Object Oriented CAE Software for the Exploration and Design of Microstructures

Stephen D. Sintay
Brigham Young University - Provo

Follow this and additional works at: https://scholarsarchive.byu.edu/etd

Part of the Mechanical Engineering Commons

BYU ScholarsArchive Citation
https://scholarsarchive.byu.edu/etd/711

This Thesis is brought to you for free and open access by BYU ScholarsArchive. It has been accepted for inclusion in All Theses and Dissertations by an authorized administrator of BYU ScholarsArchive. For more information, please contact scholarsarchive@byu.edu, ellen_amatangelo@byu.edu.
OBJECT ORIENTED CAE SOFTWARE FOR
THE EXPLORATION AND DESIGN
OF MICROSTRUCTURES

by

Stephen D. Sintay

A thesis submitted to the faculty of
Brigham Young University
in partial fulfillment of the requirements for the degree of

Master of Science

Department of Mechanical Engineering
Brigham Young University
December 2005
This thesis has been read by each member of the following graduate committee and by majority vote has been found to be satisfactory.

Date

Brent L. Adams, Chair

Date

C. Greg Jensen

Date

Alan R. Parkinson
As chair of the candidate’s graduate committee, I have read the thesis of Stephen D. Sintay in its final form and have found that (1) its format, citations, and bibliographical style are consistent and acceptable and fulfill university and department style requirements; (2) its illustrative materials including figures, tables, and charts are in place; and (3) the final manuscript is satisfactory to the graduate committee and is ready for submission to the university library.

Date

Brent L. Adams
Chair, Graduate Committee

Accepted for the Department

Matthew R. Jones
Graduate Coordinator

Accepted for the College

Alan R. Parkinson
Dean, Ira A. Fulton College of Engineering and Technology
ABSTRACT

OBJECT ORIENTED CAE SOFTWARE FOR
THE EXPLORATION AND DESIGN
OF MICROSTRUCTURES

Stephen D. Sintay
Department of Mechanical Engineering
Master of Science

Through the use of generalized spherical harmonic basis functions a spectral representation is used to model the microstructure of cubic materials. This model is then used to predict the macroscopic elastic and plastic properties of materials with cubic crystal symmetry and various sample symmetry including triclinic and axial–symmetric. Building on the work of Barnett and Asaro (1972) the influence that anisotropy has on the fatigue response of the material is also modeled. This is accomplished through using the effective elastic stiffness tensor in the computation of crack extension force $G$. The resulting material model and macroscopic property calculations are the foundation for a software package which provides an interface to the microstructure. The Microstructure Sensitive Design interface (MDSi) enables interaction with the material design process and provides tools needed to incorporate material parameters with traditional design, optimization, and analysis software. Therefore the microstructure model can be optimized concurrently with a geometric
model to further increase the overall design space. The software is then be used to explore how changes in the microstructure affect the performance of a turbine disc. The additional design space afforded by inclusion of the material parameters show that the total mass of the disk can be lowered by 9.5%. Additionally when the same geometry and loading conditions are considered and only the texture of the material is modified $G$ is reduced be more than an order of magnitude.
Contents

List of Tables xi

List of Figures xii

1 Introduction 1
1.1 Problem statement and why it is important 1
1.2 Survey of prior work 2
1.2.1 General materials design 2
1.2.2 Microstructure Sensitive Design (MSD) 4
1.3 Microstructure Sensitive Design interface (MSDi) 4

2 MSD Material Model 7
2.1 Spectral representation of texture 7
2.2 Overview of generalized spherical harmonic equations 8
2.3 Material parameters 10
2.4 Bounding the material parameters 10

3 Elastic Bounds 13
3.1 Series representation of elastic bounds 13

4 Scalable Anisotropic Yield Surface 17
4.1 Introduction 17
4.2 Rate sensitive Taylor yield model 17
4.2.1 Slip systems 17
4.2.2 Total strain rate 18
4.2.3 Polar representation of total strain rate 19
List of Tables

6.1 Key design variables used in finding the optimal design of a turbine disk in the first case study. There are 9 material parameters and 4 geometric parameters. ................................................................. 32

6.2 Key design functions and the associated objective or constraints of the first case study. Two minimization objectives for mass and crack extension force are formulated. ................................................................. 32

6.3 Design variables for the second case study. The number of applicable material parameters is variable based on the symmetry conditions imposed. The geometric parameters now represent the \((x, z)\) location of two key points that define the web of the disk. ................................................................. 33

6.4 Key design functions and the associated objective or constraints of the second case study. Two minimization objectives for mass and crack extension force are formulated. Case study two shows the addition of curvature constraints on the disk geometry. ................................................................. 33

7.1 The design variables listed comprise only the geometric parameters. The objective of this optimization is to minimize the mass. ................................................................. 38

7.2 Only the material parameters are used in the second simulation. The geometric parameters are held constant at the final value of the first simulation. The objective of this run is minimize the crack extension force \((G)\). ................................................................. 39

7.3 Common texture components found in cubic materials. These components result from known processing paths. ................................................................. 42
7.4 The common texture components listed in Table 7.3 are compared to the peak intensities of Figure 7.2 to identify what percent of the components are found in the designed texture.

7.5 The results of the third simulation are shown where both geometric and material parameters are used as design variables with the objective of minimizing the mass. The mass is reduced by 9.5%.

7.6 The starting and ending values of the design variables and analysis functions for the geometry only simulation of the second case study.

7.7 Only the material parameters are used in the second simulation of this case study. The geometric parameters are held constant at the final value of the first simulation. The objective of this run is $ming(G)$.

7.8 The common texture components listed in Table 7.3 are compared to the peak intensities of Figure 7.6 to identify what percent of the components are found in the designed texture.

7.9 Results for cubic axial–symmetric symmetry. Simulations 3 and 4 in the second case study start in different locations and find two local minima for $G$. 


# List of Figures

1.1 The integration of MSDi with traditional design and analysis software. In this way the material and geometry of a design can be optimized concurrently. ........................................... 5

2.1 The cubic orthorhombic microstructure hull for rank \( \ell = 4 \). For this symmetry and rank there are only 3 non-zero non-constant texture coefficients that allow the hull to be displayed in \( \mathbb{R}^3 \) ........................................... 11

4.1 Plot of Equation (4.20) in polar coordinates. The function is periodic with \( T = 2\pi \) ........................................... 21

5.1 A slit like crack is defined by a vector, \( \mathbf{n} \), that is normal to the crack surface and by a vector, \( \mathbf{t} \), that is perpendicular to \( \mathbf{n} \) and in the direction of the crack front. The crack plane then extends to infinity along the direction perpendicular to \( \mathbf{n} \) and \( \mathbf{t} \). ........................................... 27

6.1 Starting profile with displacement constraints and loads \( \omega \) and \( P \) ........................................... 29

6.2 Orthogonal view of the base section of disk used in analysis. A volume element is used to capture the anisotropic nature of the material. ........................................... 31

6.3 Unscaled gradients obtained from OptDesX using central difference derivatives and a step size of 0.01. ........................................... 33

6.4 Scaled gradients obtained from OptDesX using central difference derivative and a step size of 0.01. ........................................... 33
6.5 The parameters and analysis results are passed between the CAE software packages by the use of standard I/O. The optimization software writes the design variables to a file and then calls a shell script. The shell script then manages the execution order of MSDi and ANSYS. The results are then read by the optimization software to see if the objective has improved and or if the constraints were violated.

7.1 Optimal profile of the disk obtained by using only the geometric parameters. The material parameters represent an isotropic material.

7.2 The resulting material parameters represent the ODF above as defined in Equation (2.1). The sections are of constant angle $\phi_2$. The horizontal axis in each section is $\phi_1$ and the vertical axis is $\Phi$.

7.3 a) Equivalent stress distribution results from simulation 2. b) Equivalent stress distribution results from simulation 1. Modification of the material parameters appears to more evenly distribute the stress. This is most clearly seen in the highest contour region on the necked portion of the profile.

7.4 Optimal profile of the disk obtained by using the geometric parameters and the material parameters as design variables. The stress appears to be more evenly distributed across the profile.

7.5 Optimal profile of the disk obtained by using only the geometric parameters. The contours are of Von Mises eqv. stress.

7.6 A) The resulting ODF plot for the cubic triclinic material. Each section is a contour plot of intensity in Euler space. B) The resulting scale for the ODF plot C) a more precise analysis of the texture is possible by only looking at the peaks of the cubic triclinic ODF. D) the scale for the contours of the plot of peak intensities.

7.7 A) The (111) fiber texture B) The cube (001) fiber texture C) The resulting scale for the ODF plot.
Chapter 1

Introduction

1.1 Problem statement and why it is important

The set of available materials and their associated properties are fundamental to the design and manufacture methodology employed by mechanical engineers. Two limiting assumptions typically applied to this material set are that the material is homogeneous and it is isotropic. Even though these assumptions allow the engineer to continue with the design process they neglect the influence that microstructural features have on the overall performance of the engineering system. One cause of the performance variation in such a system is the anisotropic nature of individual grains and the distribution of these grains in the material. This meso-scale distribution directly affects the macroscopic material properties and therefore the performance of the system. Additionally the assumptions of isotropy and homogeneity artificially limit the overall design space. The ability to expand the design space and quantify variation in the system performance based on specific microstructure properties will provide the engineer with added control during the design process leading to improved system performance.

Microstructure Sensitive Design (MSD) (Adams, Lyon, and Henrie 2003) has the unique ability to explore all possible microstructures and therefore provide the engineer with the means to thoroughly examine and manipulate the material during the design stage. One factor limiting the incorporation of MSD into the current design methodology is that the designer can not easily manipulate the microstructure model and then see the affect of this change in the over all performance of the design. To
help the designer explore the microstructure there needs to be an interface with the material design process where accurate and efficient information can be transmitted. The designer can then use this information to explore a broader range of feasible design solutions.

When accurate information about the material is available the designer can utilize optimization techniques to explore the expanded design space provided by the incorporation of microstructure parameters. Finding an optimal material design requires specialized algorithms that are developed to efficiently explore the Fourier space (Lyon and Adams 2003). The power and flexibility of an optimization routine that incorporates MSD is the actual recovery of specific microstructures that are tailored for specific combinations of properties while exploring the entire set of microstructural possibilities.

In addition to the information and optimization tools provided in the MSD interface the designer will need to estimate the design performance based on the new material model. Many analysis packages will accept materials with anisotropic property combinations. However the form of the stiffness matrix utilized can vary between analysis packages. An interface can simplify and automate the interaction of the user with the analysis package to facilitate the overall design, optimization, and analysis process. The focus of this thesis is to define and develop a more general MSD interface (MSDi) through a set of programming tools that will allow the engineer to integrate the power of MSD with traditional optimization and analysis software. MSDi will then be implemented to explore the affect that texture will have on performance of a turbine disc.

1.2 Survey of prior work

1.2.1 General materials design

Chemistry, texture, and topology all have a significant influence on elastic plastic and fatigue properties of polycrystalline materials. Materials by design “Systems Theory” (Olson 2000) and Topology Optimization (Rozvany 2001) (Sigmund 1994) are two methods that the bring parameters of the material into the design space.
The majority of the work done in Topology Optimization is at the macroscopic level. Within this framework there is support for anisotropic materials (Rozvany 2001). The orientation of a unit cell of orthotropic material is included as a design variable (Cheng, Kikuchi, and Ma 1994). Tenek and Hagiwara (1993) optimize the material distribution within isotropic and anisotropic plates. Optimizing Extreme anisotropic properties such as a negative Poisson’s ratio can be obtained through the manipulation of material solid and void phases (Sigmund 1994). OptiStruct (Teresko 1994) is a commercial software package available for designing a material with Topology Optimization. OptiStruct allows the designer to optimize a 3D model based on several Topology design theories. Of these the most common and robust is SIMP. Tang and Chang (2001) showed that Topology Optimization can be integrated into traditional CAD based shape optimization using a geometric reconstruction technique to create solid models of the Topology Optimized structure in Solid Works.

At Northwestern University under the direction of Prof. G. Olson the Steel Research Group (SRG) was formed in 1985 with initial support from the National Science Foundation. The SRG is conducting material design experiments based on links between key microstructure systems (such as crystal grain sizes) and macroscopic properties (such as toughness and strength). It is this utilization of microstructure systems (also referred to as microstructure features) and their relation to macroscopic properties that gives "Systems Theory" its name. While many microstructure systems are considered in detail the approach remains stochastic. There is not an encompassing definition of the microstructure which is then extended to predict macroscopic properties. Rather "reciprocity" is used to associate macroscopic properties to microstructure features (Olson 1997). When available, models are used to help determine the desired microstructure features, but a description of the microstructure is not a goal of the "Systems Theory" material design process. The reciprocal system-property models are linked to material processing models wherein processing paths can be defined (Olson 1997). This link is loosely formed in that there is not an attempt to bridge the differences between models and length scales in the models. The contribution of grain orientation as a microstructure feature and its anisotropic
influence on macroscopic material properties is not considered. The theory focuses only on isotropic material response.

1.2.2 Microstructure Sensitive Design (MSD)

MSD incorporates macroscopic properties and microstructure description in a single spectral representation (Adams et al. 2002). It allows the design engineer to dictate required macroscopic properties and returns real microstructures that satisfy those requirements. One point statistical theory has been established to represent the upper and lower bounds of the elastic stiffness and compliance matrices (Henrie 2002). In addition recent work has been completed to include yield strength and nonlinear combinations of the elastic properties into other material parameters such as stress concentration factor (Lyon and Adams 2003). The theoretical foundation for Microstructure design and optimization has been explored for a compliant beam (Adams et al. 2001). Furthermore the construction of isoproperty hyper-surfaces has been established (Adams et al. 2003). As a test bed for new theory the calculation of a circular hole in an orthotropic axially loaded plate is performed using the MSD theory (Kalidindi et al. 2003) and (Lyon 2003). Kalidindi and Schoenfeld (2000) use the Taylor model and the spectral representation of the microstructure to formulate an estimate of the yield surface in FCC polycrystals. The evolution of microstructures in polycrystals can also be treated under the framework of MSD (Adams et al. 2001) and (Schoenfeld et al. 2003). Lyon (2003) incorporated the MSD model in the design of a compliant bicycle derailleurs.

1.3 Microstructure Sensitive Design interface (MSDi)

The real power of MSDi is its support for the single point statistical representation of the texture in single phase FCC materials. Through its object oriented nature it can be adapted to integrate higher order statistical models as the theory becomes more established. MSDi is able to support all processing symmetries from
triclinic to axisymmetric and unlimited rank\(^1\) although a max of \(\ell = 15\) is a reason-
able computational limit. At the core of the representation is the generalized spherical
harmonic equations (Bunge 1993) and dynamic allocation of supporting variables.

The integration of the spectral representation of the microstructure into the
design space will be accomplished through the coupling of MSDi with ANSYS and
iSIGHT. Figure 1.1 Shows the basic flow of information between the software ele-
ments. The integration accomplished via simple file I/O. Both ANSYS and MDSi are
able to read the same input file and modify the same output file.

---

\(^1\)Rank as referred to in the literature (Bunge 1993) is the maximum value of \(\ell\) in the spectral representation of the microstructure.
MSD Material Model

2.1 Spectral representation of texture

MSD is formulated to represent many local states of the microstructure [Adams et al. 2002]. These include, but are not limited to phase, composition, crystal lattice orientation, and grain size. Only orientation is considered as a local state in the development of MSDi. The other microstructure features are not supported. Through homogenization relationships the local state distribution function is related to the macroscopic properties of elasticity and plasticity [Bunge 1993] and [Adams and Olsen 1998]. A closure on the macroscopic properties can be calculated through a combination of bounds on all possible microstructures [Adams et al. 2003]. The treatment that follows is the implementation of the spectral representation of the microstructure in MDSi.

The following review of the spectral representation of the microstructure is taken from [Bunge 1993], and it provides a solid foundation for the development of the macroscopic properties in the following chapters. A polycrystalline microstructure can be represented with a Fourier series through the expansion of the Orientation Distribution Function (ODF). The ODF, $f(g)$, is expanded through the use of the generalized spherical harmonic basis functions where

$$f(g) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{+\ell} \sum_{n=-\ell}^{+\ell} F_{\ell}^{mn} T_{\ell}^{mn}(g),$$

(2.1)

and the orientation $g$ is defined as a set of Euler angles such that

$$g = \{\phi_1, \Phi, \phi_2\}.$$  

(2.2)
Integration of the orientation distribution function over all orientations is normalized such that
\[ \oint f(g)dg = 1, \quad (2.3) \]
where \( \oint \) represents the integration over Equation (2.3) in the space \( SO(3)/G \) and \( dg \) is the invariant measure \( \sin(\Phi)d\phi_1d\Phi d\phi_2 \).

The symmetries associated with the cubic crystal lattice and those symmetries created through processing techniques can be imposed on the mathematics via the harmonic function. Two columns of dots over the generalized spherical harmonic function \( T_{\ell}^{\mu\nu}(g) \) represent the specific symmetry imposed on the ODF. The right column indicates the processing symmetry and the left indicates the sample symmetry. For a cubic sample symmetry and low processing symmetry we have \( \cdot\cdot\cdot T_{\ell}^{\mu\nu}(g) \), and for cubic sample symmetry and high processing symmetry such as orthorhombic we have \( \cdot\cdot\cdot\cdot T_{\ell}^{\mu\nu}(g) \). The symmetry is further reflected in the \( m \) and \( n \) indices. The symmetric indices are changed to \( \mu \) and \( \nu \) respectively, where \( \mu \) is associated with sample symmetry and \( \nu \) is associated with processing symmetry. With the inclusion of symmetry Equation (2.1) can be rewritten where
\[ f(g) = \sum_{\ell=0}^{\infty} \sum_{\mu=1}^{M(\ell)} \sum_{\nu=1}^{N(\ell)} F_{\ell}^{\mu\nu} \cdot\cdot T_{\ell}^{\mu\nu}(g). \quad (2.4) \]
The upper limit to \( \mu \) and \( \nu \) are now functions of \( \ell \). The functions \( M(\ell) \) and \( N(\ell) \) are themselves dependent upon the symmetry conditions and are found in Figures 4.4 and 14.1 of Bunge (1993). For a finite representation of the ODF the upper value limit of \( \ell \) is chosen to be finite. It has been found that \( \ell = 4 \) is sufficient for the computation of the elastic problem and that \( \ell = 10 \) is sufficient for plasticity.

### 2.2 Overview of generalized spherical harmonic equations

The ability to represent all symmetry combinations is essential to solve the general class of design problems encountered by materials scientists and engineers. MSDi accounts for each symmetry condition and arbitrary rank \( \ell \) through an adaptation of the “CTexCalcGSHE” programming class found in the source code of the
Orientation Imaging Microscopy (OIM) software (Adams, Wright, and Kunze 1993). The actual method used to calculate the harmonic functions is different for each symmetry condition. This introduces and additional complication that must be accounted for during implementation. In OIM the functions are implemented by using \( \ell, \mu, \) and \( \nu \) as indices for all symmetric and non-symmetric functions. By adapting this convention continuity and simplicity are maintained throughout the code. This continuity comes with a cost as an ambiguity is introduced for functions which do not have both sample and processing symmetry imposed. This is the case for the Cubic Triclinic harmonic functions where by definition Triclinic is non-symmetric and the \( \nu \) index should not be used. This ambiguity is clarified in Figures 4.4 and 14.1 of Bunge (1993), where the \( M(\ell) \) and \( N(\ell) \) for the symmetric indices \( \mu \) and \( \nu \) are outlined for all cases including Triclinic. The change from \( n \) to \( \nu \) or from \( m \) to \( \mu \) for the Triclinic case is not imposition symmetry but rather an index substitution.

This work focuses on Cubic Triclinic materials where the harmonic functions are represented using \( \hat{T}_{\ell \mu \nu}^{\mu \nu}(g) \) as opposed to \( \hat{T}_{\ell \mu n}^{\mu n}(g) \). This reflects the actual implementation of the harmonic functions in MSDi.

The harmonic functions are orthogonal and when integrated over all orientations produce the following

\[
\oint \hat{T}_{\ell \mu \nu}^{\mu \nu}(g) \hat{T}_{\ell' \mu' \nu'}^{\mu' \nu'}(g) dg = \frac{1}{2\ell + 1} \delta_{\ell \ell'} \delta_{\mu \mu'} \delta_{\nu \nu'} \tag{2.5}
\]

Where * represents the complex conjugate. This property is utilized to calculate the \( F_{\ell \mu \nu} \) coefficients in Equation (2.4). They are calculated by the standard method where each side of the equation is multiplied by the complex conjugate of the basis functions and integrated over all \( g \) such that

\[
\oint f(g) \hat{T}_{\ell \mu \nu}^{\mu \nu}(g) dg = \sum_{\ell'=0}^{\infty} \sum_{\mu'=1}^{M(\ell')} \sum_{\nu'=1}^{N(\ell')} F_{\ell \mu \nu}^{\mu' \nu'} \oint \hat{T}_{\ell' \mu' \nu'}^{\mu' \nu'}(g) \hat{T}_{\ell \mu \nu}^{\mu \nu}(g) dg. \tag{2.6}
\]

Utilizing the orthogonal property of (2.5) we have

\[
F_{\ell \mu \nu} = (2\ell + 1) \oint f(g) \hat{T}_{\ell \mu \nu}^{\mu \nu}(g) dg \tag{2.7}
\]
2.3 Material parameters

The $F_{\ell}^{\mu\nu}$ texture coefficients of Equation (2.4) represent the parameters of the material. For a material that contains many orientations the coefficients can be calculated as a linear sum of the individual orientations. Consider an ODF that is only different from zero at a single orientation $g = g_0$. Apply this to Equation (2.7) and what follows is

$$F_{\ell}^{\mu\nu} = (2\ell + 1)\hat{T}_{\ell}^{\mu\nu}(g_0) \int f(g)dg$$

(2.8)

Then by using Equation (2.3) we can simplify the form such that

$$F_{\ell}^{\mu\nu} = (2\ell + 1)\hat{T}_{\ell}^{\mu\nu}(g_0).$$

(2.9)

If the ODF is obtained as a list of crystal orientations as is the case with an OIM scan then the resulting coefficients of the polycrystalline material are obtained by summing Equation $G$ and $\Delta\hat{W}$ (2.9) for all $g_i$ in the list and normalizing by the total number of points $N$ such that.

$$F_{\ell}^{\mu\nu} = (2\ell + 1)\sum_{i}^{N}\hat{T}_{\ell}^{\mu\nu}(g_i).$$

(2.10)

It is clear that in a crystalline material the $F_{\ell}^{\mu\nu}$ coefficients represent a measure of the texture. In a design environment where the texture is not known but modified to meet the needs of the application these coefficients become the parameters of the material. They are modified within the constraints imposed to improve the material properties. As will be shown in the following sections the estimated elastic, plastic and crack interaction energy are functions of these coefficients.

2.4 Bounding the material parameters

The microstructure Hull as defined by Adams et al. (2001) is all possible ODFs. In certain circumstance it can be plotted in $\mathbb{R}^3$. This is the case when the elastic response of a cubic orthorhombic material is considered. Only the first three non-constant material parameters influence elasticity. A plot of the Hull is show in Figure 2.1 One important aspect of the Hull is that it is convex in all dimensions.
All points in the Hull are represented by both single crystal or polycrystalline microstructures. The are a few locations which are only represented by polycrystals and others only represented by single crystals (Lyon 2003).

Figure 2.1: The cubic orthorhombic microstructure hull for rank $\ell = 4$. For this symmetry and rank there are only 3 non-zero non-constant texture coefficients that allow the hull to be displayed in $R^3$.

Only material parameters that reside on or within the surface of the hull are real. The bounding of the material parameters is accomplished through a specialized Gram-Schmidt orthonormalization algorithm developed by Lyon and Adams (2003). In the form adapted for MDSi the algorithm takes as input the material parameters and then determines if the material is feasible or not. The algorithm is dynamic in that it can bound an $R^n$ space and has been utilized to optimize a texture in $R^{18}$ space by Lyon (2003).
Essentially there are two steps required for implementation of the algorithm. The first step is to identify the set of single crystal points that are on the surface of the hull when considering all possible points in the hull. This is done by providing the algorithm with set of individual orientations that have been expanded into the Fourier space through (2.9). Individual orientations are chosen to span the entire space. The algorithm then takes these points and determines the set that are on the surface of the hull. The graph in Figure 2.1 is the result of such a search. The algorithm can then take as input any point in the space and return $S$. Where $S$ is defined as the distance from the point to the surface of the hull. If the point is outside the Hull then $S < 0$. If the point is on or inside the surface of the Hull then $S \geq 0$. Any point inside or on the surface of the hull is a valid real texture. This material constraint can then be defined as

$$S \geq 0.$$ (2.11)
Chapter 3

Elastic Bounds

The MSD implementation of homogenization relationships to provide an estimate for anisotropic elasticity in polycrystalline materials has been demonstrated by Henrie (2002) and Lyon (2003). MSDi builds on this foundation to provide estimates for the elastic Stiffness and Compliance tensors and in turn the upper and lower bounds of elasticity. For continuity and as a review of the fundamental principles involved the elastic bounds and the Fourier representation of them are presented again here.

The stiffness tensor implemented is in the form of generalized Hooke’s law.

\[ \sigma_{ij} = C_{ijkl} \varepsilon_{kl} \] (3.1)

where \( C_{ijkl} \) is the elastic stiffness tensor and relates stress to strain. The elastic compliance tensor is found through inversion of the stiffness tensor and also relates stress and strain where

\[ \varepsilon_{ij} = S_{ijkl} \sigma_{kl} \] (3.2)

When statistical homogenization of the microstructure is considered the effective elastic and compliance tensors can be found to relate the volume averages \( \langle \rangle \) of stress and strain such that

\[ \langle \sigma_{ij} \rangle = C_{ijkl}^* \langle \varepsilon_{kl} \rangle \] (3.3)

and

\[ \langle \varepsilon_{ij} \rangle = S_{ijkl}^* \langle \sigma_{kl} \rangle \] (3.4)

The Hill-Paul bounds for elasticity have been incorporated and utilized in one point MSD (Adams, Lyon, and Henrie 2003) and (Henrie 2002). The Hill-Paul formulation
shows that the Voigt (1928) and Reuss (1929) averages are an upper and lower bound on diagonal terms of the effective stiffness tensor of a polycrystal. Using the principles of minimum potential energy and minimum complementary energy the following bound of the diagonal elements of the effective stiffness tensor can be formed.

\[
\langle \varepsilon_{ij} \rangle \langle S \rangle^{-1}_{ijkl} \langle \sigma_{kl} \rangle \leq C^*_{ijkl} \leq \langle \varepsilon_{ij} \rangle \langle C_{ijkl} \rangle \langle \sigma_{kl} \rangle,
\]

and for the effective compliance tensor

\[
\langle \varepsilon_{ij} \rangle \langle C \rangle^{-1}_{ijkl} \langle \sigma_{kl} \rangle \leq S^*_{ijkl} \leq \langle \varepsilon_{ij} \rangle \langle S_{ijkl} \rangle \langle \sigma_{kl} \rangle
\]

A bound on the off diagonal elements can also be formulated but this bound is degraded in that they are dependent upon the bounds of the diagonal terms. MSDi provides an estimate for the elastic stiffness tensor that is ensured to be within the Hill-Paul bounds.

### 3.1 Series representation of elastic bounds

The \( \langle C_{ijkl} \rangle \) and \( \langle S_{ijkl} \rangle \) terms can be formulated as functions of the texture of the material. The development of the stiffness and compliance tensors is identical. Only the stiffness tensor will be carried further. The inner product of the ODF and orientation dependent stiffness tensor is integrated over all orientations such that

\[
\langle C_{ijkl} \rangle = \int f(g) C_{ijkl}(g) dg
\]

This is in essence texture weighted average of the elastic stiffness tensor rotated from the crystal from into the sample frame. In the crystal coordinate system the elastic stiffness tensor is a function of the material constants \( C_{11}^0, C_{12}^0, \) and \( C_{44}^0 \) (Hirth and Lothe 1968). Are simple rotations of the single crystal elastic tensor

\[
C_{ijkm} = g_{in} g_{jo} g_{kp} g_{mq} C_{nopq}
\]

and can for cubic materials can be represented in a reduced form

\[
C_{ijkm} = C_{12}^0 \delta_{ij} \delta_{km} + C_{44}^0 \left[ \delta_{ik} \delta_{jm} + \delta_{im} \delta_{jk} \right] + \left[ C_{11}^0 - C_{12}^0 - 2C_{44}^0 \right] g_{ri} g_{rj} g_{rk} g_{rm}.
\]
The function $C_{ijkl}(g)$ can be expanded using the generalized spherical harmonic equations similar to Equation (2.4) where

$$C_{ijkl}(g) = \sum_{\ell=0}^{\infty} \sum_{\mu=1}^{M(\ell)} \sum_{\nu=1}^{N(\ell)} C_{\ell(ijkl)}^{\mu\nu} \hat{T}_{\ell}^{\mu\nu}(g). \quad (3.10)$$

The coefficients $C_{\ell(ijkl)}^{\mu\nu}$ can be computed in the same way as Equation (2.7) yielding

$$C_{\ell(ijkl)}^{\mu\nu} = (2\ell + 1) \oint C_{ijkl}(g) \hat{T}^{\mu\nu}_{\ell}(g) dg \quad (3.11)$$

An estimation for Equation (3.7) can then be made through the inner product of Equation (2.4) and the conjugate of Equation (3.10) where

$$\langle C_{ijkl} \rangle = \oint f(g) C_{ijkl}^*(g) dg \quad (3.12)$$

or

$$\langle C_{ijkl} \rangle = \sum_{\ell=0}^{\infty} \sum_{\mu=1}^{M(\ell)} \sum_{\nu=1}^{N(\ell)} F_{\ell}^{\mu\nu} C_{\ell(ijkl)}^{\mu\nu} \oint \hat{T}^{\mu\nu}_{\ell}(g) \hat{T}^{\mu\nu}_{\ell'}(g) dg. \quad (3.13)$$

By using the property or orthogonality in Equation (2.5) we finally have

$$\langle C_{ijkl} \rangle = \frac{1}{2\ell + 1} \sum_{\ell=0}^{\infty} \sum_{\mu=1}^{M(\ell)} \sum_{\nu=1}^{N(\ell)} F_{\ell}^{\mu\nu} C_{\ell(ijkl)}^{\mu\nu}. \quad (3.14)$$

Here it is clear that the elastic properties of the material are influenced by the texture coefficients Equation (2.10), and that the texture coefficients are efficient material parameters. For a material that has cubic-orthorhombic symmetry the only the first three non-constant coefficients are found to have an influence on Equation (3.14). For cubic triclinic only the first nine non-constant terms will have an influence.
Chapter 4

Scalable Anisotropic Yield Surface

4.1 Introduction

The purpose of this formulation is to determine the yield criteria for an anisotropic polycrystalline material under any loading condition. The method is based on rate sensitive Taylor theory and utilizes the spectral representation of the microstructure as defined by Bunge (1993). The yield condition is defined in terms of an observable rate of plastic working. The observable rate of plastic working for a material can be determined experimentally or estimated from existing material data. This parameter defines the energy dissipation required for yielding. Through the use of a single scaling parameter the applied stress and strain rate can be modified.

4.2 Rate sensitive Taylor yield model

The yield phenomena in polycrystalline materials can be described with the rate sensitive Taylor model. This model assumes that every part of the material experiences the same strain and strain rate. Rate sensitivity as presented in the text is a power law equation with parameter $n$.

4.2.1 Slip systems

Consideration must be given to each slip system, $s$, of the single crystal. A geometric tensor

$$
\mu_{ij}^{(s)c} = \left( b_i^{(s)} n_j^{(s)} + b_j^{(s)} n_i^{(s)} \right)
$$

(4.1)
is formed to characterize these systems. The slip planes are identified by unit vectors $\hat{n}^{(s)}$ normal to the plane. The vector $\hat{b}^{(s)}$ is a unit vector in the direction of slip. Equation (4.1) is in the crystal reference frame, $\hat{e}^c_i$, and can be transformed into the macroscopic frame, $\hat{e}_i$ using direction cosines, $g_{rs}$, such that

$$
\mu^{(s)}_{ij} = g_{mi} g_{nj} \mu_{mn}^{(s)c},
$$

where

$$
g_{rs} = \hat{e}^c_r \cdot \hat{e}_s.
$$

The resolved shear stress $\tau_{RSS}^{(s)}$ acting on the slip system for a given stress state can also be expressed using Equation (4.1)

$$
\tau_{RSS}^{(s)} = \sigma_{ij} \mu^{(s)}_{ij}.
$$

Let $\dot{\gamma}^{(s)}$ denote the shear strain rate of the single crystal for slip system $s$. A power law relationship between the resolved shear stress and the strain rate is used where

$$
\frac{\dot{\gamma}^{(s)}}{\dot{\gamma}_0} = \left| \frac{\tau_{RSS}^{(s)}}{\tau_0} \right|^n \text{sign}(\tau_{RSS}^{(s)}).
$$

The reference variables $\dot{\gamma}_0$ and $\tau_0$ are predetermined material properties. They can be used to calibrate the model with the existing material data.

### 4.2.2 Total strain rate

The total strain rate of the single crystal is defined as the sum over the slip systems and can be written as

$$
\dot{\varepsilon}_{ij} = \sum_s \dot{\gamma}^{(s)} \mu^{(s)}_{ij}.
$$

Through substitution of Equation (4.5) into (4.6) we have

$$
\dot{\varepsilon}_{ij} = \sum_s \dot{\gamma}^{(s)} \left| \frac{\tau_{RSS}^{(s)}}{\tau_0} \right|^n \text{sign}(\tau_{RSS}^{(s)}) \mu^{(s)}_{ij}.
$$

Further substitution of Equation (4.4) into (4.7) yields

$$
\dot{\varepsilon}_{ij} = \sum_s \dot{\gamma}^{(s)} \left| \frac{\sigma_{ij} \mu^{(s)}_{ij}}{\tau_0} \right|^n \text{sign}(\sigma_{ij} \mu^{(s)}_{ij}) \mu^{(s)}_{ij}.
$$
Hutchinson (1976) formulates the total strain rate as the product of the tensor of creep compliances, $M^c$ and the stress tensor such that

$$\dot{\varepsilon}_{ij} = M^c_{ijpq} \sigma_{pq},$$  \hspace{1cm} (4.9)

where

$$M^c_{ijpq} = \sum_s \left( \alpha / \tau_0^{(s)} \right) \left| \frac{\sigma_{pq} \mu^{(s)}_{pq}}{\tau_0^{(s)}} \right|^{n-1} \mu^{(s)}_{ij} \mu^{(s)}_{pq}. \hspace{1cm} (4.10)$$

In this formulation he introduces an iterative numerical method to solve for $\sigma$ with a prescribed $\dot{\varepsilon}$. When $n = 1$ the Equation (4.10) can be solved directly for $\sigma_{ij}$. This is the starting point for the numerical solution. This value of $\sigma_{ij}$ is then used to calculate the value of $\Delta \sigma$ where

$$\Delta \sigma = \left( M^{c-1} \dot{\varepsilon} - \sigma \right). \hspace{1cm} (4.11)$$

As the material is incompressible $M^c$ is singular and can not be inverted. Hutchinson suggests working the problem in an alternate form through the conversion of $\sigma$ and $\dot{\varepsilon}$ into the Cauchy stress space with 5-component vectors. In this frame Equation (4.11) can be computed and the stress vector is then updated with the addition of $\Delta \sigma$. This is repeated as $n$ is incremented by 1/10 until the stopping point of $n = 10$ is reached. The result can easily be checked by calculating Equation (4.9) with the resultant value of $\sigma$. The implementation currently used in MSDi iterates to the value of $n = 10$. This is found to be sufficient. As $n = 10$ the rate sensitive model approaches that or rate insensitivity.

### 4.2.3 Polar representation of total strain rate

The total strain rate of the single crystal, $\dot{\varepsilon}$, is a second rank symmetric tensor; and therefore has six independent components. It will be shown at the end of this section that it is convenient to discretize the strain rate space that spans these six independent variables. This is most directly accomplished through the polar representation of $\dot{\varepsilon}$.

We define $\dot{\varepsilon}$ in terms of a unit strain direction, $\hat{\varepsilon}$, and a scaling parameter, $\eta$, such that

$$\dot{\varepsilon} = \eta \hat{\varepsilon}. \hspace{1cm} (4.12)$$
Where
\[ \eta = \| \dot{\varepsilon} \| = \sqrt{\dot{\varepsilon}_{ij}\dot{\varepsilon}_{ij}} \]  \hspace{1cm} (4.13)

In the frame of principal directions the strain rate, \( \dot{\varepsilon}^p \), can be represented with eigenvalues along its diagonal such that
\[ \dot{\varepsilon}^p = \eta \begin{bmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & c \end{bmatrix}. \]  \hspace{1cm} (4.14)

The selection of \( a, b, c \) and \( \eta \) determine the direction and magnitude of the strain rate imposed. We will reduce the number of independent variables from six to five by requiring volume conservation in plasticity. This constraint is imposed in Equation (4.15) where the first scalar invariant of \( \dot{\varepsilon} \) is constrained to be zero. We can reduce the independent variables further in the second scalar invariant where we require \( |\dot{\varepsilon}| = 1 \). These operations yield
\[ \dot{\varepsilon}_{ii} = 0, \]  \hspace{1cm} (4.15)

or
\[ (a + b + c) = 0 \]  \hspace{1cm} (4.16)

and
\[ \sqrt{\dot{\varepsilon}_{ij}\dot{\varepsilon}_{ij}} = 1. \]  \hspace{1cm} (4.17)

By Solving Equation (4.16) for \( c \) and substituting back into Equation (4.14) we have
\[ \dot{\varepsilon}^p = \eta \begin{bmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & -(a + b) \end{bmatrix}. \]  \hspace{1cm} (4.18)

Expansion of Equation (4.17) then yields
\[ \sqrt{2a^2 + 2b^2 + 2ab} = 1. \]  \hspace{1cm} (4.19)

Equation (4.19) is then expressed in polar coordinates where \( a = r \cos \theta \) and \( b = r \sin \theta \) we can then solve this equation for \( r \) such that
\[ r = \frac{1}{\sqrt{2 + \sin 2\theta}}. \]  \hspace{1cm} (4.20)
Substitute Equation (4.20) and the polar expressions for $a$ and $b$ into Equation (4.18) which becomes

\[
\dot{\varepsilon}^p(\theta) = \eta \begin{bmatrix}
\frac{\cos(\theta)}{\sqrt{2+\sin(2\theta)}} & 0 & 0 \\
0 & \frac{-\sin(\theta)\sqrt{2+\sin(2\theta)}}{\sqrt{2+\sin(2\theta)}} & 0 \\
0 & 0 & -\left(\frac{\cos(\theta)}{\sqrt{2+\sin(2\theta)}} + \frac{\sin(\theta)}{\sqrt{2+\sin(2\theta)}}\right)
\end{bmatrix}.
\]

(4.21)

Figure 4.1 is a plot in polar coordinates of Equation (4.20). The function is periodic with $T = 2\pi$. Through this formulation the representation of the strain mode in the principal directions is reduced to a single angular variable $\theta$ that has a domain $0 \leq \theta < 2\pi$. Van Houtte (1994) uses a similar representation which exhibits the same properties as listed in Equation (4.15) and (4.17).

Figure 4.1: Plot of Equation (4.20) in polar coordinates. The function is periodic with $T = 2\pi$

As $\dot{\varepsilon}^p$ is defined in the frame of principal directions we will apply a rotation to it such that all possible strain modes that satisfy the imposed constraints can be
The rotation operation on $\dot{\varepsilon}^p$ is defined as

\[
\begin{align*}
t_{11} & = \cos(\beta_1) \cos(\beta_3) - \sin(\beta_1) \sin(\beta_3) \cos(\beta_2), \\
t_{12} & = \sin(\beta_1) \cos(\beta_3) + \cos(\beta_1) \sin(\beta_3) \cos(\beta_2), \\
t_{13} & = \sin(\beta_3) \sin(\beta_2), \\
t_{21} & = -\cos(\beta_1) \sin(\beta_3) - \sin(\beta_3) \cos(\beta_2), \\
t_{22} & = -\sin(\beta_1) \sin(\beta_3) + \cos(\beta_1) \cos(\beta_3) \cos(\beta_2), \\
t_{23} & = \cos(\beta_3) \sin(\beta_2), \\
t_{31} & = \sin(\beta_1) \sin(\beta_2), \\
t_{32} & = -\cos(\beta_1) \sin(\beta_2), \\
t_{33} & = \cos(\beta_2).
\end{align*}
\]

This is similar to Equation (4.2) where $g$ is used as the rotation operator, but $t_{ij}$ does not have any connection to $f(g)$ or to the orientation of any single crystal. Equation (4.22) acts only on Equation (4.18) as a means to describe a complete set of strain rate modes. Any unit strain mode can now be defined by selecting values for each of the following four angles;

\[
\begin{align*}
0 & \leq \beta_1 < 2\pi, \\
0 & \leq \beta_2 < \pi/2, \\
0 & \leq \beta_3 < \pi, \\
0 & \leq \beta_4 < 2\pi.
\end{align*}
\] (4.23)

The first three angles are used to define a rotation matrix that is applied to $\dot{\varepsilon}$. The fourth is the angle $\theta$ in the polar representation of the strain mode in Equation (4.12). These combined with the magnitude comprise the independent variables needed to completely define the total strain rate.

The four dimensional space of $\dot{\varepsilon}$ can be readily discretized when the polar representation is formed. This is accomplished by simply stepping through the angles listed in Equation (4.23). This discretisation is used by MSDi to solve the yield problem for the polycrystalline material. A set of unique directions in strain rate
space are generated and stored in a text file. This list is then used to solve Equation (4.8). These steps are described in more detail in Section 4.7. In MSDi a database of solutions to Equation (4.8) was created by stepping through the \( \beta \) angles in 30° increments. This is obviously a very coarse description of the strain rate space. The intense computation required to generate the database at this coarse step size prohibits further refinement.

4.3 Rate of plastic working

The rate of plastic working \( \dot{W}_p \) is a scalar value which represents the dissipation rate of the material. We define this scalar such that

\[
\dot{W}_p = \sigma_{ij} \dot{\varepsilon}_{ij},
\]

(4.24)

or

\[
\dot{W}_p = \sum_s \frac{\sigma_{pq} \mu_{pq}(s)}{\tau_{pq}(s)} \ln \left| \frac{\sigma_{pq} \mu_{pq}(s)}{\tau_{pq}(s)} \right| \mathrm{sign}(\sigma_{pq} \mu_{pq}(s)) \sigma_{ij} \mu_{ij}(s).
\]

(4.25)

A crystalline material has an observable rate of plastic working \( \dot{W}_p^* \) such that if this value is exceeded the material will yield.

4.4 Scaling

The above treatment of yielding is formulated such that scaling can be utilized to modify \( \sigma \) and \( \dot{\varepsilon} \). Equation (4.12) introduces \( \eta \) as a parameter representing the magnitude of total strain and \( \dot{\varepsilon} \) as the unit total strain rate mode. Similarly \( \lambda \) will be used to represent the scalar parameter associated with stress such that

\[
\sigma_{ij} = \lambda \hat{\sigma}_{ij},
\]

(4.26)

where \( \hat{\sigma} \) represents the unit stress mode. The scaling of \( \sigma \) and \( \dot{\varepsilon} \) are related. Consider the substitution of Equation (4.26) into (4.25) yielding

\[
\dot{W}_p = \sum_s \frac{\lambda \hat{\sigma}_{pq} \mu_{pq}(s)}{\tau_{pq}(s)} \ln \left| \frac{\lambda \hat{\sigma}_{pq} \mu_{pq}(s)}{\tau_{pq}(s)} \right| \mathrm{sign}(\lambda \hat{\sigma}_{pq} \mu_{pq}(s)) \lambda \hat{\sigma}_{ij} \mu_{ij}(s).
\]

(4.27)

It can then be found that

\[
\eta = \lambda^n.
\]

(4.28)

This result is obtained by Hutchinson (1976).
4.5 Fourier representation of single crystal yield stress

A Fourier representation of the stress acting in the single crystal can be formulated to include the rate sensitive yield theory as outlined above. The yield stress can be expressed as a function of \( \dot{\varepsilon} \) and the orientation of the single crystal, \((g)\), such that

\[
\sigma_{ij}(\dot{\varepsilon}, g) = \sum_{\ell=0}^{4} M(\ell) N(\ell) \sum_{\mu=1}^{2\ell+1} \sum_{\nu=1}^{2\ell+1} \left( Y_{ij}(\dot{\varepsilon})\right)^{\mu\nu}_\ell \dot{T}^{\mu\nu}_\ell(g). \tag{4.29}
\]

The coefficients of Equation (4.29) can be computed in the standard fashion where

\[
(Y_{ij}(\dot{\varepsilon}))^{\mu\nu}_\ell = (2\ell + 1) \int \int \int_{SO(3)} \sigma_{ij}(\dot{\varepsilon}, g) \dot{T}^{\mu\nu}_\ell(g) dg. \tag{4.30}
\]

The value of \( \sigma_{ij}(\dot{\varepsilon}, g) \) is determined by the solution of Equation (4.8) when a specified strain mode and crystal orientation are specified. The basis functions are generalized spherical harmonic functions with the * indicating the complex conjugate. A set of the above coefficients were computed with the MSDi software.

4.6 Yield stress in polycrystalline microstructures

The main result of the previous discussion is that the yield stress of the polycrystalline microstructure can be determined via the inner product of Equation (4.29) and Equation (2.4) such that

\[
\langle \sigma_{ij}(\dot{\varepsilon}) \rangle = \int \int \int_{SO3} f(g)\sigma_{ij}(\dot{\varepsilon}, g) dg. \tag{4.31}
\]

Equation (4.31) can be approximated through the finite summation of the Fourier coefficients yielding

\[
\langle \sigma_{ij}(\dot{\varepsilon}) \rangle = \sum_{\ell=0}^{4} M(\ell) N(\ell) \sum_{\mu=1}^{2\ell+1} \sum_{\nu=1}^{2\ell+1} \frac{1}{2\ell+1} F^{\mu\nu}_\ell \left( Y_{ij}(\dot{\varepsilon})\right)^{\mu\nu}_\ell. \tag{4.32}
\]

In this way the yield stress in the polycrystalline material is a direct function of \( F^{\mu\nu}_\ell \) and \( \dot{\varepsilon} \). In general \( \dot{\varepsilon} \) is not known for the given simulation and must be identified. Section 4.7 introduces a method for identifying \( \dot{\varepsilon} \).
4.7 Determination of yielding

The determination of yielding is accomplished by comparing the calculated rate of plastic working with the observable rate of plastic working. We recall that $\dot{W}_p^*$ is a material parameter that can be measured and that $\dot{W}_p$ is our estimate. We can then formulate an inequality to determine if yielding has occurred. If

$$\dot{W}_p^* - \dot{W}_p \leq 0$$  \hspace{1cm} (4.33)

then yielding has occurred.

The following list is a summary of the steps required to incorporate the above treatment of the Taylor yield theory into finite element modelling (FEM).

1. Analyze a geometric model using FEM and obtain the results of an elastic analysis.

2. Query the FEM results for the stress mode that has the maximum equivalent stress and extract $\lambda^{\text{FEM}}$ and $\hat{\sigma}^{\text{FEM}}$ where $\lambda^{\text{FEM}}$ is the magnitude of the FEM stress mode.

3. Iterate through the discrete set of strain rate modes and find $\dot{\varepsilon}$ such that

$$\langle \hat{\sigma}_{ij}(\dot{\varepsilon}) \rangle \hat{\sigma}_{ij}^{\text{FEM}} = \text{MAX}.$$  \hspace{1cm} (4.34)

The value of $\langle \hat{\sigma}_{ij}(\dot{\varepsilon}) \rangle$ is obtained from Equation (4.32), and the (‘) over $\hat{\sigma}_{ij}(\dot{\varepsilon})$ and $\hat{\sigma}_{ij}^{\text{FEM}}$ represents the unit stress or the stress mode independent of magnitude. The magnitude of the calculated stress in the polycrystal is then $\lambda^{\text{CAL}}$.

4. Use the ratio of $\lambda^{\text{FEM}}/\lambda^{\text{CAL}}$ to scale the resulting $\dot{\varepsilon}$ and $\sigma_{ij}(\dot{\varepsilon})$ then calculate $\dot{W}_p$ and determine if yielding has occurred.
Chapter 5

Crack Extension Force

The crack extension force $G$ or toughness of a linear elastic anisotropic media is postulated by [Barnett and Asaro (1972)]. The crack extension force is formulated as a function of applied stress, elastic constants, and crack geometry. Building on the work of [Barnett and Asaro (1972)] a method for designing the material to minimize $G$ is proposed.

![Figure 5.1: A slit like crack is defined by a vector, $n$, that is normal to the crack surface and by a vector, $t$, that is perpendicular to $n$ and in the direction of the crack front. The crack plane then extends to infinity along the direction perpendicular to $n$ and $t$.](image)

Barnett and Asaro (1972) show that given a slit-like crack as in Figure 5.1 the crack extension force $G$ becomes

$$G = \frac{1}{4} \epsilon_i^A n_j^A \sigma_{sm}^A n_m K_{is}^{-1},$$

(5.1)

where $n_m$ are the components of the unit normal to the crack surface. They are specified in the sample frame. The half crack length is $c$, and $\sigma_{ij}^A$ is the far field
applied stress. The matrix $K_{mg}$ is dependant upon the effective elastic stiffness tensor (Barnett and Swanger 1971) and it can be written as

$$K_{mg} = \frac{1}{8\pi^2} \varepsilon_{jw} t_j \left( \langle C_{ngip} \rangle \langle C_{wmrs} \rangle + \langle C_{nmiip} \rangle \langle C_{wgirs} \rangle \right) \int_0^\pi z_s \left( \frac{dz_n}{d\psi} \right) M^{-1}_{ir} d\psi. \quad (5.2)$$

In Equation (5.2) $t$ is defined a unit vector in the direction of the dislocation line which lies in the plane with normal vector $n$. Additionally $z$ is any unit vector perpendicular to $t$, and $\psi$ is an angular variable in the plane $z \cdot t = 0$. The $M_{ir}$ matrix is the symmetric Christoffel stiffness matrix and is defined as

$$M_{ir} = \langle C_{irjs} \rangle z_j z_s. \quad (5.3)$$

MSDi connects the above estimate of crack extension force with the FEM-model by equating $\sigma^{FEM}$ as defined in Section 4.7 with $\sigma^A$ from Equation (5.1). With this imposed stress field the directions of $n$ and $t$ are iterated through all possible combinations such that $G$ is maximized. In this way the worst case crack extension force is considered. In some instances it may be desirable to only consider one specific crack inclination and direction. This may be the case when the processing or manufacturing methods used during fabrication are known to introduce a specific type of crack or when fatigue analysis reveals that a specific type of crack exists. The turbine disk case study outlined in Chapter 6 uses the worst case procedure specified above.
Chapter 6

Case Study: Microstructure Design of a Turbine Disk

6.1 Overview

There is an astonishing amount of design work required to produce a turbine disk. Steady state and dynamic loading conditions are considered. Operating temperature, thermal gradients and thermal stability each play a significant role. Harmonic excitations are known to cause catastrophic failure and reduce efficiency. Cyclic loads are generated from angular velocities in excess of 20,000 RPM; and as a result crack initiation and propagation are critical factors in the life of the disk. While the texture of the material may influence each of these factors this case study is limited to its effect on the elastic, plastic, and crack driving force responses of the disk. Thermal and harmonic stress effects are neglected.

Figure 6.1: Starting profile with displacement constraints and loads $\omega$ and $P$
A turbine rotor is comprised of its air-foils, rim, and disk. The rim and disk are each portions of the same part. The rim is the section of the disk that contains the fir-tree attachment points for the air-foils. The web of the disk attaches the rim to the hub, and the hub attaches the entire rotor to the shaft. Figure 6.1 is a profile of the starting disk model used in this case study. The disk is considered symmetric about the $x, y$ plane and only the unique portion is shown.

In this example the profile, with the exception of the web, is essentially constructed of line segments. The web is defined by a spline that connects the hub to the rim and passes through key points. While a case study that includes the design of the fir-tree section of the rim would prove interesting it is outside the scope of the current model. Instead of transferring the radial force that the air-foils exert on the rim through a fir-tree model this force is accounted for as a uniform pressure, $P$, on the outermost rim surface. In this way the stress mode that dominates analysis results is confined to the region of interest, namely the disk itself.

A turbine disk has cyclic geometric symmetry about its shaft allowing the stress analysis to be reduced to only a base section. Figure 6.2 shows the base section used to specify loads and displacement constraints. The base section is created by sweeping Figure 6.1 $18^\circ$ about the $z$ – axis. The volume in Figure 6.2 represents one section of disk with 20 air-foils. A 3D representation is needed in the case study as the material properties are anisotropic and must be represented by a volume element in the finite element analysis.

### 6.2 Case study 1: Procedure

Two case study scenarios were considered. In the first a multi-objective optimization problem is formulated to find the optimal geometry for a turbine disk and the optimal texture of the material that comprises the disk. Several combinations of objectives and design variables are explored to determine the influence of the texture on the performance of the turbine disc. The key design variables are listed in Table 6.1. The material parameters are defined as the non-constant Fourier coefficients for a polycrystalline material with cubic sample symmetry and no statistical symmetry.
when \( \ell = 4 \). This results in 9 non-constant terms. The geometric parameters are the \( z \) coordinate of the four key points of the spine that define the web of the disk. The upper and lower bounds for the geometric design variables are seen in Table 6.1. The bounds on the Fourier coefficients are loose and have no real significance. They are mainly used to scale the design space correctly. The real bound on the material parameters is the material constraint \( S \) as defined in Section 2.4.

The key design functions along with the objective or constraints placed on each are listed in Table 6.2. The turbine disk model in the first case study is subjected to an inertial load about the \( z \) – axis of \( \omega = 3,400 \ RPM \). Additionally a static load of \( P = 25 MPa \) is applied to the outer surface of the rim.

Both OptDesX and iSIGHT were used to explore the model for the first case study. Scaled and unscaled Gradient information for the design variables and functions were obtained from OptDesX. The unscaled gradients in Figure 6.3 and the

Figure 6.2: Orthogonal view of the base section of disk used in analysis. A volume element is used to capture the anisotropic nature of the material.
Table 6.1: Key design variables used in finding the optimal design of a turbine disk in the first case study. There are 9 material parameters and 4 geometric parameters.

<table>
<thead>
<tr>
<th>Description</th>
<th>Variable</th>
</tr>
</thead>
<tbody>
<tr>
<td>Material Parameters</td>
<td>$F_i$ with $i=1..9$</td>
</tr>
<tr>
<td>(Section 2.3)</td>
<td></td>
</tr>
</tbody>
</table>
| Geometric parameters ($m$)         | $0.00762 \leq Z_4 \leq 0.034$
|                                    | $0.00762 \leq Z_5 \leq 0.034$
|                                    | $0.00762 \leq Z_6 \leq 0.034$
|                                    | $0.00762 \leq Z_7 \leq 0.034$

Table 6.2: Key design functions and the associated objective or constraints of the first case study. Two minimization objectives for mass and crack extension force are formulated.

<table>
<thead>
<tr>
<th>Description</th>
<th>Variable</th>
<th>Objective/Constraints</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total mass ($kg$)</td>
<td>$M$</td>
<td>$\min(M)$</td>
</tr>
<tr>
<td>Crack extension force ($J/m^2$)</td>
<td>$G$</td>
<td>$\min(G)$</td>
</tr>
<tr>
<td>Change in rate of</td>
<td>$\Delta W$</td>
<td>$0 &lt; \Delta W$</td>
</tr>
<tr>
<td>plastic working ($W$)</td>
<td>$S$</td>
<td>$0 &lt; S$</td>
</tr>
<tr>
<td>Material Constraint</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Scaled gradients in Figure 6.4 show that there is significant interaction among the variables and functions. It is evident that $G$ and $\Delta W$ are sensitive to changes in all design variables.

6.3 Case study 2: Procedure

Based on the results of the first case study a second case study was formulated to further explore the models. In the second case study the geometric model is refined to include curvature constraints and the treatment of plasticity is reduced to a constraint on Von Mises equivalent stress. Additionally a material with cubic crystal symmetry and axial–symmetric sample symmetry is explored. The key design variables are listed in Table 6.3 where the changes in geometric and material parameters are shown. Only one material parameter is needed to represent the highly symmetric cubic axial–symmetric material properties. Their are still four geometric parameters but they are now the $(x, z)$ position of two key points that define the web of the disk. The key design functions along with the objective or constraints placed on each for
Figure 6.3: Unscaled gradients obtained from OptDesX using central difference derivatives and a step size of 0.01.

<table>
<thead>
<tr>
<th></th>
<th>Mass</th>
<th>Toughness</th>
<th>Dissipation</th>
<th>Hull</th>
</tr>
</thead>
<tbody>
<tr>
<td>F1</td>
<td>0.00000</td>
<td>5.468824</td>
<td>-1044.247</td>
<td>-0.02647039</td>
</tr>
<tr>
<td>F2</td>
<td>0.00000</td>
<td>-1.320455</td>
<td>-115.3553</td>
<td>0.46439089</td>
</tr>
<tr>
<td>F3</td>
<td>0.00000</td>
<td>-4.256472</td>
<td>93.29393</td>
<td>-0.02584103</td>
</tr>
<tr>
<td>F4</td>
<td>0.00000</td>
<td>3.311111</td>
<td>215.3370</td>
<td>0.8870570</td>
</tr>
<tr>
<td>F5</td>
<td>0.00000</td>
<td>-4.97778</td>
<td>562.0674</td>
<td>-0.1462063</td>
</tr>
<tr>
<td>F6</td>
<td>0.00000</td>
<td>2.164815</td>
<td>257.5370</td>
<td>-0.08588889</td>
</tr>
<tr>
<td>F7</td>
<td>0.00000</td>
<td>6.463354</td>
<td>224.4491</td>
<td>-0.1633664</td>
</tr>
<tr>
<td>F8</td>
<td>0.00000</td>
<td>2.334146</td>
<td>-156.4927</td>
<td>-0.1534146</td>
</tr>
<tr>
<td>F9</td>
<td>0.00000</td>
<td>6.814554</td>
<td>426.3498</td>
<td>-0.1707317</td>
</tr>
<tr>
<td>Z4</td>
<td>0.00000</td>
<td>82.355653</td>
<td>570.8257</td>
<td>0.000000</td>
</tr>
<tr>
<td>Z6</td>
<td>228.6687</td>
<td>-79.66637</td>
<td>5136.557</td>
<td>0.000000</td>
</tr>
<tr>
<td>Z8</td>
<td>239.4586</td>
<td>80.65530</td>
<td>-1616.39</td>
<td>0.000000</td>
</tr>
<tr>
<td>Z7</td>
<td>378.7979</td>
<td>1061.742</td>
<td>-12613.7</td>
<td>0.000000</td>
</tr>
</tbody>
</table>

Figure 6.4: Scaled gradients obtained from OptDesX using central difference derivative and a step size of 0.01.

<table>
<thead>
<tr>
<th></th>
<th>Mass</th>
<th>Toughness</th>
<th>Dissipation</th>
<th>Hull</th>
</tr>
</thead>
<tbody>
<tr>
<td>F1</td>
<td>0.00000</td>
<td>38.96000</td>
<td>-35.90044</td>
<td>-0.4522613</td>
</tr>
<tr>
<td>F2</td>
<td>0.00000</td>
<td>-2.50500</td>
<td>-2.54950</td>
<td>5.251750</td>
</tr>
<tr>
<td>F3</td>
<td>0.00000</td>
<td>-3.87500</td>
<td>1.83131</td>
<td>-0.2512863</td>
</tr>
<tr>
<td>F4</td>
<td>0.00000</td>
<td>8.34000</td>
<td>5.301350</td>
<td>12.03518</td>
</tr>
<tr>
<td>F5</td>
<td>0.00000</td>
<td>-31.09530</td>
<td>13.56255</td>
<td>-1.89425</td>
</tr>
<tr>
<td>F6</td>
<td>0.00000</td>
<td>5.04150</td>
<td>6.55450</td>
<td>-1.20530</td>
</tr>
<tr>
<td>F7</td>
<td>0.00000</td>
<td>7.70000</td>
<td>6.172580</td>
<td>0.557280</td>
</tr>
<tr>
<td>F8</td>
<td>0.00000</td>
<td>6.05000</td>
<td>-6.02100</td>
<td>-1.683417</td>
</tr>
<tr>
<td>Z4</td>
<td>1.40000</td>
<td>13.65000</td>
<td>8.793450</td>
<td>1.789794</td>
</tr>
<tr>
<td>Z5</td>
<td>1.70000</td>
<td>-1.10000</td>
<td>0.10000</td>
<td>0.000000</td>
</tr>
<tr>
<td>Z6</td>
<td>2.10000</td>
<td>1.15000</td>
<td>0.770050</td>
<td>0.000000</td>
</tr>
<tr>
<td>Z7</td>
<td>2.50000</td>
<td>24.61500</td>
<td>-1.86200</td>
<td>0.000000</td>
</tr>
</tbody>
</table>
the second simulation are listed in Table 6.4. The turbine disk model in the second case study is subjected to an inertial load about the \( z \)-axis of \( \omega = 1,500 \) RPM. Additionally a static load of \( P = 10MPa \) is applied to the outer surface of the rim.

Table 6.3: Design variables for the second case study. The number of applicable material parameters is variable based on the symmetry conditions imposed. The geometric parameters now represent the \((x, z)\) location of two key points that define the web of the disk.

<table>
<thead>
<tr>
<th>Description</th>
<th>Variable</th>
</tr>
</thead>
<tbody>
<tr>
<td>Material Parameters</td>
<td>( F_i ) with ( i = 1 ) for Cubic Axial–Symmetric, ( i = 9 ) for Cubic Triclinic</td>
</tr>
<tr>
<td>Geometric parameters (m)</td>
<td>( 0.035 \leq X_1 \leq 0.11 )</td>
</tr>
<tr>
<td></td>
<td>( 0.005 \leq Z_1 \leq 0.035 )</td>
</tr>
<tr>
<td></td>
<td>( 0.035 \leq X_2 \leq 0.11 )</td>
</tr>
<tr>
<td></td>
<td>( 0.005 \leq Z_2 \leq 0.035 )</td>
</tr>
</tbody>
</table>

6.4 Process integration

The data passed between each CAE software package is accomplished by standard file I/O. The execution order of MSDi and ANSYS is managed in the shell script. Figure 6.5 describes in greater detail the data flow between each program and during the computation of the analysis functions.

Table 6.4: Key design functions and the associated objective or constraints of the second case study. Two minimization objectives for mass and crack extension force are formulated. Case study two shows the addition of curvature constraints on the disk geometry.

<table>
<thead>
<tr>
<th>Description</th>
<th>Variable</th>
<th>Objective/Constraints</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total mass (kg)</td>
<td>( M )</td>
<td>min( (M) )</td>
</tr>
<tr>
<td>Crack extension force (kJ/mm²)</td>
<td>G</td>
<td>min( (G) )</td>
</tr>
<tr>
<td>Yielding (Von Mises)</td>
<td>( \sigma^{FEM} )</td>
<td>( \sigma^{FEM} &lt; 150MPa )</td>
</tr>
<tr>
<td>Material Constraint</td>
<td>( S )</td>
<td>( 0 &lt; S )</td>
</tr>
<tr>
<td>Geometric Curvature</td>
<td>( \Delta Z_1 )</td>
<td>( 0 &lt; \Delta Z_1 )</td>
</tr>
<tr>
<td></td>
<td>( \Delta Z_2 )</td>
<td>( 0 &lt; \Delta Z_2 )</td>
</tr>
</tbody>
</table>
Figure 6.5: The parameters and analysis results are passed between the CAE software packages by the use of standard I/O. The optimization software writes the design variables to a file and then calls a shell script. The shell script then manages the execution order of MSDi and ANSYS. The results are then read by the optimization software to see if the objective has improved and or if the constraints were violated.
Chapter 7

Results and Discussion of Results

To determine the influence that texture plays on the performance of the disk, several simulations were created for each case study. All explorations were accomplished by using the Generalized Reduced Gradient (GRG) optimization method. In general, as a base line the mass of the disk, \( M \), is minimized using only the geometric parameters as design variables. Following this baseline other combinations of objectives, constraints and design variables are used.

7.1 Case study 1: Geometry only

The baseline for the first case study is set by an optimization with the objective of minimizing mass, where only the geometric parameters are used as design variables. The material parameters are set as an isotropic microstructure. This is the equivalent of a material that is only represented by the Elastic modulus, \( E \), and Poisson’s ratio, \( \nu \). The starting and ending values for each of the geometric parameters and the analysis functions for this first simulation are listed in Table 7.1. The active constraints on this simulation are the upper and lower bounds on the geometric parameters and that \( 0 < \Delta \dot{W} \).

The optimization analyzed approximately 250 feasible designs. The resulting mass of 0.785kg is a 23.5% reduction. The resulting profile and stress distribution can be seen in Figure 7.1. The stepped nature of the web profile is possibly an artifact of the spline used to model the geometry as there were no curvature constraints formulated for this geometry. None of the geometric parameters are brought to their lower bound therefore the limiting constraint can only be \( 0 < \Delta \dot{W} \) as the other
Table 7.1: The design variables listed comprise only the geometric parameters. The objective of this optimization is to minimize the mass.

<table>
<thead>
<tr>
<th>Design variables/Analysis functions</th>
<th>Initial value</th>
<th>Final value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$z_1(m)$</td>
<td>0.034</td>
<td>0.02741</td>
</tr>
<tr>
<td>$z_2(m)$</td>
<td>0.030</td>
<td>0.02280</td>
</tr>
<tr>
<td>$z_3(m)$</td>
<td>0.026</td>
<td>0.01800</td>
</tr>
<tr>
<td>$z_4(m)$</td>
<td>0.022</td>
<td>0.00935</td>
</tr>
<tr>
<td>$M(kg)$</td>
<td>1.0273</td>
<td>0.785</td>
</tr>
<tr>
<td>$G(kJ/mm^2)$</td>
<td>15,714</td>
<td>16,858</td>
</tr>
<tr>
<td>$\Delta \dot{W}(J/s)$</td>
<td>7185.4</td>
<td>5259.6</td>
</tr>
<tr>
<td>$S$</td>
<td>NA</td>
<td>NA</td>
</tr>
</tbody>
</table>

The analysis functions were not bounded for this optimization.

The min and max values of the Von Mises equivalent stress, $(\sigma_{VM})$, are respectively $\sigma_{VM}^{min} = 85 MPa$ and $\sigma_{VM}^{max} = 440 MPa$. The max value of stress is in the range of yield stress for nickel and nickel alloys as show by Callister (1997). It is however significantly higher than $\sigma_y = 148 MPa$ which is the yield strength for commercially pure Nickel 200. In Figure 7.1 $\sigma_{VM}^{max}$ is located on the thin portion of the web while $\sigma_{VM}^{min}$ is located on the rim on the surface that represents the joint between two adjacent turbine wheels.

7.2 Case study 1: Cubic triclinic material

Following the optimization of the geometry a “material only” exploration is conducted with min($G$) as the objective. The design variables consist only of the material parameters. The geometric parameters are held constant at the final values listed in Table 7.1. In this way the influence of the material texture on $G$ and $\Delta \dot{W}$ can be determined. The starting location of the material is the isotropic case where all the material parameters are exactly zero. The result of this run can be seen in Table 7.2. The resulting value of $G$ is 1,095 kJ/mm$^2$. This is more than an order of magnitude reduction in energy per unit area.

The material parameters listed in Table 7.2 represent $f(g)$ as defined in Equation (2.1). A graphical representation of $f(g)$ known as an Orientation Distribution
Figure 7.1: Optimal profile of the disk obtained by using only the geometric parameters. The material parameters represent an isotropic material.

Table 7.2: Only the material parameters are used in the second simulation. The geometric parameters are held constant at the final value of the first simulation. The objective of this run is minimize the crack extension force ($G$).

<table>
<thead>
<tr>
<th>Design variables/Analysis functions</th>
<th>Initial value</th>
<th>Final value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$F_1$ $F_2$</td>
<td>0.0 0.0</td>
<td>-0.7488 -0.4992</td>
</tr>
<tr>
<td>$F_3$ $F_4$</td>
<td>0.0 0.0</td>
<td>-0.4992 0.0254</td>
</tr>
<tr>
<td>$F_5$ $F_6$</td>
<td>0.0 0.0</td>
<td>0.8626 -0.4602</td>
</tr>
<tr>
<td>$F_7$ $F_8$</td>
<td>0.0 0.0</td>
<td>-1.0063 0.3656</td>
</tr>
<tr>
<td>$F_9$</td>
<td>0.0</td>
<td>-0.7592</td>
</tr>
<tr>
<td>$M(kg)$</td>
<td>0.785</td>
<td>0.785</td>
</tr>
<tr>
<td>$G(kJ/mm^2)$</td>
<td>16.858</td>
<td><strong>1,095</strong></td>
</tr>
<tr>
<td>$\Delta W(J/s)$</td>
<td>5259.6</td>
<td>6770.8</td>
</tr>
<tr>
<td>$S$</td>
<td>6.84</td>
<td>3.708</td>
</tr>
</tbody>
</table>
Function Plot, or ODF plot is shown in Figure 7.2. A reference scale for the contours is provided to the right of the plot. The negative minimum value should be ignored as it is an artifact of the auto scaling procedure in the OIM software. The positive maximum value should be interpreted as multiplication factor on a random texture. For example, the max value of 3.3 as seen in Figure 7.2 means that the max contours are $3.3 \times$ random. Using the OIM software the peak intensities of the ODF plot in Figure 7.2 are selected for further analysis in Section 7.3.

Figure 7.2: The resulting material parameters represent the ODF above as defined in Equation (2.1). The sections are of constant angle $\phi_2$. The horizontal axis in each section is $\phi_1$ and the vertical axis is $\Phi$.

Figure 7.3 shows the resulting profile for the second simulation side by side the profile of the first simulation. Modification of the material parameters seem to have an evening effect on the stress distribution in the profile. When the profile sections of the first two simulations are compared side by side as in Figure 7.3 it is clear that in the region of $\sigma_{VM}^{\text{max}}$ the intensity has been relaxed. The relaxation is accomplished through the modification of the $\langle C_{ijkl} \rangle$. 
In addition to the relaxing effect seen in Figure 7.3 the modification of \(\langle C_{ijkl}\rangle\) is seen to have a marked effect on \(G\). In Equations (5.1) through (5.3) \(\langle C_{ijkl}\rangle\) couples with itself, the Christoffel stiffness matrix \(M_{ir}\), and the far field applied stress \(\sigma_{ij}\), where the latter two terms are known to be functions of \(\langle C_{ijkl}\rangle\) as shown in Equations (3.1) and (5.3). It becomes clear by inspection that modification of the effective elastic properties have a significant influence on \(G\). As \(G\) is non-linear with respect to \(\langle C_{ijkl}\rangle\) it is not a simple matter to determine what form of the stiffness tensor is desired to minimize \(G\). In this second simulation \(\sigma_{ij}^{\text{max}} = 434 Mpa\) which is essentially identical to the results of the first simulation. This small change in the far field applied stress is not enough to account for the reduction of \(G\). This leaves the coupling of \(\langle C_{ijkl}\rangle\) in Equation (5.2) as a reasonable source. A significant result of this simulation is that the GRG algorithm is able to effectively use the materials parameters to explore this nonlinear objective function.

![Figure 7.3](image-url)

Figure 7.3: a) Equivalent stress distribution results from simulation 2. b) Equivalent stress distribution results from simulation 1. Modification of the material parameters appears to more evenly distribute the stress. This is most clearly seen in the highest contour region on the necked portion of the profile.
7.3 Case study 1: Microstructure analysis

Microstructure features including texture are influenced by manufacturing processing paths\(^1\) [Humphreys and Hatherley (2000)] show that there are a number of texture components which frequently appear from known processing paths. Table 7.3 lists these common components and their Euler angles. The components as listed in Table 7.3 are specified in the crystal frame for simplicity where as the peak intensities identified from Figure 7.2 are not. As it is necessary to compare the peaks of the designed texture to the common components the latter must have the cubic symmetry operations applied to them. Additionally it is not likely that the peak intensities will be exactly identical to any of the common components therefore it is routine to specify an angular deviation to the common components. For example if a peak in the designed texture is believed to be near the Brass component then a comparison to Brass and a 10° deviation from Brass should correctly identify the peak.

Table 7.3: Common texture components found in cubic materials. These components result from known processing paths.

<table>
<thead>
<tr>
<th>Texture Component</th>
<th>Euler angles (deg)</th>
<th>(\phi_1)</th>
<th>(\Phi)</th>
<th>(\phi_2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cube</td>
<td>0.0 0.0 0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>10° RD Cube</td>
<td>0.0 10.0 0.0</td>
<td>0.0</td>
<td>10.0</td>
<td>0.0</td>
</tr>
<tr>
<td>20° RD Cube</td>
<td>0.0 20.0 0.0</td>
<td>0.0</td>
<td>20.0</td>
<td>0.0</td>
</tr>
<tr>
<td>30° RD Cube</td>
<td>0.0 30.0 0.0</td>
<td>0.0</td>
<td>30.0</td>
<td>0.0</td>
</tr>
<tr>
<td>Goss</td>
<td>0.0 45.0 0.0</td>
<td>0.0</td>
<td>45.0</td>
<td>0.0</td>
</tr>
<tr>
<td>Brass</td>
<td>35.0 45.0 0.0</td>
<td>35.0</td>
<td>45.0</td>
<td>0.0</td>
</tr>
<tr>
<td>Dillamore (D)</td>
<td>90.0 27.0 45.0</td>
<td>90.0</td>
<td>27.0</td>
<td>45.0</td>
</tr>
<tr>
<td>Copper</td>
<td>40.0 65.0 26.0</td>
<td>40.0</td>
<td>65.0</td>
<td>26.0</td>
</tr>
<tr>
<td>S</td>
<td>65.0 75.0 34.0</td>
<td>65.0</td>
<td>75.0</td>
<td>34.0</td>
</tr>
</tbody>
</table>

The result of comparing these common texture components for all the peaks in Figure 7.2 are shown in Table 7.4 for deviations of 20°, 25°, and 30°. Each peak intensity is only identified once and the percentage of peaks that are associated with

\(^1\)A processing path for a material is defined as a list of manufacturing steps that may include but are not limited to; rolling, annealing, forging, and quenching.
the texture components are listed. For all deviations $\leq 20^\circ$ not a single peak was identified to be associated with the common texture components. At a $25^\circ$ deviation some peaks begin to be identified with the Cube, Goss, and S components. At a $30^\circ$ deviation 25% of the peaks are found to associate with the Dillamore component. From this analysis it can be seen that while there is a texture in the material is not closely related to those in Table 7.3 and it is therefore not readily apparent what processing steps are required to produce this texture or how to obtain its predicted benefits.

Table 7.4: The common texture components listed in Table 7.3 are compared to the peak intensities of Figure 7.2 to identify what percent of the components are found in the designed texture.

<table>
<thead>
<tr>
<th>Texture Component</th>
<th>% of Component in specified deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>20$^\circ$</td>
</tr>
<tr>
<td>Cube</td>
<td>0.0</td>
</tr>
<tr>
<td>10$^\circ$ RD Cube</td>
<td>0.0</td>
</tr>
<tr>
<td>20$^\circ$ RD Cube</td>
<td>0.0</td>
</tr>
<tr>
<td>30$^\circ$ RD Cube</td>
<td>0.0</td>
</tr>
<tr>
<td>Goss</td>
<td>0.0</td>
</tr>
<tr>
<td>Brass</td>
<td>0.0</td>
</tr>
<tr>
<td>Dillamore (D)</td>
<td>0.0</td>
</tr>
<tr>
<td>Copper</td>
<td>0.0</td>
</tr>
<tr>
<td>S</td>
<td>0.0</td>
</tr>
</tbody>
</table>

7.4 Case study 1: Geometry and material

The third and final simulation for the first case study includes both the material parameters and geometric parameters as design variables with an objective of minimizing the mass. The starting values for the design variables in this simulation are the ending value of the second simulation. The results can be seen Table 7.5. Not one of the nine material parameters have changed in value, but Each of the geometric parameters have changed. One geometric parameter $z_4 = 0.0076$ is brought to its
lower bound. The resulting mass $M = 0.7388kg$ is a 9.5% reduction from the first simulation and the active constraints in the problem appear to be the lower bound of $z_4$ and $\Delta \dot{W}$.

Table 7.5: The results of the third simulation are shown where both geometric and material parameters are used as design variables with the objective of minimizing the mass. The mass is reduced by 9.5%.

<table>
<thead>
<tr>
<th>Design variables and Analysis functions</th>
<th>$\min(M)$</th>
<th>$z_i$ and $F_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Initial</td>
<td>Final</td>
</tr>
<tr>
<td>$z_1(m)$</td>
<td>0.02741</td>
<td>0.02587</td>
</tr>
<tr>
<td>$z_2(m)$</td>
<td>0.02280</td>
<td>0.02124</td>
</tr>
<tr>
<td>$z_3(m)$</td>
<td>0.01800</td>
<td>0.01597</td>
</tr>
<tr>
<td>$z_4(m)$</td>
<td>0.00935</td>
<td>0.00760</td>
</tr>
<tr>
<td>$M(kg)$</td>
<td>0.785</td>
<td><strong>0.7388</strong></td>
</tr>
<tr>
<td>$G(kJ/mm^2)$</td>
<td>1,095</td>
<td>1,754</td>
</tr>
<tr>
<td>$\Delta \dot{W}(J/s)$</td>
<td>6770.8</td>
<td>739.4</td>
</tr>
<tr>
<td>$S$</td>
<td>3.708</td>
<td>3.708</td>
</tr>
</tbody>
</table>

The resulting profile can be seen in Figure 7.4. The stress distribution of this final design is more uniform than either of the previous simulations. From the contour plot of equivalent stress in Figure 7.4, it is seen that the much of the profile is under the same level of stress. It is through coupling shape and material performance that this stress distribution is possible. The min and max values of the Von Mises equivalent stress are respectively $\sigma_{V_M}^{min} = 92Mpa$ and $\sigma_{V_M}^{max} = 517Mpa$. The dissipation rate of the material is brought to the final value of $\Delta \dot{W} = 739.4$ in this simulation. This is almost an order of magnitude lower than the final value of the other simulations. This corresponds to the increase of $\sigma_{V_M}^{max}$ as would be expected from the outline given in Section 4.7.

Modification of the material parameters will not change volume or density of the disk. They only influence of the material parameters on the problem is to modify the yield constraint, $\Delta \dot{W}$, and the elastic response of the material. The gradient
based search methods were not able to effectively explore the effects of the material parameters on the constraints during this third simulation. One explanation for this effect is that while the material can do much to relieve stress it is the geometry that ultimately has the largest influence on stress concentration.

In an attempt to guide the optimization to effectively search the entire design space random search methods were employed. Simulated annealing and Genetic Algorithms in iSIGHT were both unsuccessful at searching this space. They were unable to effectively chose feasible material parameters. They each consistently chose materials where the hull measure constraint in Table 6.2 was violated. This resulted in premature termination of the attempts.

While the material parameters did not play a direct role in the third simulation it would seem that this final geometry is possible only when the material parameters
are included in the overall design. This portion of the geometric design space is opened by consideration of additional material properties. In this case study consecutive repetition of simulations one and two could possibly result in further improvements in both objectives.

7.5 Case study 2: Geometry only

In general it was found in the final simulation of the first case study that the material parameters did not have an effect on the minimum mass solution. Additionally the geometric parameters had a much greater influence on the stress state found in the model such that $\sigma^{FEM}$ was dominated by the geometry of the disk. In light of these results it was determined that in this simulation the goal would be to implement the objectives of $\min(M)$ and $\min(G)$ sequentially rather than in parallel. This would allow a closer look at the influence of material symmetry on $G$. The changes in the design variables and analysis function in this second case study are discussed in Section 6.3.

Again a base line is set such that minimizing mass is the objective and only the geometric parameters are active as design variables. The material parameters are set as an isotropic microstructure. The starting and ending values for each of the geometric parameters and the analysis functions for this first simulation are listed in Table 7.6. The active constraints on this simulation are the upper and lower bounds on the geometric parameters and the yielding constraint. The resulting profile can be seen in Figure 7.5. The max Von Mises stress of $\sigma^{FEM}(MPa) = 149.39$ is in the web.

7.6 Case study 2: Cubic triclinic material

Following the optimization of the geometry a “material only” exploration is conducted with $\min(G)$ as the objective and cubic triclinic material symmetry. The design variables consist only of the material parameters. The geometric parameters are held constant at the final values listed in Table 7.6. In this way the influence of the material texture on $G$ can be determined. The starting location of the material
Table 7.6: The starting and ending values of the design variables and analysis functions for the geometry only simulation of the second case study.

<table>
<thead>
<tr>
<th>Design variables/Analysis functions</th>
<th>Initial value</th>
<th>Final value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$X_1(m)$</td>
<td>0.065</td>
<td>0.0634</td>
</tr>
<tr>
<td>$Z_1(m)$</td>
<td>0.030</td>
<td>0.0192</td>
</tr>
<tr>
<td>$X_2(m)$</td>
<td>0.08</td>
<td>0.08</td>
</tr>
<tr>
<td>$Z_2(m)$</td>
<td>0.026</td>
<td>0.0071</td>
</tr>
<tr>
<td>$M(kg)$</td>
<td>1.0218</td>
<td>0.6153</td>
</tr>
<tr>
<td>$G(kJ/mm^2)$</td>
<td>784</td>
<td>12,205</td>
</tr>
<tr>
<td>$\sigma_{FEM}(MPa)$</td>
<td>140.36</td>
<td>149.39</td>
</tr>
<tr>
<td>$S$</td>
<td>NA</td>
<td>NA</td>
</tr>
</tbody>
</table>

Figure 7.5: Optimal profile of the disk obtained by using only the geometric parameters. The contours are of Von Mises eqv. stress.
is the isotropic case where all the material parameters are exactly zero. The result of this run can be seen in Table 7.7. The resulting value of $G$ is 521 kJ/mm$^2$. This result is similar to that in Section 7.2 where again there is a large reduction in energy per unit area over that of the isotropic material with the exact same geometry and loading conditions.

Table 7.7: Only the material parameters are used in the second simulation of this case study. The geometric parameters are held constant at the final value of the first simulation. The objective of this run is $ming(G)$

<table>
<thead>
<tr>
<th>Design variables/ Analysis functions</th>
<th>Initial value</th>
<th>Final value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$F_1$ $F_2$</td>
<td>0.0 0.0</td>
<td>-0.3778  -0.2615</td>
</tr>
<tr>
<td>$F_3$ $F_4$</td>
<td>0.0 0.0</td>
<td>-0.2125  -0.2047</td>
</tr>
<tr>
<td>$F_5$ $F_6$</td>
<td>0.0 0.0</td>
<td>0.4908   -0.3311</td>
</tr>
<tr>
<td>$F_7$ $F_8$</td>
<td>0.0 0.0</td>
<td>-0.3578  0.1062</td>
</tr>
<tr>
<td>$F_9$</td>
<td>0.0</td>
<td>0.0697</td>
</tr>
<tr>
<td>$M(kg)$</td>
<td>0.6153</td>
<td>0.6153</td>
</tr>
<tr>
<td>$G(kJ/mm^2)$</td>
<td>12,205</td>
<td>521</td>
</tr>
<tr>
<td>$\sigma^{FEM}(MPa)$</td>
<td>149.39</td>
<td>149.8</td>
</tr>
<tr>
<td>$S$</td>
<td>6.84</td>
<td>5.34</td>
</tr>
</tbody>
</table>

The material parameters listed in Table 7.7 represent $f(g)$ as defined in Equation (2.1). A graphical representation of $f(g)$ or ODF plot is shown in Figure 7.6A. A reference scale for the contours is provided to the right of the plot in Figure 7.6B. The positive maximum value should be interpreted as multiplication factor on a random texture. For example, the max value of 1.9 as seen in Figure 7.6B means that the the max contours are $1.9 \times$ random. This weak texture is an artifact of the truncation of the harmonic series expansion at $\ell = 4$. When the peak intensities of Figure 7.6A are listed and plotted by themselves then then the texture become much sharper. For this simulation these peak intensities are shown in Figure 7.6C.

To determine what common texture components are present in the designed material the peak intensities in Figure 7.6C are compared with the common texture components shown in Table 7.3. The results are presented in Table 7.8 where the
Figure 7.6: A) The resulting ODF plot for the cubic triclinic material. Each section is a contour plot of intensity in Euler space. B) The resulting scale for the ODF plot. C) A more precise analysis of the texture is possible by only looking at the peaks of the cubic triclinic ODF. D) The scale for the contours of the plot of peak intensities.
values are for deviations of 10°, 15°, and 20° from the standard components. Each peak intensity is only identified with one component and the percentage of peaks that are associated with the standard components are listed. It is found that the designed material has a strong “S” texture component with some appearance of Goss and Brass.

Table 7.8: The common texture components listed in Table 7.3 are compared to the peak intensities of Figure 7.6 to identify what percent of the components are found in the designed texture

<table>
<thead>
<tr>
<th>Texture Component</th>
<th>% of Component in specified deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>10°</td>
</tr>
<tr>
<td>Cube</td>
<td>0.0</td>
</tr>
<tr>
<td>10° RD Cube</td>
<td>0.0</td>
</tr>
<tr>
<td>20° RD Cube</td>
<td>0.0</td>
</tr>
<tr>
<td>30° RD Cube</td>
<td>0.0</td>
</tr>
<tr>
<td>Goss</td>
<td>0.0</td>
</tr>
<tr>
<td>Brass</td>
<td>0.0</td>
</tr>
<tr>
<td>Dillamore (D)</td>
<td>0.0</td>
</tr>
<tr>
<td>Copper</td>
<td>0.0</td>
</tr>
<tr>
<td>S</td>
<td>16.3</td>
</tr>
</tbody>
</table>

7.7 Case study 2: Cubic axial–symmetric material

The third and fourth simulations of case study 2 include only the cubic axial–symmetric material parameter as a design variable. The starting point for the design is the ending point of the simulation found in Section 7.5. The objective is min(G). As there is only one material parameter for this symmetry condition it allows for further exploration of the design space. The material parameter for the third and fourth simulations is started in two different locations to determine if there is a local minimum of the objective. The starting and ending values for these simulations can be seen in Table 7.9. The reduction in G is still significant for each simulation, and two local minima for G are found.
Table 7.9: Results for cubic axial–symmetric symmetry. Simulations 3 and 4 in the second case study start in different locations and find two local minima for $G$.

<table>
<thead>
<tr>
<th>Design Variables/Analysis Functions</th>
<th>Initial 3</th>
<th>Final 3</th>
<th>Initial 4</th>
<th>Final 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>$F_1$</td>
<td>0.0</td>
<td>-0.5461</td>
<td>5.0</td>
<td>0.1889</td>
</tr>
<tr>
<td>$M(kg)$</td>
<td>0.6153</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>$G(kJ/mm^2)$</td>
<td>12,205</td>
<td>910</td>
<td>1,520</td>
<td>528</td>
</tr>
<tr>
<td>$\sigma^{FEM}(MPa)$</td>
<td>149.39</td>
<td>150.0</td>
<td>146</td>
<td>149.2</td>
</tr>
<tr>
<td>$S$</td>
<td>6.84</td>
<td>4.5</td>
<td>1.4</td>
<td>6.12</td>
</tr>
</tbody>
</table>

The two textures that result from the Cubic Axial–symmetric simulation are exactly complimentary of each other. This is best seen in the sections of the ODF plot shown in Figure 7.7 where the constant section is $\phi_1$. This allows for clear identification of the two fiber textures. Only the first section of the plot is shown as all the others are identical. Figure 7.7.A is a $\langle 111 \rangle$ fiber and Figure 7.7.B is a Cube $\langle 001 \rangle$ fiber. The $\langle 111 \rangle$ fiber is the result of the simulation three and the Cube fiber is from simulation four. These fibers are standard in the literature (Humphreys and Hatherley 2000) and can be produced in many materials from known processing paths.

Figure 7.7: A) The $\langle 111 \rangle$ fiber texture B) The cube $\langle 001 \rangle$ fiber texture C) The resulting scale for the ODF plot
Chapter 8

Conclusions and Recommendations

A model of a material with arbitrary crystal and sample symmetries is formulated such that the texture is represented by Fourier series expansion. The coefficients, $F^\mu_\nu_\ell$, of this expansion then become the material parameters. For a Face Centered Cubic (FCC) material elastic, plastic and crack driving force responses of the material are expressed and functions of $F^\mu_\nu_\ell$. The material parameters are bounded by a multidimensional convex Hull. Further a method for determining if a point in this space lies within the Hull is utilized to ensure that during optimization a measure the the feasibility of the material is consistent and accurate. These tools and models comprise the MSDi object oriented software package. The software has been successfully compiled and executed on multiple platforms including Microsoft Windows XP, HPUX, and various other UNIX and Linux varieties. A significant computational expense was demanded when generating the database information for the yield model. This limited the resolution of the yield model. Future work that utilizes parallel processing techniques will significantly improve this.

While the Fourier representation of the material allows the material to enter into the realm of multidisciplinary design and optimization it is limited it is ability to accurately represent the material properties. For the turbine disk case study the series representation was truncated at $\ell = 4$. This is sufficient for elasticity but more terms are needed for plasticity.

With a parametric material successfully represented in MSDi it is possible to include geometric and material parameters concurrently as design variables in traditional CAE optimization and analysis software. This is demonstrated through
a case study on the design of a turbine disk. Using shell scripts and file I/O a multidisciplinary optimization loop was created to examine the influence of material texture in the performance of a turbine disk. Two case studies each with three optimization scenarios were formulated. The first simulation of each case study only included the geometric parameters as design variables with an objective to minimize the mass of the disk. This first simulation set a baseline for the following simulations where the material parameters are included to explore the crack driving force response and mass of the disk respectively.

When the material parameters are considered the crack driving force response of the disk, $G$, is improved by more than an order of magnitude in all simulations. This is a significant result that occurs through the coupling of the multiple elements of $\langle C_{ijkl} \rangle$ and their interaction with the far field applied stress.

A textured material is obtained as a result of the first case study but it is not associated with any of the common texture components listed in Table 7.3. It is not readily known how to produce this material and take advantage of its predicted benefits. The material parameters appear to expand the design space when minimizing the mass. This is through indirect effects of relaxing the yield constraint, $\Delta \dot{W}$, and modifying the elastic response of the material. When the designed material was the starting position in the third simulation the mass was reduced by 9.5%. Though indirect the texture does influence the shape optimization of the disk. This result should also be explored further as the database of yield coefficients become more refined.

The second case study also generated textured material results. In the cubic triclinic simulation of Section 7.6 the texture was found to have a strong $S$ component. In the cubic axail–symmetric simulations of section 7.7 the $\langle 111 \rangle$ and Cube $\langle 001 \rangle$ fibers are identified as the best performing materials. These results are significant as these textures and the processing paths required to produce them are known in the literature (Humphreys and Hatherley 2000).

Gradient based optimization techniques were effective in exploring both the material design space and the geometric design space. Random based search methods however were not effective. The random search methods were not able to successfully
chose feasible designs. The problem primarily arose from the complex nature of bounding the material parameters through the use of the convex Hull. A Decoupling of the geometric parameters and the material parameters into two simulations was an solid strategy to obtain feasible solutions.

These results are obtained for Nickel and are likely not the same for other Cubic materials that have different anisotropic elastic behavior. Additionally the reduction in $G$ by an order of magnitude is believed to influence the fatigue life of the spinning disk but it must be acknowledged that it only is one of many factors involved.
Bibliography


