flow, can occur. These lattice blocks can deform under applied macroscopic loading conditions. This deformation can be any general combination of rotation, stretching, bending, or any higher-order distortion. As also seen from Fig. 3.1, for the macroscopic solid to attain its final deformed shape, relative glide (or displacement) between lattice blocks may occur, which is what describes plastic flow.

In continuum mechanics, the motion of a solid under large deformations is generally described by a deformation gradient, $F$, relating a material element, $dX$, in the reference configuration, to its image, $dx$, in the current configuration, i.e.:
\[ dx = F dX \] \quad (3.1.1)

The gradient \( F \) admits the Kroner-Lee (Kroner (1960), Lee and Liu (1967)) decomposition

\[ F = F^e F^p \] \quad (3.1.2)

\( F^p \) pertains to the plastic part of deformation, which maps \( dX \) to an intermediate and unstressed configuration, and \( F^e \) is the corresponding elastic part, mapping the element \( F^p dX \) from the intermediate configuration to \( dx \) in the current configuration.

To help account for incompatibilities, discontinuities, and fracture surfaces, we propose to decompose the deformation gradient as

\[ F = F^{\text{Lattice}} F^{\text{Flow}}, \] \quad (3.1.3)

where \( F^{\text{Lattice}} \) will be assumed to account for all elastic and inelastic distortions that are intrinsic to the lattice blocks, and \( F^{\text{Flow}} \) will account only for plastic flow, or the relative glide between the undistorted lattice blocks. Lattice blocks will be assumed as embedded within a material element, as shown in Fig. 3.2. This proposed decomposition provides a clear distinction between plastic flow and plastic strains that
occurs due to the presence of dislocations within the crystalline solid, as postulated by Nemat-Nasser (2009). Generally, plasticity associated with the flow of matter, i.e. the glide of lattice blocks, can be sustained by the generation and annihilation of dislocations, rather than by the continuous storage of dislocations. Plastic flow can therefore lead to macroscopic strains of the order of a several hundred percent, without altering the final dislocation density in the material (Nemat-Nasser (2009)). However, plastic strains due to dislocations stored within the crystalline solid (or lattice blocks) to accommodate internal incompatibilities are usually only of the order of the associated elastic strains, i.e. of the order of $10^{-3}$ in metals (Nemat-Nasser (2009)).

### 3.1.2 Physical description of $F^{\text{Flow}}$

As noted earlier, the glide of lattice blocks is accounted for by the distortion $F^{\text{Flow}}$. Glide, as shown in Fig. 3.2, occurs by the relative displacement of blocks in the intermediate configuration B. No gaps between the displaced blocks are assumed to appear in the figure, but this does not generally have to be true. In fact, as shown in Fig. 3.3, if glide occurs along multiple planes (as indicated by the red arrows), small gaps, or displacement discontinuities, can occur between lattice blocks, resulting in a non-compact configuration, i.e. a configuration that is not simply connected (Kroner (1981)). Consider for example a corner point that is shared by multiple lattice blocks, as shown in Fig. 3.3. When a displacement gap or hole opens up, displacements will no longer be unique at that point, as each block will have a different displacement for its
corner. The distortion $F_{\text{Flow}}$ is usually therefore incompatible. i.e. it is a distortion that is not compatible with the existence of a unique displacement field (Kroner (1981)), and does not map into a compact configuration (Anthony and Azirhi (1995)). We note that $F_p$ will, therefore, also be in general incompatible.

We emphasize that we are considering continuous crystals in this formulation, for otherwise the glide of lattice blocks would not be topologically preserving, and continuum mechanics would generally be invalid as a deterministic description of glide (Anthony and Azirhi (1995), Kroner (2001)). However, if we only consider glide in an average sense, by allowing lattice blocks to be smeared out in the continuum, then the resulting continuous distributions of plastic distortion is what would be characterized by $F_{\text{Flow}}$.

3.1.3 Physical description of $F^{\text{Lattice}}$

The change in shape, or orientation, of lattice blocks is specified by $F^{\text{Lattice}}$. In general, $F^{\text{Lattice}}$ is decomposed into an elastic part ($F^e$), and an inelastic part ($F^I$) as

$$F^{\text{Lattice}} = F^e F^I$$

(3.1.4)

As $F^e = R^e U^e$ (Nemat-Nasser (2009)), the elastic part accounts for both lattice rotation and lattice stretch. $F^I$ will be assumed to account for all inelastic processes that are
intrinsic to lattice blocks. Examples of such inelastic processes can be twinning (Hull and Bacon (2006)), or distortions from geometrically necessary dislocations (GND) induced by the bending or torsion of crystals (Nye (1953)). Multiple inelastic processes can then be accounted for multiplicatively as:

\[ F^I = F^I_n F^I_{n-1} \ldots F^I_1 , \]  

assuming \( n \) such inelastic processes.

As with any continuum, it is assumed that the compact reference configuration is mapped by a compatible deformation \( F \) to the current configuration, which is therefore also compact. As we have seen, \( F^{\text{Flow}} \) is not in general compatible, since plastic flow is in general not sufficient for the continuum to attain a compact current configuration. In such a case, elastic distortions in the lattice blocks have to be activated, so that the current configuration would remain compact (see Fig. 3.3). Hence, \( F^{\text{Lattice}} \) must evolve in just the right manner such that the product \( F^{\text{Lattice}} F^{\text{Flow}} \) is compatible (cf. Kroner (1981)).

To summarize, in this decomposition, we have two separate terms for inelasticity, \( F^{\text{Flow}} \) and \( F^I \), the term \( F^I \) being lumped in \( F^{\text{Lattice}} \). Based on length scales, \( F^{\text{Flow}} \) characterizes macro or mesoscopic strain fields, consistent with plastic flow. Whereas, \( F^I \) combines the effects of local microscopic inelastic deformation mechanisms.
From an alternative standpoint, $F^{\text{Flow}}$ will account for plastic processes that do not alter the solid's macroscopic internal energy; its purpose being only to accommodate externally applied deformations. As plastic flow does not require the storage of dislocations, so the internal state of the material, defined by dislocation densities, could remain unchanged, and the internal energy of the material would thus also be unaltered. Furthermore, even when plastic flow is accompanied by dislocation storage, it would be in the form of statistically stored dislocations (SSDs) with zero net burgers vector, and thus would have no contribution to the macroscopic energy. On the other hand, due to internal incompatibilities that arise within the solid (or lattice blocks), some inelasticity will take place to minimize stored energy. For such inelastic processes, we have $F'$. For example, GNDs or twinning would entail a storage of dislocations of the same sign in the lattice (Nye (1953)), which would result in a net burgers vector that relaxes stored energy.

3.2 Failure and a Proposed Crack Criterion

In the proposed formulation, the necessary and sufficient condition for the compatible deformation of the macroscopic crystalline solid is the first-order differential form of the compatibility law (Kroner (1981)),

$$\text{Curl}(F^{\text{Lattice}} F^{\text{Flow}}) = 0$$  \hspace{1cm} (3.2.1)
Compatibility ensures the uniqueness of displacements at any material point in the solid. Hence, a displacement discontinuity arises when the macroscopic deformation gradient is no longer compatible; a condition which can be characterized by a (non-zero) discontinuity-strength parameter, \(\kappa\), as:

\[
\kappa \equiv \text{Curl}(F^{\text{Lattice}} F^{\text{Flow}}) \tag{3.2.2}
\]

There are, however, two shortcomings that hinder the direct use of Eq. 3.2.2 as a fracture criterion. The first is that it requires the calculation of higher-order strain derivatives, i.e. the curl. The second is that it has the unit of curvature, the interpretation of which, in the context of fracture, is not of immediate relevance.

We can overcome these shortcomings in Eq. 3.2.2 by using the integral form of the incompatibility law, which is obtained by application of Stokes’ theorem (cf. Kroner (1981)) to \(\kappa\), yielding:

\[
\delta \equiv \oint_C F^{\text{Lattice}} F^{\text{Flow}} \, dX \tag{3.2.3}
\]

The criterion for crack nucleation would thus correspond to a critical displacement incompatibility, \(\delta_{\text{Crit}}\), which can be identified with the size of a nucleating crack. Note that any non-zero value of \(\delta_{\text{Crit}}\) would indicate crack nucleation. However, due to the
likelihood of self-welding (Weertman (1998)), the value of $\delta_{\text{crit}}$ should be sufficiently removed from zero.

3.3 Numerical Implementation of the Theory

3.3.1 Computational scheme for the criterion $\delta$

Since $F$ is by definition compatible, we can rewrite $\delta$ as:

$$\delta \equiv \int_C (F - F^{\text{Lattice}} F^{\text{Flow}}) dX \quad (3.3.1)$$

Note that the integrand is non-zero only when the decomposition $F^{\text{Lattice}} F^{\text{Flow}}$ is not equal to $F$. For efficient finite-element implementation, we use element integration-point values of $F$, $F^{\text{Lattice}}$ and $F^{\text{Flow}}$. We further assume that an inequality occurring at the integration-point persists throughout the element, whose initial characteristic length is defined as $L_0^e$. In this way, we can simplify $\delta$ to an equivalent scalar measure ($\delta_s$) as

$$\delta_s \equiv \left\| F - F^{\text{Lattice}} F^{\text{Flow}} \right\| L_0^e \quad (3.2.3)$$
An example of $\delta_s$ is shown in Fig. 3.4 for quadrilateral elements undergoing one-dimensional stretch, with $L'_0$ taken along the x-axis. Specifically, if $^2F > F^\text{Lattice} F^\text{Flow}$, a macroscopic gap will nucleate in the solid, since local element deformations cannot sustain the global requirements on $F$. If, on the other hand, $F^\text{Lattice} F^\text{Flow} > F$, an overlap between neighboring elements would occur, though this is not a likely scenario.

As we shall show in the following sections, $F^\text{Lattice} \equiv R^r F^I$, and $F^\text{Flow} = F^{-1} F^p$. Therefore, the fracture criterion in its simplest form becomes:

$$\delta_s \equiv \| F - R^r F^p \| L'_0$$

(3.2.4)

Hence, based on the Kroner-Lee decomposition, $F^I$ need not be computed explicitly to apply the fracture criterion. But to illustrate the generality of our approach, we will calculate $F^I$ as a sub-problem to obtain insights from its relevant physical processes.

### 3.3.2 Computational scheme for $F^\text{Flow}$

As noted earlier, $F^\text{Flow}$ corresponds to macroscopic plastic flow (see Fig. 3.2) and is given by

---

2 If $A$ and $B$ are $n \times n$ matrices, we define $A > B$ as: $a_{ij} \geq b_{ij}$ for $i,j = 1...n$, and $\exists p,q \in \{1...n\}$ such that $a_{pq} > b_{pq}$. 

The computation of $F^I$ discussed in § 3.3.4. To compute $F^p$, we use the polar decomposition $F^p = R^p U^p$. We obtain $R^p$ at increment $n + 1$ using the recursive formula:

$$R^p_{n+1} = \Delta R^p_{n+1} R^p_n,$$  \hspace{1cm} (3.3.2)

where $\Delta R^p_{n+1}$ is computed from the Hughes-Winget formula (Hughes and Winget (1980)), using the plastic spin, $W^{pl}$, which calculated from the crystalline plasticity constitutive model (Eq. 2.2). $U^p$ is computed from the plastic deformation rate $D^p$, as the crystalline plasticity model is rate-dependent, by

$$U^p = \left(1 + 2 \int_0^t F^T D^p F \, dt\right)^{1/2}$$ \hspace{1cm} (3.3.3)

The argument under the square root is the plastic part of the right Cauchy-Green strain tensor ($C^p$), which is positive definite. $U^p$ and $C^p$ are therefore coaxial tensors, and $U^p$ is obtained by taking the positive square-root of the eigenvalues of $C^p$, as outlined in (Belytschko, et al. (2008)). For the computation of eigenvalues and eigenvectors, we
use the QR algorithm in the *Eispack* FORTRAN Library (Garbow, *et al.* (1977)). A flow chart summarizing the computation of both $F^{\text{Flow}}$ and $F^{\text{Lattice}}$ is shown in Fig. 3.5.

### 3.3.3 $F^{\text{Lattice}}$ and the Computation of $F^e$ for the Fracture Criterion

We have defined $F^{\text{Lattice}}$ as the combination of elastic and inelastic processes that distort lattice blocks, i.e. $F^{\text{Lattice}} = F^e F^{I}$, as shown in Fig. 3.2. Here we describe how to calculate, $F^e$ and in the next section we give an example of how $F^I$ can be calculated.

For our finite element implementation, we begin from the Kroner-Lee decomposition of $F$. Now, $F$ is calculated from the nodal displacements, which assume the deforming solid is compact. $F^p$, on the other hand, is calculated from the constitutive behavior at the element level. It is then tacitly assumed that, for $F$ to be compatible, $F^e = FF^p$. Such an assumption on $F^e$ might not always be valid. What is needed, therefore, when using the Kroner-Lee decomposition, is to verify this assumption with an independent calculation of $F^e$, to monitor the onset of fracture or displacement discontinuity.

Since $F^e = R^e U^e$, the lattice stretch can be negligible when elastic strains are very small; e.g. in crystalline metals, where elastic strains are only on the order of approximately $10^{-3}$. For such a case, $F^e$ is then equivalent to lattice rotation $R^e$ (cf. Gurtin (2006), Nemat-Nasser (2009)). Hence, we can obtain the relation with $U^e = 1$, 


30
\( F^e = R^e. \) \hspace{1cm} (3.3.4)

The independence of this relation can be further understood by considering its dependent counterpart from the Kroner-Lee decomposition,

\[ F^e = FF^{-p}, \text{ assuming } U^e = R^{eT} FF^{-p}. \] \hspace{1cm} (3.3.5)

From equation 3.3.5 for \( F^e \), it is clear that no guarantee exists such that \( U^e \) would only generate elastic strains corresponding to the small elastic values. In other words, the Kroner-Lee decomposition assumes that for the material to remain compact, it can generate elastic strains of any magnitude. By dropping \( U^e \) from the calculation of \( F^e \), therefore, we enforce the condition that elastic strains are negligible. We emphasize, however, that the assumption \( U^e = 1 \) is only used in determining the failure criterion \( \delta \).

To obtain \( R^e \) at increment \( n+1 \) we again use the recursive formula,

\[ R^e_{n+1} = \Delta R^e_{n+1} R^e_n, \] \hspace{1cm} (3.3.6)

where \( \Delta R^e_{n+1} \) is computed from the Hughes-Winget formula, using the lattice spin \( W^* \).
3.3.4 $F_{\text{lattice}}$ and the computation of $F^I$: A sub-problem for GNDs

The physical processes defining $F^I$

As we noted earlier, $F^I$ does not need to be computed explicitly for the application of the fracture criterion. However, if we choose to calculate $F^I$, we need to determine the specific inelastic processes that can occur. For instance, we have pointed earlier to twinning as a candidate process. The form for $F^I$ defining twinning transformation can be found in Sutton and Balluffi (2006). We note that twinning occurs in body centered cubic (BCC), hexagonal close-packed (HCP) crystals (Hull and Bacon (2006)), and nanocrystalline face centered cubic (FCC) crystals (Chen, et al. (2003)). We might expect, on the other hand, geometrically necessary dislocation (GND) densities for the aluminum alloys that have been investigated in this study. GNDs are nucleated and stored in a crystal lattice that is subjected to bending or torsion to relax strain gradients (Kubin and Mortensen (2003)). GNDs, insofar as they are associated with strain (or stress) gradients, reflect a higher-order effect (Kroner (1963)). In the context of large deformations, therefore, where the leading term (i.e. plastic flow) is comparatively large, GND densities can be significantly smaller than statistically stored dislocation (SSD) densities. SSDs will thus dominate the $\rho_m$ and $\rho_{im}$ densities in Eq. 2.2.6.

Nonetheless, to show the general utility of our approach, we will obtain $F^I$ by solving a sub-problem for GNDs as summarized in Fig. 3.5.

The general approach for calculating the GND densities is as follows:
Compute the shear strain gradients ($\nabla \gamma$) of each active slip system.

For every active slip system, $\alpha$, compute the necessary screw ($\rho_\parallel$) and edge ($\rho_\perp$) dislocation densities using the equations, (Gurtin (2006), Rezvanian, et al. (2007)):

$$
\rho_\parallel^\alpha = \tilde{1}^\alpha \cdot \nabla \gamma^\alpha \\
\rho_\perp^\alpha = -\tilde{s}^\alpha \cdot \nabla \gamma^\alpha \quad \text{(No sum on indices),} \quad (3.3.7)
$$

where $\tilde{1}^\alpha$ is the dislocation line vector, and $\tilde{s}^\alpha$ is the slip direction, both defined with respect to the current configuration.

Compute the corresponding Nye dislocation tensor, $G_{ij}^\alpha$, from the decomposition (Gurtin (2006)):

$$
G_{ij}^\alpha = \rho_\parallel^\alpha \tilde{s}^\alpha \otimes \tilde{s}^\alpha + \rho_\perp^\alpha \tilde{1}^\alpha \otimes \tilde{s}^\alpha \quad \text{(No sum on indices)} \quad (3.3.8)
$$

Solve for the necessary displacements, $\vec{u}_i^{\text{GND}}$, using the relation, cf. (Sutton and Balluffi (2006)):

$$
u_i^{\text{GND}} = \int_A G_{ij}^\alpha b_j^\alpha \, dA \quad \text{(Sum on all repeated indices),} \quad (3.3.9)
$$

where $\vec{b}^\alpha$ is the burgers vector for the slip system, and is aligned with $\tilde{1}^\alpha$ for the screw dislocation densities, or $\tilde{s}^\alpha$ for the edge dislocation densities. $A$ is the current area of the element.

$F^I \equiv F^{\text{GND}}$ is thus defined as the deformation gradient computed from $\vec{u}^{\text{GND}}$

$$
F^{\text{GND}} = I + \frac{\partial u^{\text{GND}}}{\partial X} \quad (3.3.10)
$$

**Details and Simplifications to the calculation of $F^{\text{GND}}$**

We begin by noting that shear slip ($\gamma$), from which $\nabla \gamma$ is to be computed, is not the total shear slip computed from the large deformation theory ($F^p$). The reason is, as noted by Nye (1953), GNDs cannot not account for the sliding of lattice blocks. With
large deformations, \( F^p \) is decomposable into \( F^{\text{GND}} \) (with net burgers vector due to GNDs) and \( F^{\text{Flow}} \) (with zero net burgers vector due to SSDs), and it is expected that \( F^{\text{Flow}} \) would usually dominate. Hence, the shear slip \( \gamma \), computed from \( F^p \), would overestimate the values anticipated by GND theory in proportion to \( F^{\text{Flow}} \). It is therefore needed to define a shear-slip \( \gamma^{\text{GND}} \), i.e. that part of plasticity associated with a net burgers vector, in order to yield the appropriate magnitudes and trends of GND formation.

In our implementation, we assume that shear slip associated with GNDs is a micro-plasticity due to internal incompatibilities in the lattice, and would thus only be of the order of associated elastic strains (Nemat-Nasser (2009)). We approximate \( \gamma^{\text{GND}} \) on slip system \( \alpha \) from the elastic strains in the element projected on the slip system, as

\[
\gamma^{\text{GND}}_{(\alpha)} = \varepsilon^e_{(\alpha)},
\]

(3.3.11)

where component \( \varepsilon^e_{(\alpha)} \) is defined by

\[
\varepsilon^e_{(\alpha)} = \bar{n}^\alpha \cdot E^\varepsilon \cdot \bar{s}^\alpha \quad \text{(No sum on } \alpha \text{)},
\]

(3.3.12)
with \( E_i^e = \int_0^t \sigma_i^e \, dt \) the elastic strain tensor for the element, \( \bar{\eta}^\alpha \) the slip normal and \( \bar{s}^\alpha \) the slip direction, all defined with respect to the current configuration.

This approximation parallels the formulation for GND densities in terms of stress-vector gradients (Weertman (1998)), for instance:

\[
\rho_{x}^{GND} = \frac{1 - \nu}{G} \nabla \cdot \sigma_x, \tag{3.3.13}
\]

where \( \rho_{x}^{GND} \) is the \( x \)-component of the GND density, \( G \) is the shear modulus, \( \nu \) is Poisson's ratio, and \( \sigma_x \) is the \( x \)-component of the stress vector. That is, recognizing that stress in any elasto-plastic solid is fully defined by the elastic strains leads to

\[
\rho_{x}^{GND} = \frac{1 - \nu}{G} \nabla \cdot \sigma_x = \nabla \cdot \left( \frac{1 - \nu}{G} \sigma_x \right) = \nabla \cdot \varepsilon^e_x, \tag{3.3.14}
\]

which further confirms the approximation of \( \gamma^{GND} \) by the elastic strains.

To calculate the gradients (\( \nabla \gamma^{GND}_\alpha \), and \( F^{GND} \)) we extrapolate integration-point values of shear slip \( \gamma^{GND}_\alpha \) and displacements \( \bar{u}^{GND} \) to the nodes. We start from:

\[
[B(\bar{\xi})u]_{ij} \mathbf{e}_i \otimes \mathbf{e}_j \quad \text{(Sum on repeated indices),} \tag{3.3.15}
\]
where $\mathbf{B}$ is the strain interpolation matrix defined with respect to the current configuration (Belytschko, et al. (2008)), $\xi$ is the nodal coordinate vector defined in the parent element, $\mathbf{u}$ is the nodal displacement matrix, and $(\mathbf{e}_i \otimes \mathbf{e}_j)$ is the Lagrangian dyad. The strain component $\varepsilon^\alpha(\xi)$, defined in the plane with normal $\bar{n}^\alpha$ and in direction $\bar{s}^\alpha$, is

$$
\varepsilon^\alpha(\xi) = B_{ik}(\xi)u_{kj} \quad \text{(Sum on repeated indices)}
$$

(3.3.16)

Hence, the nodal shear slip, $\gamma^\text{GND}_\alpha(\xi)$, can be obtained from its integration-point value, $\gamma^\text{GND}_\alpha(0)$, and the aligned element strain components, $\varepsilon^\alpha(\xi)$, by the following scaling relation:

$$
\gamma^\text{GND}_\alpha(\xi) = \gamma^\text{GND}_\alpha(0) \cdot \varepsilon^\alpha(\xi)/\varepsilon^\alpha(0) \quad \text{(No sum on indices)}
$$

(3.3.17)

Similarly, to extrapolate integration-point GND displacements, $\bar{\mathbf{u}}^\text{GND}(0)$, to the nodes, we use the following scaling relation with the shape function, $N$, as

$$
\bar{u}^\text{GND}_{(j)} = \bar{u}^\text{GND}_{(j)}(0)\left(N_k(\xi)u_{k(j)}/N_l(\xi)u_{l(j)}\right) \quad \text{(No sum on } j; \text{ sum on } k \text{ and } l)
$$

(3.3.18)
We can then obtain $\nabla \gamma_{\alpha}^{GND}$ and $F^{GND}$ at the integration-point by differencing $\gamma_{\alpha}^{GND}(\xi)$ and $\ddot{u}_{GND}^{GND}(\xi)$. For differencing to be meaningful, we note that at least linear variations in strain within an element should be anticipated. In two dimensions, this would at least require the use of bilinear four-node quadrilateral (Q4) elements.

### 3.4 Numerical Generation of Failure Surfaces

When the failure criterion is met, there are various finite-element techniques to treat the failed element, and to generate the corresponding failure surfaces. For instance, *interelement crack* methods (Camacho and Ortiz (1996), Xu and Needleman (1994)) could be used, which rely on node separation. However, the crack path would then be confined to element edges, which would not properly account ductile crack profiles, such as with crack blunting. Moreover, when simulating fracture of microstructures at very small length-scales, it would not be reasonable to require for the crack-tip opening radius at nucleation to be infinitesimal. We, therefore, use the *element removal* method. Briefly, element removal involves the ‘deletion’ of an element’s contribution to the global system of equations, by zeroing the strains passed into the flagged element and zeroing the stresses passed out from it (Hibbitt, *et al.* (2007)). In this implementation, an element is flagged for removal when the condition,

$$\delta_{\text{Crit}} / L \geq 0.5$$

(3.4.1)
is met; i.e. when the magnitude of the incompatibility corresponds to half the current characteristic length (\( L^c \)) of any element. To avoid spurious mesh dependence on element size (Song, et al. (2008)) we have scaled the element removal criterion by \( L^c \). The value \( 0.5 \) is chosen arbitrarily; it essentially implies that the size of the incompatibility is half the element size when the element is removed.

To avoid sudden numerical instabilities in the mesh, once flagged for removal the element is numerically unloaded over a span of \( 500 \) increments. Unloading follows the recursive formula:

\[
\sigma_{ij}^{n+1} = \xi \sigma_{ij}^n, \tag{3.4.2}
\]

where \( \sigma_{ij} \) is the Cauchy stress tensor, \( \xi < 1 \) is an arbitrary factor related to the rate of unloading (which we set as: \( \xi = 0.995 \)), and \( n \) is increment number.
3.5 Figures

(a) Lattice block

(b) Crystalline solid undergoes
- rotation
- stretch
- flow (Plastic)
- curvature, H.O.T.

Figure 3.1: Crystalline solid deforming by bending
Figure 3.2: Proposed decomposition of the deformation gradient $F$

\[ F = F^e F^p \]
\[ = F^e F^I \cdot F^{-I} F^p \]
\[ F \equiv F^{\text{Lattice}} F^{\text{Flow}} \]

$\phi_*(X) \equiv F$
Figure 3.3: Compact configurations and compatible distortions

\[ F^p = F^I F^{Flow} \]

( Incompatible )

\[ F^e \]

( Incompatible )

Holes open up

compact

( compatible )
Figure 3.4: Graphical presentation of the simplified failure criterion, for a Q4 element. E1, E2 and E3 are element labels. $\delta_s$ is the size of the gap which opens up when $F_{\text{Lattice}} F_{\text{Flow}}$ is not sufficient to account for the whole of $F$.
Figure 3.5: Flow chart for the computation of $F^{LATTICE}$ and $F^{FLOW}$.
Chapter 4

The Role of Rationally Oriented $\Omega$ and $\theta'$ in the Localization of Deformation

In this chapter we conduct dynamic finite element simulations to investigate the microstructural mechanisms related to the high strength and ductile behavior of 2139-Al, and their effect on the overall behavior of this alloy. The specialized microstructurally-based crystalline plasticity model (§ 2.2) is combined with the new rational orientation scheme for $\Omega$ and $\theta'$ precipitates (§ 2.3) to develop a model with an explicit crystallographic and morphological representation the crystals. The material properties used in this study are summarized in Table 2.1, § 2.5.

4.1 The Model

The multiple-slip dislocation-density based crystal plasticity formulation was implemented within the framework of the explicit dynamic finite-element program ABAQUS\Explicit to investigate the behavior of a polycrystalline aggregate representative of 2139-Al under large compressive inelastic strains and strain-rates. An 18-grain aggregate with dimensions of 100 $\mu$m $\times$100 $\mu$m (Figure 4.1) was used, where
the grain size was of a maximum of 1,000 µm². Random Euler angles were assigned for relative grain misorientations that did not exceed 10°. The Ω and θ’ precipitates were placed near the centroid of each grain based on the crystallographic formulations (i.e., having aligned their thickness and long directions in accordance with their rational orientation relationships with respect to each grain, and then projecting these directions in 2D).

The aggregate was subjected to nominal axial strain-rates ranging from 10⁻³ s⁻¹ to 10⁴ s⁻¹ by applying a velocity along the normal direction. Symmetry boundary conditions were applied for a 2D plane-strain deformation (Figure 4.1). A convergent mesh of 6500 elements was used. Four-node bilinear plane-strain quadrilaterals, with one-point integration and enhanced assumed-strain hourglass control were used. For representative behavior, results for an applied strain-rate of 10⁴ s⁻¹ will be presented in this chapter.

4.2 Discussion of Results

The contours of accumulated plastic slip are shown in Figure 4.2. The maximum accumulated plastic strain is 1.4 with most of the maximum accumulations occurring at the precipitate-matrix interfaces. The curves for the comparison between the precipitate-free Aluminum and the 2139-Al indicate that the presence of precipitates has a significant effect on plastic slip behavior and distribution. Specifically, the
precipitates are clearly shear-deformable. This is consistent with experimental observations (Koda, et al. (1963), Li and Wawner (1998), Nourbakhsh and Nutting (1980)). The slip within the θ’ and Ω precipitates has not resulted in slip concentration as is often observed with shearable particles (Nourbakhsh and Nutting (1980), Polmear (2006b), Sanders and Starke (1982)). This could be due to the precipitates continuing to harden, and also acting as physical barriers that impede the matrix from forming large connected zones of intense plastic strain. Moreover, the finite element model, though constrained in plane-strain, showed plastic strain on multiple slip-systems in the Ω and θ’ precipitates. Therefore, slip in the precipitates was not planar, and shearing did not localize as would otherwise be expected (Polmear (2006c)).

The corresponding adiabatic temperature changes are shown in Figure 4.3. The Ω precipitates along the selected evaluation path have a lesser increase in temperature than the θ’ phase or the matrix, which indicates that these precipitates may delay thermal softening of the 2139-Al alloy. This, combined with the diffuse plastic slip accumulation, is another indication of 2139-Al’s ductility and lack of susceptibility to shear-strain localization.

The contours in Figure 4.4 show the immobile dislocation density corresponding to slip system (111)[0\overline{1}1] in the matrix, which is the most active matrix system, and the immobile dislocation density corresponding to the most active system (110)[\overline{1}2\overline{1}] for the precipitates. The contours indicate that the matrix slip system has saturated to $10^{14}$ m$^{-2}$ over most grains. This saturation actually occurred in most of the grains, at a
nominal strain of approximately 12%, which is approximately equivalent to the true strain at which softening is first observed in the experimental stress-strain curves.

It is also seen that the dislocation densities attain maximum values at precipitate-free triple junction points and at precipitate-matrix interfaces. From the curve it is seen that peaks in the immobile dislocation densities are at the matrix-Ω interfaces. This accumulation at the precipitate interfaces further indicates the incompatibility of slip in the surrounding matrix with Ω precipitates, similar to experimental observations (Li and Wawner (1998), Nie and Muddle (2001), Nourbakhsh and Nutting (1980)), for \{100\}_α and \{111\}_α precipitates. This accumulation, however, does not occur for the θ' precipitates along the selected path. Furthermore, the largest immobile dislocation density for Ω precipitates is at 40% of the value in the matrix and θ', which have both saturated. This is therefore an indication that Ω precipitates can add further strength and ductility through the interrelated mechanism of material hardening and dislocation density generation.

The evolution of the reference shear stress values is shown in Figure 4.5. It is clear from the contours that the Ω precipitates generally harden more than the surrounding matrix, and often more than the θ' precipitates. The curves in Figure 4.5 show hardening peaks within the Ω precipitate well above those for the θ' precipitates or the matrix for the selected path. Hence, the Ω precipitates have a marked effect on strengthening the alloy, and it is more pronounced than that of the θ' precipitates. It is
clear, however, that different grain orientations would align $\theta'$ and $\Omega$ differently with respect to the loading direction, and could thus favor $\theta'$ hardening more than $\Omega$. Hence, the effectiveness of precipitate strengthening of the alloy is dependent on crystallographic orientation of the grains, which governs the relative precipitate orientations with respect to the loading of the aggregate; a dependence that is consistent with experimental observations and predictions (Nie and Muddle (2001), Nie, et al. (1996)). The presence, therefore, of both $\theta'$ and $\Omega$, acting on different crystallographic orientations in the alloy, could be expected to enhance the strength and strain-hardening response (Polmear (2006c)) for the various grain orientations in the polycrystalline aggregate.

4.3 Conclusions

The predictions from the microstructural finite element model indicated that the precipitates continue to harden, and also act as physical barriers that impede the matrix from forming large connected zones of intense plastic strain. This understanding is predicated on the accurate representation of the crystallography of the precipitates and the matrix. Moreover, the multiplicity of active slip systems resulted in the shearing of the precipitates, and this multiplicity also inhibited shear strain localization. As the predictions have indicated, the combined effects of $\theta'$ and $\Omega$, acting on different crystallographic orientations, enhance the strength and strain-hardening response of
the alloy. The $\Omega$ precipitates had lower temperature increases than the matrix, and therefore could delay thermal softening. Furthermore, dislocation densities in $\Omega$ have not saturated. Hence, $\Omega$ had the inherent capacity of increasing strength and ductility to the alloy through the interrelated mechanisms of hardening, and sustained ductility through precipitate shearing.
4.4 Figures

Figure 4. 1: 18 grain aggregate, with $\theta'$ and $\Omega$ precipitates, subjected to an applied strain rate of $10^4 \text{ s}^{-1}$ on the upper surface and with symmetry boundary conditions at the left and bottom edges.
Figure 4.2: Contour plot of plastic slip at a nominal strain of 25%. (b) Plastic slip comparison between 2139-Al and precipitate-free Al along path shown in (a)
Figure 4.3: Adiabatic temperature increase comparison between 2139-Al and precipitate-free Al along selected path, showing the temperature build up is lowest inside the Ω precipitates.
Figure 4.4: (a) Contour plot of immobile dislocation density normalized by the initial density for (111)[0 1 1] slip system in the matrix and (110)[1 1 2] in the precipitates at a nominal strain of 25% (i.e. most active slip systems) (b) Comparison of dislocation densities for most active slip systems between 2139-Al and precipitate-free Al along path shown in (a)
Figure 4.5: (a) Contour plot of reference shear stress normalized by static yield at a nominal strain of 25% (b) Comparison of reference shear stress (normalized by static yield) between 2139-Al and precipitate-free Al along path shown in (a)
Chapter 5

Zooming on an $\Omega$ Precipitate

Our objective from this chapter was to identify the microstructural mechanisms controlling the $\Omega$ precipitates’ contribution to the high strength and ductility of Al-Cu-Mg-Ag alloys subjected to high impact loading conditions. We conduct microstructurally-based finite element (FE) simulations for a single $\Omega$ platelet, based on the specialized crystalline plasticity formulations of Chapter 2. The material properties used in this study are summarized in Table 2.2, § 2.5.

5.1 The Model

The matrix crystal was assumed to have dimensions of 0.5 $\mu$m $\times$ 0.5 $\mu$m as shown in Fig. 5.1. An $\Omega$ precipitate was placed at the centroid of an aluminum crystal, with its thickness and long directions aligned in accordance with its rational orientation relationship to the matrix. The precipitate size was taken as 4.5 nm $\times$ 95 nm, which is consistent with the physically observed scales from the TEM characterization images (Elkhodary, et al. (2009a)).
The aluminum crystal was assigned Euler angles of \((35^\circ, 70^\circ, 30^\circ)\) in the Bunge convention with respect to the sample axes (RD, ND, TD), consistent with aluminum plates (Polmear (2006a)). Periodic boundary conditions were applied for a 2D plane-strain deformation mode (Fig. 5.2). For representative high strain-rate behavior, results for an applied strain-rate of \(5 \times 10^4\) s\(^{-1}\) will be presented. A convergent mesh of 4500 four-node bilinear plane-strain elements was used with one-point integration and enhanced assumed-strain hourglass control.

5.2 Discussion of Results

5.2.1 Dislocation-Density Evolution

The Al/Ω interface is a source of dislocation densities. Fig. 5.3 (a) shows the generation of dislocation densities in the \((\overline{1}1\overline{1})[011]_\text{Al}\) slip system from the tips of the Ω precipitate, labeled as step 1. Fig. 5.3 (b) shows the propagation of a dislocation density level of fixed value along the interface and into the matrix (labeled as 2). The propagated dislocation density is predominantly aligned with, but also normal to, the Ω broad-face. Fig. 5.3 (c) shows the same dislocation density spread uniformly across the matrix (labeled as 3). It also shows the generation of a new dislocation density at the tip (labeled as (1)), which will then follow the prior sequence: (1)-(3). We note that sequence (1)-(3) varies in duration with applied strain, however, it is typically very
rapid, spanning small increments in strain; for example, the increment of strain is 0.2% in Fig. 5.3. This result indicates the rapid propagation of dislocation densities from the tips of the Ω precipitate along its entire broad face, prior to spreading into the matrix. This result is also consistent with that for dislocation evolution obtained by MD calculations (Elkhodary, et al. (2010c)). We note that the Ω broad face is always aligned with a habit plane from the {111} matrix planes, which are also slip planes for the matrix, hence the favorable propagation of dislocation densities along the Ω broad face. For precipitates aligned differently, e.g. θ' precipitates, whose habit plane is a {010} matrix plane (Elkhodary, et al. (2009c)), propagation of dislocation densities along the broad face would not be as favorable. This rapid and preferential propagation of dislocation densities along the Ω broad face permits a rapid distribution of deformation along its entire length, without localizing to a particular segment of the precipitate. This result can explain the multiplicity of shear cuttings of thin Ω precipitates observed in the TEM image (Elkhodary, et al. (2010c)), Fig. 5.4, which indicates that the Ω platelet is sheared more or less uniformly along its length (smearing out localization at the atomic level where dislocations cut). In contrast, for instance, θ' precipitates exhibit plastic buckling (Elkhodary, et al. (2009a), Embury (1985)) where deformation essentially localizes to a segment of the precipitate.

As shown in Fig. 5.5 (a), due to the difference in crystal structure between Ω precipitates (I4/mcm) and the matrix (FCC), slip is incompatible; i.e. for plasticity to
traverse a precipitate, a change in slip vectors is needed. In Fig. 5.5 (b), the green circles correspond to the slip vectors in the matrix crystal adjacent to the precipitate, while the magenta circles correspond to those in Ω, the stereographic projection being centered on the load axis. It is clear, therefore, that large changes in burgers vector orientations (as well as lengths) are required for plasticity to traverse the precipitate. Due to the intensive interspersion of Ω precipitates in every matrix crystal in the alloy, and as a result of this incompatibility of slip, Ω precipitates act as an obstacle to plastic deformation, and will therefore also result in alloy strengthening. Furthermore, due to the multiple shear cuttings of Ω, the deformation is not localized at the macro-scale, and alloy ductility is improved (Elkhodary, et al. (2010b)).

5.2.2 Effect of unrelaxed misfit strains at the Al/Ω interface

Aluminum alloys with Ω precipitates have large unrelaxed misfit tensile strains in the thickness direction of the Al/Ω interface, which are localized at the tips of Ω precipitates, where the interface is semi-coherent. On the basis of lattice misfits between Ω and Al, these tensile strains were estimated to be as large as 8% at the tip of the Ω platelet (Fonda, et al. (1992)), while experimental measurements revealed these tensile strains could vary with platelet thickness and attain values up to 30% (Hutchinson, et al. (2001)). It has never been quantified how these tensile strains can further affect behavior at high strain rates. To investigate the effects of these tensile
strains on precipitate deformation, unrelaxed tensile strains were introduced in the finite element model as an initial state, which we model as follows. As shown in Fig. 5.6, the finite element model constitutes initially of the Al matrix, without attaching the Ω precipitate. Its surfaces, those that enclose the Ω precipitate, are pulled on with linearly varying displacement profiles as shown (Fig. 5.6 (b)). In this manner, we impart a nominal tensile strain in the matrix that localizes near the tip of the Ω precipitate, and which decays to zero within 50 burgers vectors from its tip. Having induced this tensile strain distribution in the matrix, the Ω precipitate is then attached to the Al matrix by application of tie constraints (Hibbitt, et al. (2007)) along their common surfaces, with node-to-node correspondence, as shown by the dotted lines in Fig. 5.6 (c). Once tied, the tensile strains in the matrix will redistribute to the precipitate, and the matrix-precipitate system will find a new equilibrium, which will correspond to the initial state we use to represent the unrelaxed misfit strains. Fig. 5.7 shows this initial state, corresponding to a nominal tensile strain of 5%. A corresponding maximum shear strain of 5% occurs at the Ω precipitate tips (Figure 5.7(a)). Associated with this strain is the normal tensile stress shown in 5.7(b), with a maximum value of 350 MPa. A corresponding localized increase in dislocation densities occurs at the tip of the Ω precipitate for system $(\overline{1}11)[011]_{Al}$, as shown in 5.7(c). This local increase of dislocation densities is consistent with the presence of misfit dislocations at a semi-coherent interface (Fonda, et al. 1992, Hutchinson, et al. 2001).
Fig. 5.8 compares accumulated plastic shear slip in an initially strain-free model with that in the ‘pre-strained’ model (i.e., the model with unrelaxed misfit strains, or Fig. 5.7, as its initial state). The curve is for a nominal compressive strain of 7% along an evaluation path that cuts through $\Omega$, as is shown in the inset. It is clear that the pre-strained matrix undergoes less shear slip on average, and that slip is less localized. The fluctuations along the path in the pre-strained condition are related to the initially non-uniform dislocation densities along the path, as can be seen from Fig. 5.7 (c). It is also seen that the precipitate undergoes shear slip that is more comparable with the surrounding matrix for the pre-strained condition than for the strain-free condition. A pre-strained interface therefore has the effect of uniformly distributing plastic deformation and inhibiting localized behavior.

Fig. 5.9 shows the corresponding comparison of the reference shear strengths ($\tau_{ref}$) of the crystals (Eqn. 4). It is seen that $\tau_{ref}$ is on average higher for the pre-strained condition than the strain-free condition. Moreover, the shear strengths in $\Omega$ and the adjacent matrix are comparable. The observed fluctuations in $\tau_{ref}$ are again related to the non-uniformity of dislocation densities at the precipitate interface (Fig 5.7(c)). The $\Omega$ precipitate, therefore, is less of a local stress raiser in the pre-strained condition. This results in the increased homogeneity of strengthening seen in Fig. 5.10.
5.3 Conclusions

The FE microstructurally-based model indicates that dislocation densities generated from the tip of an Ω precipitate rapidly propagate, first along the Al/Ω interface, then into the matrix. The experimentally observed *stepladder* deformation of Ω can be understood in terms of this mechanism, which rapidly propagates dislocation densities along the favorably oriented Al/Ω interface, thus leading to the uniform distribution of shear cuttings of the Ω precipitate. This rapid generation-propagation mechanism was also consistent with the MD simulations (Elkhodary, *et al.* (2010c)) for discrete dislocations, which accounts for the Al/Ω interface coherency and energies. Finally, along with this mechanism, the unrelaxed tensile-strains at the Al/Ω interface have the effect of inhibiting localization of plastic strains and stresses under impact loading, and result in higher strength of Al-Cu-Mg-Ag alloys.
5.4 Figures

Figure 5. 1: HRTEM image of a deformed $\Omega$ platelet in a 2139-Al impacted plate. The $\Omega$ platelet is cut multiple times by dislocations cutting through it, forming this stepladder configuration.
Figure 5.2: Model of the Aluminum crystal with an imbedded Ω precipitate. The Aluminum matrix is 0.5 μm × 0.5 μm and the Ω precipitate is 4 nm × 95 nm. The left and right boundaries are periodic, the upper edge is subjected to an applied strain rate of 50,000 s⁻¹, and the lower edge is fixed.
Figure 5.3: Generation of dislocation densities at the tip of the Ω platelet. This marks the beginning of a sequence (labeled (1)). (b) Propagation of dislocation densities aligned with and normal to the Ω broad face (labeled (2)). (c) Dislocation densities spread uniformly into the matrix (labeled 3); also, generation of new dislocation densities at the tip of Ω (again, labeled (1)).
Figure 5.4: (a) Close up view of the matrix and elements used in stereographic projection (b). (b) Stereographic projection of slip directions for matrix and $\Omega$ elements, looking down the loading axis. Circular symbols are on the upper hemisphere, and square symbols are on the lower hemisphere.
Figure 5.5: (a) Application of 5% tensile strain on the matrix surfaces at the Al/Ω interface. (b) Closeup view of the surfaces at Al/Ω interface showing the applied displacement profile near the Ω platelet tips, which decays over a span of 50 burgers vectors (bv) away from the tips. (c) After the load is removed, the surfaces of Ω and Al are fixed together by application of tie-constraints as shown (dotted), with node-to-node correspondence.
Figure 5. 6: The state of the matrix and corresponding to the load described in Figure 6. (a) A maximum plastic shear slip of 5% results at the tips of . (b) The associated normal tensile stress ($\sigma_{22}/E_{Al}$), with $\sigma_{22} = 350$ MPa maximum value. (c) The corresponding mobile dislocation densities on slip system with a maximum value of $2.38 \times 10^{12} \text{ m}^2$. 
Figure 5.7: Comparison of plastic shear slip ($\gamma_p$) at a nominal compressive strain of 7% along an evaluation path that cuts through $\Omega$ as shown in the inset.
Figure 5.8: Comparison of reference shear strength ($\tau_{Ref}/E_{Al}$) at a nominal compressive strain of 7% along an evaluation path that cuts through $\Omega$ as shown in the inset.
Figure 5.9: Contours of reference shear strength ($\tau_{Ref}/E_{Al}$) for the cases with (b) and without (a) initial strain.
Chapter 6

Localization with Nano-sized $\Omega$ and $\theta'$ Precipitates, versus Micron-sized Mn-Dispersoids

In this brief chapter we investigate the role of precipitate and dispersoid length scales in the Al-Cu-Mg-Ag microstructure. In particular, how localization of deformation is affected by the interspersion of nano-sized $\Omega$ and $\theta'$ precipitates in the microstructure, as compared with the micron-sized Mn-bearing dispersed particles.

6.1 The Models

The behavior of a polycrystalline aggregate representative of 2139-Al under large compressive strains and strain-rates was investigated for different strain-rates. In this chapter, we will present results for an applied strain-rate of $50 \times 10^3$ s$^{-1}$.

A 17-grain aggregate with dimensions of $30 \, \mu m \times 30 \, \mu m$ was modeled, Fig. 6.1, where the grain size was taken on average as $90 \, \mu m^2$, and Euler angles consistent with rolled aluminum plates were used, with relative grain misorientations ranging between $10^\circ$-$15^\circ$. $\Omega$ and $\theta'$ precipitates were interspersed in each grain, at a 1:1 ratio for an area fraction of 4%. Precipitate dimensions were $1000 \, nm \times 34 \, nm$, to be consistent with
observed length scales for precipitates. The Mn-bearing particles were taken as 2 µm × 3 µm for a 5% area fraction. Material properties used in this study were based on the

A two-dimensional plane-strain analysis was conducted, with symmetry boundary
conditions applied. Four-node bilinear plane-strain quadrilaterals, with one-point
integration and hourglass control were used, with a convergent mesh of 60,000 elements.

6.2 Discussion of Results

Figure 6.2(a) shows the 17-grain aggregate, where the grains have been labeled
for clarity. Figure 6.2(b) shows plastic shear slip contours for a nominal compressive
strain of 7%. Figure 6.3(a) (cf. grains 8 and 17) shows that the addition of dispersed
particles results in increased localization of shear slip. The maximum accumulated
shear slip is 25% greater than in the matrix without dispersed particles (cf. Figure
6.2(b)). Conversely, the addition of precipitates (2% Ω, 2% θ’) results in a more diffuse
distribution of shear slip (cf. Figure 6.3(b)), with a maximal value corresponding to
60% that in the matrix devoid of precipitates.

These results indicate that the presence of nano-sized precipitates can inhibit
shear strain localization in the matrix, thereby contributing to the ductility and
toughness of the alloy without incipient shear-strain localization. The larger micro-
sized particles, however, moderately intensify strain localization, as is consistent with known results for large secondary phase particles (Brown and Stobbs (1971)), which could be detrimental to alloy ductility. However, both precipitates and dispersed particles increase the strength of the alloy (Polmear (2006b)).

6.3 Conclusions

It has been shown that nano-sized precipitates can inhibit shear-strain localization in aluminum, which can significantly increase the ductility and toughness of the alloy. Micro-sized inclusions and dispersed particles, however, moderately intensify strain localization, which could be detrimental to alloy ductility and toughness.
6.4 Figures

(a) ~ 800 Nano-sized Precipitates
(b) 9 Micron-sized Dispersoids

Figure 6.1: (a) Polycrystal with Ω and θ’ precipitates. (b) Polycrystal with Mn-bearing dispersoids.
Figure 6.2: (a) 17-grain aggregate with grains labeled. (b) Shear slip accumulation at a nominal compressive strain of 7%. Maximum shear slip = 0.8 (intense red contours).
Figure 6.3: (a) Shear slip contours in the 17-grain aggregate, with 9 dispersed particles constituting a 5% area fraction of the sample. Maximum shear slip = 1.0 (b) Shear slip contours in the 17-grain aggregate, with collectively 760 Ω and θ' precipitates constituting a 4% area fraction of the sample. Maximum shear slip = 0.5
Chapter 7

Fracture: Brittle and Ductile Single Crystals

In this chapter we investigated and the validity of the fracture criterion with two single aluminum FCC crystals: one with brittle behavior, the other ductile behavior. The properties are summarized in Table 2.2. The primary aim of this chapter is to demonstrate that the proposed fracture criterion offers a unified approach for the modeling of brittle and ductile modes, yielding results that are in good agreement with well-known experiments. We also investigate the evolution and interaction of GND densities with dynamic loads, as well as stationary and moving cracks.

7.1 The Model

The finite-element mesh for both crystals is shown in Fig. 7.1. It should also be noted that brittle behavior is obtained by using a significantly higher reference stress in comparison with the ductile case. The dimensions are 500 µm × 500 µm with a pre-crack on the left side of length 125 µm, and an initial crack opening of 3 µm. The crystals have an orientation consistent with rolled aluminum plates, with Euler angles (53°, 90°, 68°). A nominal tensile strain rate of 5000 s⁻¹, is imparted by a constant velocity. A convergent mesh of approximately 30,000 bi-linear quadrilateral elements
with single-point integration and relax-stiffness hourglass control was used. Mesh convergence was determined by overall stress response, crack size and propagation.

7.2 Discussion of Results

7.2.1 Crack Paths

As seen from Fig. 7.2, the failure modes of the two crystals are significantly different. The brittle crystal has a horizontal crack directly ahead of the initial crack. In comparison, the ductile has a crack path of approximately $43^\circ$ from the horizontal, which is close to the plane of maximum shear. Hence, the failure criterion, $\delta$, is capable of capturing both ductile and brittle modes of failure. This follows from the equation 

$$\delta = \|F - R^EF^p\|L_0,$$

where in the limit of elastic (brittle) behavior, simply $F^p \rightarrow 1$. Moreover, the strain to failure or rupture is approximately 9% for the brittle case and 14% for the ductile case. This difference is directly related to the longer crack paths and slower crack velocities in the ductile case.

7.2.2 Crack Velocities

Fig. 7.3 shows a surface plot for the propagation of the brittle crack at different time increments. The crack velocity slightly increases during propagation, from $0.21c_A$ to $0.22c_A$, where $c_A$ is the elastic dilatational wave speed for aluminum. This value is
consistent with the experimental measurements of brittle crack velocities in metals (Bluhm (1969)), which range between $0.2c_0$ to $0.4c_0$, with $c_0$ being the elastic wave speed in that metal, for Mode I cracks.

Fig. 7.3 further indicates that the incompatibility $\delta_s$ always attains its maximum at the crack-tip as expected. However, up until a crack length of $0.4W$, where $W$ is the model’s width, $\delta_s$ values predominantly build up behind the crack front (Fig. 8 (b)), and are steeply localized at the crack surfaces. After the crack has grown beyond $0.4W$, $\delta_s$ distribution becomes much more widespread, Fig. 7.3 (c), and the difference between $\delta_s$ at the crack tip and farther afield becomes less steep. Thus, we can identify two stages of brittle crack propagation. In stage 1, crack propagation is stable and the crack surface appears smooth. In stage 2, crack propagation becomes unstable and the surface becomes irregular, as labeled in Fig. 7.2. This is because as the $\delta_s$ distribution becomes more spread, unstable crack propagation becomes more probable, since the criterion for failure can be attained in any number of elements in the vicinity of the crack tip.

Crack propagation in the ductile aluminum crystal is shown in Figure 7.4. Crack propagation can be described by distinct stages. Fig. 7.4 (a–b) show an initiation and “pop-in” (Bluhm (1969)) of the crack, which is short-lived, spanning a time-increment from $t = 2.17\mu s$ to $t = 5.01\mu s$, at which time the crack is arrested. Fig. 7.4 (c) shows the arrested crack blunts from time $t = 5.01\mu s$ to $t = 10.62\mu s$ and then crack propagation resumes. The propagation, after this stage, is slow and stable, with an average crack
velocity of $v_{crack} = 0.025c_{Al}$, up until time $t = 12.83\mu s$ (Fig. 7.4 (d)). Finally, rapid propagation ensues, Fig. 7.4 (e), with average crack velocity $v_{crack} = 0.12c_{Al}$, until catastrophic failure is attained at time $t = 13.27\mu s$. Fig. 7.5 summarizes schematically these predicted stages for ductile crack propagation. We note that these stages correspond to those experimentally observed for the dynamic fracture of rate-sensitive metals with relatively short edge cracks, and under constant deflection conditions (Bluhm (1969)). The crack arrest we predict, further, coincides with a change in fracture mode, i.e. from vertical extension to blunting and shear, as is expected in specimens subjected to constant deflection (Bluhm (1969)), i.e. the constant velocity boundary conditions that are employed in this model. Crack propagation becomes rapid only when $\delta$ traces a narrow band of intense incompatibility ahead of the crack tip, which compromises the resistance of the crystal to crack propagation, enabling the crack to grow rapidly along this weakened path of incompatibility (Fig. 7.4 (d)).

7.2.3 Distribution of State Variables for the Ductile Single Crystal

Fig. 7.6 (a) shows the contours for lattice rotation ($\psi_{12}$) for the ductile aluminum crystal. We see that lattice rotations attain their extreme values along the crack faces. This is expected since as the crack propagates in a ductile crystal, localized plastic shear slip is activated ahead of the crack tip, which magnifies lattice reorientation in the elements following the plastic flow. Fig. 7.6 (b) represents $\tau_{ref}$, which corresponds to the work hardening in the crystal, normalized by Young’s modulus ($E$). We see that
work hardening localizes around the crack. We also see that hardening is more intense at the spot where the crack was arrested. This is consistent with the build up of $\rho_{\text{im}}$, Fig. 7.6 (c), in the plastic zone ahead of the crack tip, which result in the work hardening of crystals (Eq. 2.2.5). Also, we see from Fig. 7.6 (d) the accumulated plastic shear slip ($\gamma^p$) localize around the crack, confirming the ductility of the failure mechanism. Furthermore, associated with this plastic work is an adiabatic temperature increase, also seen localized around the crack (Fig. 7.6 (e)). Hence, the field variables defining the state of the ductile crystalline solid evolve around the crack as expected from ductile failure.

7.2.4 Ductile crystal without a pre-crack

We also investigated the ductile aluminum crystal, without an edge crack. We wanted to test the ability to initiate a crack in the crystalline solid, without the presence of a pre-crack. A contour plot for $\delta_s$ evolution is shown in Fig. 7.7, which also shows crack initiation and evolution. The general trend is a build up of displacement incompatibility, $\delta_s$, at the corners of the model, and its propagation into the solid. In Fig. 7.7 (b), we see that $\delta_s$ is again aligned with the plane of maximum shear, and builds up to its critical value in two bands, one emanating from the lower left corner, and the other from the top right corner. In Fig. 7.7 (c), we see the growth of cracks initiating from these corners. The nominal strain in the crystal in Fig. 7.7 (c) is 30%, which is seen to not have led to catastrophic failure, and is indicative of the high ductility of the
aluminum single crystal. In Fig. 7.8 we show the corresponding evolution of $\rho_{\text{tot}}$, i.e. the total (summing over all slip-systems) immobile dislocation densities in the crystal, and again see that they localize in the neighborhood ahead of the crack tip, resulting in work hardening in the ductile crystal.

### 7.2.5 GND Density Evolution

**Ductile crystal without a pre-crack**

We have mentioned in the theory section that GND processes can account for incompatibilities associated with stress gradients, and are therefore accounted for separately by solving the $F'$ sub-problem. We investigated how large stress gradients that arise from wave propagation can generate GNDs. The evolution of the absolute values of screw GND densities in slip system $(1\bar{1}1)[011]$ is shown in Fig. 7.9. The GND densities result in loops during the first 500 ns of the simulation. Moreover, the densities in the red contours correspond to a value of the order of $10^7$ m$^{-2}$. As dislocation densities represent the dislocation content per unit area, the dislocation content contained in the red elements thus yields a value of order one, i.e. a single dislocation spread over the red elements, which suggests that the GND density lines correspond to the continuum description of actual dislocations.

The GND density lines follow the steepest peripheries of the shear stress wave (i.e. the largest gradients in stress), as seen from Fig. 7.10 (a-b), while forming either closed loops, or lines whose ends are at the boundaries. Actual dislocation lines, which are
required to conserve the burgers vector, must also form in loops or lines whose ends are on the boundaries, or that intersect other dislocations (Kelly, et al. (2000)). We further note that the purpose of GND densities is to accommodate gradients in stress by generating a burgers tensor, which can always be associated with a burgers vector, as shown in (Gurtin (2002)). Hence, it is necessary for the GND density lines to obey the conservation rule of the burgers vector they create, which is consistent with their arrangement into the loops and lines seen in Fig. 7.9. Having interpreted these GND density lines as the continuum equivalent of actual dislocations, we can see that they accordingly delineate the slipped portion of the crystal from those regions that have not slipped. Since the loads are applied at the boundaries, we therefore expect slip to propagate inwards from the boundaries and into the crystal interior. Indeed, as can be seen from Fig. 7.9 (b-g), the GND density lines generally propagate inward from the boundaries into the crystal. In doing so, we see that these line segments may join to form loops, which can shrink and annihilate as seen in Fig. 7.9 (h). That no GND densities should be left behind is consistent with the final uniformity of the deformation, since the gradients introduced by the passing stress waves are only transient in nature. Subsequent passes of the stress waves induce only mild gradients, and no further GND density loops were predicted during the remainder of the simulation.

We note, however, that due to the plane strain nature of the simulation, the out-of-plane components of the stress gradients must be zero. As the slip system in which
looping occurs is generally not aligned with the plane of applied strain, we notice rapid alternation in sign of GND densities, both edge and screw, along the length of the loops and lines, as seen in Fig. 7.11. They shift from positive (red) to negative (blue) such that the net out-of-plane motion is zero.

Finally, we note that as the simulation progresses and crack nucleation and propagation take place, no further GND densities seem to form in lines or loops or to associate with the crack, as seen in Fig. 7.12. Hence, GND densities do not seem to be associated with dynamic cracks. We will explore this result further in the light of the following model with a pre-crack.

**Ductile crystal with a pre-crack**

For the model with a pre-crack, Fig. 7.13 shows the contour plot for the absolute values of total screw GND densities. It is clear that the predominant arrangement of screw GND densities around the crack tip is in the form of GND density loops. These loops are again the continuum equivalent of the experimentally observed dislocation loops that form at crack tips, and at the same length scales (Chiao and Clarke (1989), Michot, et al. (1994)). In Fig. 7.13, dislocation densities evolving on different slip systems do not overlap, permitting a separate identification of the loops. That is, the inner loop, labeled 1 in Fig. 7.13, forms on slip system $(1 \bar{1} 1)[101]$, while the dislocation densities labeled as 2 form on slip system $(1 \bar{1} 1)[011]$. 

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From Fig. 7.13 (a-c) we can identify the different stages of formation of a screw dislocation density loop on slip system (1̅11)[011]. First, three dislocation density lines are emitted from the crack tip to the top and bottom free surfaces, labeled as 2_I-III (Fig. 7.13 (a)). Then, we see the branches 2_I and 2_II approach each other to surround the inner loop (labeled as1, Fig. 7.13 (b)). We also see that branch 2_II splits into two parts: 2^a_II, which escapes from the right boundary, and 2^b_II, which is what approaches branch 2_I. In Fig. 7.13 (c) we see branches 2^b_II and 2_I join to form loop 2. A new branch 2_IV breaks off and, as shown in Fig. 7.13 (d), exits through the upper surface. This loop formation process, Fig. 7.13 (a-c), takes place over a span of 100ns. For the next 1.2 $\mu$s, Fig. 7.13 (d-f), no new loops form. Instead, loops 1 and 2 shrink, becoming more elongated along the plane of maximum shear, as indicated by the arrow in Fig. 7.13 (e). Note that both loops are pinned at the crack tip and do not travel away from it. At $t=2.39$ $\mu$s, the crack tip moves as pop-in takes place, releasing both loops from their pinning Fig. 7.13 (e). When this happens, we see that Loop 1 shrinks to indiscernible size, as densities of opposite signs cancel each other. Loop 2, on the other hand, opens up once unpinned and travels towards the right boundary (Fig. 7.13 (f)).

After pop-in, the crack is arrested and blunts, as we showed in Fig. 7.4. During this arrest and blunting phase a dislocation density loop from the new crack tip is emitted (Fig. 7.14 (a)). The GND density loop is aligned with the plane of maximum shear. In Fig. 7.14 (b), the crack has resumed propagation, and we see that no new loops formed during this phase. Moreover, the loop’s topside is absorbed into the crack as it
propagates along the plane of maximum shear, leaving behind a half-loop. The half-loop associated with the newly generated surface is consistent with experimental observations (Caillard and Martin (2003)) of half loops emanating from surface indents. Fig. 7.14 also shows the edge GND densities, and indicates GND density lines have both screw and edge components.

From the results for GNDs, we can conclude that the GND density loops formed are sessile (being pinned to the crack tip), and are associated with static crack tips. Moving cracks, on the other hand, do not result in the formation of GND densities. GND densities form in order to accommodate incompatibilities ahead of the crack tip. When incompatibilities build up at the crack front rapidly and strongly enough to propagate a crack (i.e. $\delta_s \geq \delta_{s,Crit}$), then GND formation serves no purpose and does not occur.

7.3 Conclusions

A new crack criterion, $\delta_s$, based on displacement incompatibilities in crystalline solids, has been proposed and tested as a unified approach to model fracture in ductile and brittle single crystals. The predictions from our models for crack paths and crack velocities have been found to be in good agreement with experimental data in the literature. Moreover, the various stages of ductile crack propagation have been captured by our model, including crack arrest and blunting. The criterion $\delta_s$ was also shown to be capable of nucleating ductile cracks, without the need for a pre-crack.
From the results for the GND sub-problem, we found that GND density lines and loops form with the passage of the initial stress waves in the crack-free model, but are subsequently annihilated as the deformation is uniform (i.e. the associated stress gradients are only transient). Furthermore, sessile GND density loops are predicted to form at the tip of the stationary edge crack. Moving cracks, on the other hand, did not result in the formation of GND densities. The reason is GND densities form in order to accommodate incompatibilities ahead of the crack tip. When incompatibilities build up at the crack front rapidly and strongly enough to propagate a crack (i.e. $\delta_s \geq \delta_{s,\text{Crit}}$), then GND formation serves no purpose and does not occur.
Figure 7.1: Model of edge-cracked crystal
Figure 7.2: (a) Fractured brittle crystal. (b) Ruptured ductile crystal
Figure 7.3: Snapshots of the brittle fracture process

(a) $t = 7.67 \mu s$
(b) $t = 7.96 \mu s$
(c) $t = 8.11 \mu s$

$v_{crack} = 0.21 c_{Al}$
$v_{crack} = 0.22 c_{Al}$
Figure 7.4: Snapshots of the ductile fracture process
Figure 7.5: Schematic of stages of ductile fracture
Figure 7.6: State variables for ruptured ductile crystal
Figure 7.7: Evolution of the incompatibility $\delta_s$ and the crack for the ductile crystal without a pre-crack

(a) $\varepsilon_{nom} = 15.1\%$

(b) $\varepsilon_{nom} = 22.3\%$

(c) $\varepsilon_{nom} = 28.2\%$
Figure 7.8: Evolution of immobile dislocation densities (where SSDs are preponderant) in the cracking ductile crystal

(a) $\varepsilon_{nom} = 15.1\%$

(b) $\varepsilon_{nom} = 22.3\%$

(c) $\varepsilon_{nom} = 28.2\%$
Figure 7.9: The evolution of screw GND dislocation density loops in slip system $(\bar{1}11)[011]$ with the passage of the initial stress waves. The red contours correspond to a GND density on the order of $10^9$ m$^{-2}$. 
Figure 7.10: The GND density lines attempt to follow the steepest peripheries (i.e. largest gradients) on the shear stress waves. (a) The steepest gradients on the shear wave (dark blue) are traced out to clarify the correspondence with the GND loop shown underneath. (b) The red peripheries of the shear stress wave drive the inward motion of the GND density lines from the corners and surfaces. Red contours represent a GND density on the order of $10^9$ m$^{-2}$. 
Figure 7.11: The alternating signs of the screw and edge components of the GND density lines to accommodate the plane strain deformation. The red and blue contours represent GND densities on the order of $10^9 \text{ m}^{-2}$. 
Figure 7.12: No new GND densities (blue contours: \(<10^5 \text{ m}^{-2}\)) predicted with the growth of the ductile cracks
Figure 7.13: The evolution stages of screw GND dislocation density loops from the edge crack. The red contours represent a GND density on the order of $10^9$ m$^{-2}$. 

$\mathbf{1: } \rho_{\{111\}[101]}$, \hspace{1cm} \mathbf{2: } \rho_{\{111\}[011]}$
Figure 7.14: (a) New GND dislocation density loop emitted from the blunting crack (b) no new loops formed with propagating crack; instead the top side of the loop is absorbed in the newly created surface, leaving behind a half-loop. The red contours represent a GND density on the order of $10^9$ m$^{-2}$. 
Chapter 8

Polycrystalline Dynamic Failure

In this section, we investigate intergranular and transgranular failure in initially crack-free polycrystalline aluminum; the material properties used are as listed in Table 2.2. The major objective for this chapter is to investigate crack nucleation sites, and propagation paths at different strain-rates and for different grain sizes.

8.1 The Model

Two models were used, as shown in Fig. 8.1. The Euler angles for the grains are randomly assigned, but consistent with rolled aluminum plates (Polmear (2006b)) and with a minimum misorientation of 10° (i.e. low angle boundaries) between neighboring grains. The first model (Fig. 8.1 (a)) is an aggregate with 45 grains, and the second model (Fig. 8.1 (b)) is an aggregate with 287 grains. Both models are 5 mm × 5 mm, and are subjected to a nominal strain rate of 200/s, imparted by application of a constant velocity. To investigate strain rate effects, a nominal strain rate of 20/s is applied with the coarse grained aggregate.
8.2 Discussion of Results

8.2.1 Coarse Grains versus Fine Grains

Grain refinement significantly improves the tensile behavior of the polycrystal. From the stress-strain curves in Fig. 8.2, we see that the maximum tensile stress, $\sigma_{22}^{TS}$, at a strain rate of 200 s$^{-1}$ for the coarse grained aggregate is 271 MPa, at a nominal strain of 11.85%, and 292 MPa at a nominal strain of 15.75 % for the fine grained aggregate. The tensile toughness (the area underneath the curves) is 46% greater for the fine grained aggregate.

In Fig. 8.3, we compare crack paths of the coarse grained aggregate with the fine grained aggregate at the strain rate of 200 s$^{-1}$. For the coarse grained aggregate, there is one crack running across the failed model. For the fine grained aggregate, we see the emergence of secondary cracks (circled), which do not coalesce with the primary crack. Hence, for the fine grained aggregate, it is the competition among these different crack sites that retards the primary crack from growing to a catastrophic size, which enhances the polycrystal’s resistance to failure.

In Fig. 8.4, the accumulated plastic shear slip ($\gamma^p$) is shown as a surface plot; the darkest color corresponding to $\gamma^p = 1$ and the lightest to $\gamma^p = 0.05$. From Figs. 8.4 (a-b), we see that $\gamma^p$ strongly localizes on the crack faces, further indicating how ductility is controlling crack growth. For both coarse and fine grained aggregates, slip traces can be seen. These slip traces correspond to localization of plastic shear slip, and hence are
an indication of the generally non-uniform deformation of grains at this high strain rate. These slip traces are consistent with optical microscopy observations, (Fig. 8.5), for Al-2139. We can also see that the slip traces either originate at triple junctions and evolve into the grains, or remain localized near the grain boundaries (Fig. 8.4 (a)). This suggests indicates that ductile failure can originate from triple junctions or grain boundaries, and propagate along the slip traces into the grains. In fact, Fig. 8.6 compares in the coarse grains the accumulated plastic shear strains, $\gamma^p$ with incompatibility, $\delta_s$, which defines the failure.

The crack path evolution for both the coarse (Fig. 8.7) and fine grained aggregates are shown in Figs. 8.7-8.8. These two figures only show the grains in which the cracks grow, and the grains are colored for clarity. These figures indicate that crack nucleation occurs at different times near the triple junctions (circled), or at or near the grain boundaries (arrows), and that they subsequently grow in a predominantly transgranular mode, until they coalesce into a dominant crack that cuts along the different grains' slip traces, which is roughly inclined with the planes of maximum shear. Ductile failure, hence, initiates along intergranular sites, and then propagates transgranularly for these low angle aggregates. Furthermore, displacement incompatibilities ($\delta_s$) result in the nucleation of cracks at the triple junctions and grain boundaries. Our predictions for the fine grained aggregates indicate more crack nucleation occurs at the triple junctions as compared with the grain boundaries. This is due to larger incompatibilities associated with the meeting of three different lattice
orientations at a junction. As junctions become more interspersed in the microstructure with grain refinement, therefore, it becomes easier to originate a crack at the nearest triple junction, whose $\delta_s$ builds up more rapidly.

8.2.2 Distribution of State Variables

The contours for lattice rotation ($\psi'_{12}$) for coarse and fine grained aggregates are shown in Figs. 8.9 (a) and 8.10 (a). We see that lattice rotations attain their maximum values along the crack faces. This is because, as a crack propagates in ductile crystals, localized plastic shear slip is activated ahead of the crack tip, which magnifies lattice reorientation in neighboring regions as they follow the plastic flow. Fig. 8.9 (b) and Fig. 8.10 (b) show the work hardening ($\tau_{ref}$) normalized by Young’s modulus ($E$) for the coarse and fine grained aggregates. The work hardening localizes around the crack. $\tau_{ref}$ is proportional to the total immobile dislocation densities, cf. Fig. 8.9 (c) and Fig. 8.10 (c), which are responsible for the work hardening of the crystal (Eq. 2.2.5). Also as indicated from Fig. 8.6 (b) the accumulated plastic shear slip ($\gamma^p$) localizes near the crack, confirming the ductility of the crack propagation mechanism. Furthermore, associated with plastic work is an adiabatic temperature increase ($\Delta T$), also seen localized around the crack (Fig. 8.9 (d), Fig. 8.10 (d)). Hence, the field variables defining the crystalline solid’s state evolve around the ductile crack as expected, further confirming the viability of failure criterion $\delta_s$. We also note, by comparing Figs. 8.9 -
that the relevant plasticity variables evolve to substantially larger values in the fine grains than in the coarse grains, which is another indication that grain refinement enhances plastic processes in polycrystals, furthering their ductility.

### 8.2.3 Rate Effects on Coarse Grains

From the stress-strain curves in Fig. 8.2, we see that the maximum tensile strength $\sigma_{22}^{TS}$ for an applied strain rate of 20/s is 277 MPa, at a nominal strain of 13.4%. The toughness is thus 20% higher than that for an applied strain of 200/s.

The crack path for this strain rate is shown in Fig. 8.11. The extent of cracking at 20/s is significantly less than that at 200/s. At 20/s the grain outlined in yellow does not border an intergranular crack, and that outlined in blue has no transgranular crack. Moreover, the grain outlined in green deforms extensively, but remains intact. For an applied strain-rate of 200/s, this grain is seen to have completely failed. At the lower strain rate, the crack path is more curved, and mainly propagates along the grain boundaries (see the grains outlined in red). Hence, at this lower strain-rate, the dominant mode of propagation is intergranular. Furthermore, from the grain outlined in thick black (Fig. 8.11), we note that once the crack has cut across this grain and impinges on the boundary with the grain below it (outlined in green), it is arrested and blunted (see circled, Fig. 8.11). The arrest of the crack is what allows the grain outlined in green to deform much more extensively than what occurred at 200/s. The lower crack propagation velocity, associated with lower strain rates (see time labels in Fig.
8.11), and crack arrest allows for more plastic deformation to occur. In Fig. 8.12, a comparison between the accumulated plastic shear slip \((\gamma'')\) for both strain rates, confirms more plastic deformation ahead of the arrested crack at the lower nominal strain-rate. This contributes to the overall increase in ductility and toughness of the polycrystal as shown in Fig. 8.2, i.e. at the macroscopic level.

The state variables for the grains at 20/s are shown in Fig. 8.13. At an applied strain-rate of 20/s there is more lattice rotation, hardening, and (adiabatic) temperature rise in the grains, in comparison with the 200/s case. The increase is as a result of increased plastic deformation (Fig. 8.12). The dislocation densities, however, saturate to comparable values for both cases. The distribution of these state variables at 20/s is generally not as localized around the primary crack in comparison with the 200/s case, which indicates that failure of the polycrystal at lower strain rates is less susceptible to being dominated by a single propagating crack. Multiple crack sites can dissipate energy (cf. Fig. 8.11), which can retard the growth of the primary crack, improving the resistance of the polycrystals to failure at these lower strain-rates.

8.3 Conclusions

A new crack criterion, \(\delta_s\), based on displacement incompatibilities in crystalline solids, has been tested to model fracture in polycrystalline aggregates, at different strain-rates and for different grain sizes. The predictions from our models indicate
crack preferentially nucleate at the triple-junctions or grain boundaries in an intergranular mode, but propagate in a predominantly transgranular mode. Specifically, the ductile fracture path was found to follow the slip traces inside the grains. By varying grain sizes from coarse to fine, we predicted a general improvement in the tensile behavior and fracture resistance of the microstructure, which relates to the dissipation of more energy from competing crack sites, as the grains are refined. Moreover, at lower strain rates, the enhancement of tensile behavior of the coarse grained microstructure was predicted as a result of more plastic activity around the cracks, which permits for more energy dissipation through the process of propagating fracture across the microstructure.
8.4 Figures

(a) 45 Coarse Grains

(b) 287 Fine Grains

Figure 8.1: (a) Coarse grained polycrystalline model (b) Fine grained polycrystalline model
Figure 8.2: Stress-strain behavior for 45 grains at 20/s and 200/s, and for 287 grains at 200/s
Figure 8.3: Crack paths in ruptured coarse and fine grained models
Figure 8.4: Slip traces appearing in coarse and fine grained models
Figure 8.5: Optical microscopy image of 2139-T8 Al grains showing slip traces in grains around a micro-crack
Figure 8.6: Strong correlation between slip traces and incompatibility $\delta_s$
Figure 8.7: Crack path evolution in the coarse grained model
Figure 8.8: Crack path evolution in fine grained model
Figure 8.9: State variables in ruptured coarse grained model
Figure 8.10: State variables in ruptured fine grained model
Figure 8.11: Effect of strain rate on crack path and extent in the coarse grained model
Figure 8.12: Comparison of accumulated plastic shear slip at 20/s and 200/s for the coarse grained model

(a) 45 Grains, 20 s\(^{-1}\)

(b) 45 Grains, 200 s\(^{-1}\)
Figure 8.13: State variables for ruptured coarse grained model at 20/s
Chapter 9

Dynamic Failure and Microstructural Effects

In this chapter we investigate failure in a single aluminum matrix crystal containing dispersed particles and precipitates; the material properties used are as listed in Table 2.2. The objective of this chapter was to study the role of the different secondary phases in crack nucleation and propagation in the Al-Cu-Mg-Ag microstructure at a high strain rate. In particular we investigate the effect of these secondary phases on the tensile behavior (strength, strain-to-failure, toughness) and the dynamic damage tolerance of the microstructure, whether initially defect-free, or with an edge-crack.

9.1 The Model

The model size is 500 µm × 500 µm, as shown in Fig. 9.1. The Euler angles for matrix crystal are consistent with rolled aluminum plates (Polmear (2006b)). The model is subjected to a strain rate of 5000 s⁻¹. In these simulations, however, we do not retain the nano-sized dimensions of the Ω and θ' precipitates and Mn-bearing dispersed particles (dispersoids) found in 2139-Al (Elkhodary, et al. (2010b)); instead only their crystallographic properties and morphologies were taken into account to avoid a prohibitive computational cost. Hence, the Ω crystals were taken as 40 µm × 1 µm, θ' as
32 µm × 3 µm, and the Mn-bearing dispersoids as 44 µm × 22 µm, thus preserving their experimentally observed aspect ratios (Elkhodary, et al. (2010b)).

We begin by investigating four models. The first model corresponds to a single crystal with only Ω and θ’ precipitates at a ratio of 1:1, interspersed as a regular array throughout the matrix crystal (Fig. 9.1 (a)). Model 2 corresponds to a crystal with Mn-bearing dispersoids, also arranged in an array spanning the matrix (Fig. 9.1 (b)). Model 3 corresponds to a single crystal with precipitates and dispersed particles (Fig. 9.1 (c)). Model 4 is like model 3, but with a volume fraction of Mn-bearing dispersoids that has been reduced from 8% to 3.5%.

We also investigated failure in a single crystal with a pre-crack with different arrangements of dispersed particles and precipitates as shown in Fig. 9.2. Fig. 9.2 (a) corresponds to an array of Mn-bearing dispersoids and Fig. 9.2 (b) to an array of Ω and θ’ precipitates ahead of the crack tip. The crack is modeled as an essentially sharp line of discontinuity; the crack tip radius is zero, corresponding to a single node, and the crack surfaces subtend the tolerance angle of 0.002°. Moreover, to ensure its dominance, the pre-crack spans half the model’s width, as shown in the figure. Convergent meshes containing at least 12,500 elements were used for the models in Fig. 9.1, and 9,000 elements for the models in Fig. 9.2; the elements were four-noded quadrilaterals with reduced integration and relax-stiffness hourglass control.
9.2 Discussion of Results

9.2.1 Fracture with precipitates in the microstructure

The first result, Fig. 9.3, shows the stress-strain curves for the model with Ω and θ' precipitates (Fig. 9.1 (a)) and for the matrix only. The salient results from these curves are given in Table 9.1.

From Fig. 9.3 and Table 9.1, it is seen that precipitates enhance alloy strength by a significant percentage, without reducing the strain at failure. However, at least at the macroscopic level, the tensile toughness is seen not to be affected.

To further understand these interrelated effects at the microstructural scale, we compare state variable evolution for model 1 with that for the matrix only (Fig. 9.4 and Fig. 9.5 respectively). As seen from the figures, deformation is much more uniform in model 1, in comparison with the pure matrix, which can be seen by comparing the left edge of both models; when there are no precipitates, the matrix necks at the lower left corner. When we compare lattice rotations (ψ₁₂) between these two models (Fig. 9.4 (a) and Fig. 9.5 (a)), we see that the precipitates Ω and θ' rotate with opposite senses, resulting in a symmetric and homogenized deformation mode. We also see that the precipitates harden (τ_{ref}) at higher values in comparison with the pure matrix (Fig. 9.4 (b) and Fig. 9.5 (b)). Hardening occurs as a result of the evolution of the immobile dislocation densities (ρ_{im}^{tot}) summed over all the slip planes of the crystals (Eq. 2.2.5). As seen from Fig. 9.4 (c) and Fig. 9.5 (c), the immobile densities for model 1 are higher.
than for the pure matrix. The uniform precipitate distribution results in this uniform hardening, making an alloy with precipitates less susceptible to local deformation and necking, as reflected in the accumulated plastic shear slip ($\gamma^p$) contours (Fig. 9.4 (d) and 9.5 (d)). The maximum adiabatic temperature rise ($\Delta T$) (Figs. 9.4 (e) and 9.5 (e)) is significantly lower with precipitates in comparison with the pure matrix, which indicates that a microstructure with $\Omega$ and $\theta'$ is also significantly less susceptible to localized thermal softening.

From Fig. 9.3 and Table 9.1, however, we also see that $\Omega$ and $\theta'$ result in the rapid unloading of the stress-strain curve, which indicates reduced dynamic damage tolerance. Fig. 9.6 compares the accumulated plastic shear slip ($\gamma^p$) for the pure matrix and model 1 at the nominal strain of 25%. Without the presence of precipitates, the matrix deforms intensely around the advancing crack tip, which also allows for crack blunting, as can be seen in Fig. 9.6 (a). In contrast, for model 1, the precipitates inhibit the matrix from deforming as much by stiffening the overall microstructure, thus permitting less plastic deformation ahead of the crack tip for the dissipation of energy, which deteriorates the dynamic damage tolerance.

9.2.2 Fracture with the addition of Mn-bearing particles to the microstructure

The effects of adding Mn-bearing dispersoids to a microstructure (as outlined in Figs. 9.1 (b-d)) are summarized Table 9.2.
As seen from Fig. 9.7, the Mn-bearing dispersoids increase the strength of the alloy for all three cases. However, they have a negative effect on the maximum values for stress \(\sigma_{TS}^{22}\), strain \(e_{TS}^{75}\), and greatly decrease the tensile toughness, as seen in Table 9.2. The reason for the deterioration of the mechanical properties of the microstructure is the promotion of the void-sheet mechanism (Reed-Hill (1973), Rogers (1960)) by these coarse Mn-bearing dispersoids, which controls ductile failure. Fig. 9.8 shows the accumulated plastic shear slip \(\gamma^p\) contours for model 2. As we can see in Fig. 9.8 (a), Mn-bearing particles nucleate voids from their corners, labeled 1-3, within a band of localized shear (red). In Fig. 9.8 (b) we see the formation a void-sheet between these Mn-bearing dispersoids, as well as the nucleation of more voids, labeled 4-5, in another shear localization band. In Fig. 9.8 (c) we see the splitting of the void-sheets to form large cracks. Hence, it is clear that Mn-bearing particles drive this void-sheet mechanism, which evolves very rapidly in the microstructure, just over the span of 1 \(\mu s\), and thus reduces its tensile properties. Nonetheless, we can see from the slower stress unloading for models 2-4 (Fig. 9.7) that the dynamic damage tolerance of the microstructure is much improved with Mn-bearing particles, than with the precipitates \(\Omega\) and \(\theta'\) only. We will elaborate on this particular result presently, as we discuss the results of the pre-cracked models.

Now, to compare the three cases containing Mn-bearing particles we plot the primary state variables for each in Figs. 9.9 – 9.11. We see that adding Mn-bearing dispersoids to the microstructure with precipitates has not significantly affected the
overall uniformity of deformation, as can be judged from the straight left edges in Fig. 9.10 – 9.11. However, with the larger volume fractions of Mn-bearing dispersoids there are more crack nucleation sites, and the more easily the cracks coalesce into a dominant crack, which explains the deterioration in tensile behavior of the microstructure seen in the curves in Fig. 9.7. This result is consistent with experimental observation (Walsh, et al. (1989)).

Furthermore, for models 2 – 4 in Figs. 9.9 – 9.11, we see that the lattice rotations ($\psi_{12}^\nu$) attain their extreme values at the interfaces between the matrix and the Mn-bearing particles, thus dominating the lattice re-orientation of the matrix, the precipitates in models 3 and 4 being eclipsed. In Fig. 9.10 we see that bands of lattice rotations (green) link up due to the close proximity of the dispersoids, and that the cracks tend to follow these (green) lattice reorientation bands and link up.

We further see for models 2 – 4 (Figs. 9.9 – 9.11) that the work hardening parameter ($\tau_{reff}$) is much larger in the dispersoids than in the matrix, albeit not as large as the precipitates. This explains their contribution to the higher strength of the microstructure, as noted from the higher corresponding stress-strain curves in Fig. 9.7. Also, the immobile dislocation densities ($\rho_{im}^{tot}$), summed over all slip systems, and accumulated plastic shear slip ($\gamma^p$) inside the dispersoids (Figs. 9.9 – 9.11) do not evolve significantly during the simulation, which indicates that Mn-bearing crystals, unlike precipitates, are non-shearable. Instead, their failure occurs by pullout from the matrix along the shorter ends, as can be noted in Fig. 9.10 and Fig. 9.11. This result is
consistent with experimental observations for large Mn-bearing particles in aluminum alloys (Walsh, et al. (1989)). Moreover, the adiabatic temperature rise (ΔT) at the interface between the matrix and the Mn-bearing dispersoids for models 2 – 4 is significantly larger than at the interface with precipitates (cf. model 1), which indicates that dispersoids make the microstructure more susceptible to localized thermal softening.

Looking more closely at the deformed microstructure for model 3, Fig. 9.12, we can note the different deformation and failure modes of the precipitates and dispersoids. First, we predict plastic buckling of θ' precipitates. This phenomenon has been observed experimentally (Embry (1985)), as well as predicted in our earlier work (Elkhodary, et al. (2010a)), and relates to θ' accommodating the deformation of the adjacent matrix, while not being aligned with slip directions of the matrix. On the other hand, Ω, whose broad face is aligned with the (111)_{M} matrix slip plane, is seen to elongate. Examining the rational orientation of Ω with respect to the matrix crystal, we found that there are two active Ω slip systems, [001](110)_{Ω} and [111](110)_{Ω}, with plane normals coincident with the (111)_{M} matrix plane; therefore, slip for these systems is fully directed along the Ω broad face, which explains the predicted elongation. We note, however, that Ω precipitates in our models are much coarser than in actual aluminum alloys, where they are only a few unit cells thick (Knowles and Stobbs (1988)); hence,
this propensity for elongation would not be expected to leave the precipitates intact in real alloys.

We can also see from Fig. 9.12 (model 3) that precipitates deform heavily, when the adjacent matrix localizes, and are easily cut through by the crack. On the other hand, dispersed particles are not visibly deformed, and the crack does not cut through them, but instead works its way around them. It appears, therefore, that crack propagation resistance of microstructures is predominantly by virtue of the dispersoids. We explore this result further by running simulations for models 5 & 6, with the dominant pre-cracks, shown in Fig. 9.2. The resulting stress-strain curves are given in Fig. 9.13, and summarized in Table 9.3.

As seen from Fig. 9.13 and Table 9.3, Mn-bearing dispersoids have a much more favorable effect on all the mechanical behavior of the microstructure when there is a dominant pre-crack in the region. Clearly, no real alloy is free from flaws, and therefore, it is necessary to have a certain amount of dispersed particles in the microstructure to resist the propagation of pre-cracks, as it is evident that precipitates are incapable of resisting crack propagation, but actually seem to deteriorate the tensile behavior of the microstructure in the presence of the pre-crack (Table 9.3).

To understand this change in trend from the models without a pre-crack, Fig. 9.14 – 9.16 show the deformed pre-cracked models (i.e. the pre-cracked pure matrix and models 5 & 6) with their primary state variables. Our first prediction is that the crack paths are significantly different for the three pre-cracked models, reflecting different
propagation mechanisms. For the pure matrix case, Fig. 9.13, we see the crack grows along what is essentially the plane of maximum shear, and branches towards the end of the model; one branch arresting and blunting (the top one), and the other forming a void-sheet. For the case with Ω and θ' precipitates (model 5), Fig. 9.14, we see that the crack is initially deflected vertically, away from the zone with precipitates, due to the general increase in strength of the microstructure with the precipitates ahead of the crack tip. As the crack grows, it turns back in the direction of maximum shear, and cuts through the precipitates on its path. For the case of Mn-bearing dispersoids (model 6), however, the process is different. The single dispersoids ahead of the crack tip deflects the crack, making it grow vertically downward, where it is arrested, corresponding to the plateau in the stress-strain curve in Fig. 9.13. The arrested crack then resumes its growth along the direction of maximum shear, as expected with ductile cracks. As the crack grows, we see that it traces its path in between the dispersed particles; in fact, as the crack branches towards the end, it does so around a dispersed particle. From these predictions it follows that Mn-bearing particles are capable of deflecting cracks, while the precipitates Ω and θ' cannot.

Moreover, we predict a trend change in state variables as compared with the cases without a pre-crack (i.e. models 2 - 4). For Mn-bearing dispersoids (model 6, Fig. 9.16) the lattice rotations (ψ₁₂), work hardening (τ_ref), total immobile dislocation densities (ρ_total), accumulated plastic shear slip (γ′′) and adiabatic temperature rise (ΔT), are more spread out in the deforming matrix than in either model 5 (Fig. 9.15) or the pre-
cracked pure matrix (Fig. 9.14). In fact for model 5, with the $\Omega$ and $\theta'$ precipitates (Fig. 9.15), the state variables localize around the faces of the propagating crack. Hence, the Mn-bearing particles promote plastic processes in the microstructural regions with dominant pre-cracks, while precipitates localize plasticity in the vicinity of dominant pre-cracks, deteriorating the microstructure’s resistance to crack propagation.

9.3 Conclusions

We conclude from our simulations that precipitates have a positive effect on the tensile behavior of a microstructure in absence of initial cracks or flaws, promoting strength and toughness. Once a crack appears, however, their role becomes detrimental to the microstructure’s dynamic damage tolerance. On the other hand, dispersoids primarily contribute by promoting the dynamic damage tolerance, especially when a microstructure that has initial micro-cracks, by resisting crack propagation. Dispersoids, however, also nucleate cracks, reducing the tensile toughness of the alloy. They should therefore be in small volume fractions and well interspersed to minimize interactions that lead to void-sheet formation. Nonetheless, no alloy can be defect-free, especially in ballistic applications where damage is always expected in some regions of the microstructure, thus the combination of Mn-bearing particles to resist crack propagation with $\Omega$ and $\theta'$ precipitates to enhance strength and toughness is what is needed for optimal strength, toughness and dynamic damage tolerance.
### 9.4 Tables and Figures

**Table 9.1: Mechanical Properties for the Matrix and the Matrix with Ω and θ’.**

<table>
<thead>
<tr>
<th>Mechanical Property</th>
<th>Ω &amp; θ’ (Model 1)</th>
<th>Pure Matrix</th>
</tr>
</thead>
<tbody>
<tr>
<td>Maximum tensile strength, $\sigma_{TS}$ (MPa)</td>
<td>569</td>
<td>488</td>
</tr>
<tr>
<td>Corresponding nominal strain, $\varepsilon_{TS}$ (%)</td>
<td>22.8</td>
<td>22.8</td>
</tr>
<tr>
<td>Tensile Toughness (MJ/m$^3$)</td>
<td>59.8</td>
<td>~59</td>
</tr>
<tr>
<td>Dynamic Damage Tolerance</td>
<td>Very Poor</td>
<td>Very Good</td>
</tr>
</tbody>
</table>
Table 9.2: Mechanical Properties after addition of Mn-bearing dispersoids.

<table>
<thead>
<tr>
<th>Mechanical Property</th>
<th>7.7% Dispersoids (Model 2)</th>
<th>7.7% Dispersoids, 3.5% Ω &amp; θ' (Model 3)</th>
<th>3.5% Dispersoids, 3.5% Ω &amp; θ' (Model 4)</th>
</tr>
</thead>
<tbody>
<tr>
<td>σ_{TS} (MPa)</td>
<td>447</td>
<td>466</td>
<td>484</td>
</tr>
<tr>
<td>ε_{TS} (%)</td>
<td>15.9</td>
<td>11.9</td>
<td>14.4</td>
</tr>
<tr>
<td>Tensile Toughness (MJ/m³)</td>
<td>~37</td>
<td>29.592</td>
<td>38.470</td>
</tr>
<tr>
<td>Dynamic Damage Tolerance</td>
<td>Good</td>
<td>Poor</td>
<td>Very Good</td>
</tr>
</tbody>
</table>
Table 9.3: Mechanical Properties with a Dominant Pre-crack, models 5 & 6.

<table>
<thead>
<tr>
<th>Mechanical Property</th>
<th>Pure Matrix</th>
<th>Ω &amp; θ' (Model 5)</th>
<th>Dispersoids (Model 6)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sigma^{TS}$ (MPa)</td>
<td>196</td>
<td>192</td>
<td>239</td>
</tr>
<tr>
<td>$\varepsilon^{TS}$ ( % )</td>
<td>12.2</td>
<td>6.4</td>
<td>16.8</td>
</tr>
<tr>
<td>Tensile Toughness (MJ/m$^3$)</td>
<td>35.08</td>
<td>17.86</td>
<td>49.52</td>
</tr>
<tr>
<td>Dynamic Damage Tolerance</td>
<td>Good</td>
<td>Very poor</td>
<td>Very good</td>
</tr>
</tbody>
</table>
Figure 9.1: Four models of the microstructure, without a pre-crack. Light blue corresponds to coarse θ’ precipitates, light orange corresponds to coarse Ω precipitates brick-red corresponds to coarse Mn-bearing particles.
Figure 9.2: Two models of a pre-cracked microstructure. (a) with coarse Mn-bearing particles, (b) with $\Omega$ and $\theta'$ precipitates
Figure 9.3: Stress-strain comparison of pure matrix and matrix with $\Omega$ and $\theta'$.
Figure 9.4: State variables for pure matrix at the nominal strain of 22.8%
Model: (1) \((\Omega \text{ & } \theta' \text{ precipitates only})\)

Figure 9.5: State variables of microstructure with \(\Omega\) and \(\theta'\) precipitates at the nominal strain of 22.8%
Figure 9.6: Comparison of the accumulated plastic shear slip for the pure matrix and model 1 at 25%
Figure 9.7: Stress-strain behavior with coarse Mn-bearing particles in the microstructure
Figure 9.8: The void-sheet mechanism of ductile fracture, driven by Mn-bearing dispersed particles
Figure 9.9: State variables for ruptured microstructure with Mn-bearing particles only (model 2)
Figure 9.10: State variables for ruptured microstructure with 7.7% Mn-bearing particles and 3.5% Ω and θ’ precipitates (Model 3)
Figure 9.11: State variables for ruptured microstructure with 3.5% Mn-bearing particles and 3.5% Ω and θ’ precipitates (Model 4)
Figure 9.12: Ruptured microstructure for model 3, showing different deformation modes for the $\Omega$ and $\theta'$ precipitates, as well as un-deformed Mn-bearing particles.
Figure 9.13: Stress-strain behavior for models with an edge-crack
Figure 9.14: State variables for ruptured pure matrix with an edge crack
Figure 9.15: State variables for ruptured microstructure with $\Omega$ and $\theta'$ precipitates and an edge crack (model 5)
Model: (6) (Mn – dispersoids only)

Figure 9.16: Ruptured microstructure with Mn-bearing particles and an edge-crack (model 6)
Chapter 10

Recommendations for Future Research

1- Length scale effect on microstructural dynamic damage tolerance

Our results from Chapter 9 for $\Omega$ and $\theta'$ did not consider their nano-scale. In actual Al-Cu-Mg-Ag alloys, these precipitates are usually only a few unit cells thick. Following our analysis of Chapter 6, the spacing between the nano-precipitates is smaller than what the waves from the applied loads can resolve into, forcing the matrix to deform a multitude of precipitates in its attempt to localize, leading to an inhibition of shear localization. It would thus be very informative to investigate the effect of the nano-scaling of precipitates on crack propagation and alloy dynamic damage tolerance, seeing their particularly poor performance at the micron scale.

2- Boundary conditions

We have used in this dissertation a combination of different boundary conditions. We noticed that zooming on the microstructure as such small length scales, however, always introduces boundary effects that should not appear in most of the material bulk. It is thus preferable to devise a set of boundary
conditions that would not affect the modeled microstructure with reflections or dispersions, in other words, quiet boundaries. Many methods have been proposed for such an end, mostly introducing specialized elements at the boundaries. Our preliminary research, however, indicates the method of submodeling (Hibbitt, et al. (2007)) is the best candidate for our aims. The rate and amplitude at which waves pass through the model, and at which they are reflected can be well controlled to match realistic conditions. Moreover, the nature of the applied loads in a particular region of the material is that it is transferred from the surrounding material multi-axially. This multi-axial state of loading can be accurately captured by submodeling.

3- Contact surfaces with friction

Throughout chapters 7 – 9 we have investigated crack propagation under tensile loading. However, in ballistic applications, compressive loading is expected to dominate. In order to properly account for fracture paths under compression, it is necessary to account for the mutual impingement of the failed surfaces, which necessitates a contact algorithm that is alert to the generation of new surfaces anywhere in the microstructure. Our preliminary research indicates the use of the general contact algorithm (Hibbitt, et al. (2007)) with 3D brick elements in 3D plane-strain simulations offers promising results. Further research into the coupling of this general contact algorithm with descriptive friction models is
thus paramount for the modeling of extensive deformations and fracture in compression.

4- **Failure Surface Generation**

Our numerical simulations have made use of the *element removal* method to generate fracture surfaces. This method is very simple and versatile, however it poses severe limitations on the maximum resolution of a crack, thus requiring very fine meshes. Moreover, the large distortions involved with elements for ductile materials often lead to numerical instabilities, which are only aggravated by the sudden removal of the elements at the crack tip. Thus, a new surface generation method that does not rely on element removal should be pursued for the modeling of fracture in microstructures. Perhaps even more immediately, more research needs to be conducted on the *unloading* of elements, considering both the physical and numerical aspects of the matter.

5- **Microstructure homogenization based on slip incompatibility**

Our simulations have been performed using parallel methods (domain decomposition). In fact, as the time integration scheme is explicit for our dynamic models, these simulations are considered *embarrassingly parallel*. Nonetheless, the cost of running simulations of only a few micrometers of a microstructure, while using dozens of processors, can often be in terms of weeks of runtime. In particular, 3D simulations are rarely feasible. There is therefore
great need to employ some homogenization scheme, based on the findings of our
detailed models, to simulate models that are more consistent with actual
application length scales. As our findings indicate that *incompatibility of slip* in
between dissimilar crystals (based on our rational orientation scheme) is
responsible for most of the predicted strengthening and inhibition of
localization, it is recommended to pursue a homogenization scheme based on
this incompatibility.
References


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