Multi-Scale Modeling of Anisotropic Polycrystalline Plasticity in a Shaped Charge Liner

by

Matthew J. Busche

B.S., University of Illinois, Urbana-Champaign (2000)

Submitted to the Department of Mechanical Engineering
in partial fulfillment of the requirements for the degree of

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Abstract

Polycrystalline microstructure often plays an important role in determining the macroscopic behavior of metals. This work is motivated by the case of a spin-formed shaped charge liner. When these liners are compressed and inverted by detonation of an explosive charge, the resulting jet of material exhibits a distinct rotation. There is no asymmetry at the macroscopic level that would suggest a source of this rotation, and it is in fact a result of microstructurally-induced plastic anisotropy. Procedures are outlined for calculating this anisotropy using orientation imaging microscopy (OIM) and multi-scale modeling techniques.

OIM observations are used to create a statistical characterization of the shaped charge liner's microstructure consisting of its polycrystalline texture (grain orientations) and neighbor correlation, a construct meant to capture the spatial arrangement of grains and grain boundary character. These statistics are used to generate a 3D representative volume element consisting of many discrete grains and respective orientations. The deformation of this representative aggregate is simulated using crystal plasticity within each grain. The results of these simulations are used to fit the parameters of an anisotropic yield function that can be used in macro-scale continuum simulations employing anisotropic plasticity. Prototypical macro-scale simulations were performed, and the results exhibit the expected rotation.

Thesis Supervisor: David M. Parks
Title: Professor of Mechanical Engineering
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Chapter 1

Introduction

1.1 Spin Compensation in Shaped Charge Liners

A shaped charge consists of an explosive charge with a hollow cavity lined by a thin layer of metal (Figure 1-1). This metal liner is typically conical and can be made of copper, tantalum, or other ductile metals (Figure 1-2). When the explosive charge detonates, the liner collapses and forms a high velocity jet (Figure 1-3 and 1-4). The velocity of this jet can exceed 10 km/s (Walters and Zukas, 1988), and the penetrating energy of the jet makes the shaped charge useful in military applications.

The particular shaped charge liner considered in this work is a copper liner manufactured using a spin forming process. Spin forming, also known as shear forming or rotary extrusion, is a manufacturing process used to make axisymmetric forms. A rotating workpiece is drawn over a mandrel by a round tool. The work piece is deformed until the inner surface conforms to the mandrel (Figure 1-5).

When a shaped charge liner is manufactured with a spin forming process, the jet that results has been shown to exhibit a rotation, as indicated in Figure 1-4 (Wiener et al., 1993). In practice this jet rotation is used for spin compensation. Often in military applications, a shaped charge munition is
fired from a rifled barrel to impart rotation for aerodynamic stability. However, the rotation of the shaped charge can degrade the performance of the jet. Spin compensation counters this effect by canceling the rotation of the shaped charge with an equal and opposition rotation in the jet.

The concept of spin compensation dates to the 1950's, and numerous studies have been made on the mechanisms of jet rotation (Zernow and Simon, 1954; Simon and Martin, 1958; Glass et al., 1959; Gainer and Glass, 1962; Held, 1990). It has been proposed that jet rotation could be caused by either residual stresses or material anisotropy imparted to the liner during manufacturing. Chou and Segletes showed that of residual stress relief, elastic anisotropy, and plastic anisotropy, only plastic anisotropy could lead to rotational velocities of the magnitude observed (Chou and Segletes, 1989; Segletes, 1990).

Plastic anisotropy leads to jet rotation by creating a coupling of normal and shear deformation. The compressive strains associated with liner collapse result in small but significant shear strains that lead to jet rotation. The plastic anisotropy of the liner is the result of its microstructure, which is in turn the result of the manufacturing processes used to create it. Given that the macroscopic behavior of the material is a result of its microstructure, it would be desirable to be able to model that relationship.

1.2 A Multi-scale Modeling Approach to Simulation of Spin Compensation

The spin compensation of shaped charge liners is just one example of a problem where the microstructure of a metal affects its macroscopic behavior. One classic example is earing in deep drawn aluminum (Tucker, 1961). When cups are drawn from rolled aluminum sheet, the rim is not uniform as would be expected from a symmetric operation on an isotropic material. The
rolled texture of the sheet leads to anisotropic behavior and the formation of “ears” (Figure 1-6). This phenomenon has been successfully modeled through use of crystal plasticity constitutive modeling (Becker et al., 1993; Balasubramanian and Anand, 1996).

This work examines spin compensation in a shaped charge liner, an example where a fairly subtle effect due to microstructural influence is critical to the performance of the system. A successful simulation of shaped charge liner collapse would need to incorporate the microstructurally-induced plastic anisotropy. However, the techniques outlined herein could also be applicable to many problems where it is desirable to include the effect of microstructure on macroscopic material behavior.

In general, it would be useful to be able to observe the microstructure of a metal, and then, based on these observations, have the capacity to accurately predict its macroscopic behavior. In an attempt to advance this goal, this work develops multi-scale modeling techniques for the simulation of jet rotation in shaped charge liners. This multi-scale framework can incorporate anisotropy in macroscopic simulations as calculated from direct measurements of microstructure.

The multi-scale approach consists of four distinct steps. The first is to use orientation imaging microscopy (OIM) to observe and characterize the microstructure of the liner. The objective of this step is to capture the relevant statistical character that is responsible for the observed macroscopic behavior. The statistics gathered from the 2D data are extrapolated to a form suitable for characterizing 3D grains. This step is detailed in Chapter 2.

In the second step of the multi-scale framework, the microstructural characterization is used to create a model representative volume element (RVE). This volume element consists of a polycrystal aggregate generated to represent the microstructure characteristics captured in the OIM data. The construction of this representative aggregate is discussed in Chapter 3.
The third step of the multi-scale framework is to interrogate the elastic-plastic response of the model aggregate using crystal plasticity simulations. In this step the representative volume element acts as a virtual test sample, hopefully behaving as the real material would. The fourth and final step is to use the stress response of the representative polycrystalline aggregate to compute the parameters for an anisotropic plastic yield function that is suitable for macro-scale simulations. Steps three and four are described in Chapter 4.

Chapter 5 contains discussion of the results for various calculations of the yield surface and prototypical macro-scale simulations. These simulations test the effectiveness of the multi-scale modeling approach in predicting spin during a shaped charge liner collapse and explore issues relating to the representation of the microstructure in the RVE. The final chapter contains conclusions and directions for further research.
Figure 1-1: Simplified schematic of a shaped charge.

Figure 1-2: A spin-formed copper shaped charge liner.
Figure 1-3: Collapse of a spin-formed shape charge liner captured by high-speed photography (Winer et al., 1993).
Figure 1-4: Jet formation, note that gridlines slope down to the left, indicating a slight rotation (Winer et al., 1993).
Figure 1-5: Spin forming process for shaped-charge liners (Segletes, 1990).

Figure 1-6: Earing in a drawn aluminum cup (Anand, 1996).
Chapter 2

Microstructure Characterization and Modeling

A full characterization of the polycrystalline microstructure of the shaped charge liner would encompass all aspects of grain orientation, grain topology, and spatial correlations of grains. In referring to “polycrystalline microstructure,” all aspects of dislocation structure that otherwise might be considered as part of a microstructural characterization are excluded, and future references to “microstructure” refer only to polycrystalline microstructure.

The particular microstructure present in the shaped charge liner is the result of a combination of forming procedures, most notably rolling and spin forming. The result of these forming procedures is that the microstructural character is non-random to the extent that the macroscopic response of the material is changed from the isotropic response that would be observed for a material with entirely random microstructure. The macroscopic response becomes anisotropic and results in a spinning jet upon detonation.

At the scale of a few grains, there is of course a great deal of variance in the actual grain orientations and topology in any local neighborhood of grains. However, at the macroscopic scale, and from one liner to the next, the
average response of the material, and the rotation of the jet, is consistent. This would imply that there are relevant statistical quantities that could be used to characterize the microstructure and their effects on the macroscopic behavior of the system.

The goal of the microstructure characterization is to determine the appropriate statistics and extract them in a useable form from experimental specimens of a shaped charge liner. The full characterization of microstructure must be reduced to a more useable and accessible form. The particular microstructure statistics that this work considers are grain texture and spatial correlation, and the tool used to determine these statistics is orientation imaging microscopy.

2.1 Orientation Imaging Microscopy

Orientation imaging microscopy (OIM) is a variation on scanning electron microscopy that allows sampling crystal orientations (Adams and Olson, 1998; Schwarzer 1997). It functions by reflecting an electron beam off a polished surface of the specimen. (Figure 2-1). The electron beam interacts with the crystal lattice, and the portion of electrons that is reflected forms an electron backscattered diffraction (EBSD) pattern (Figure 2-2), also known as a Kikuchi pattern (Kikuchi, 1928). Automated image processing and specimen indexing allows the determination of crystal orientation over a regular spatial grid.

The use of OIM to create model microstructures in finite element simulations is not new. However, previous researchers have limited their simulations to two dimensions (Bhattacharyya et al., 2001; Becker, 1998). This limitation comes from the fact that, while OIM allows the compilation of various statistics relating to microstructure, the information is available only as a 2D material cross section. It is in fact possible to perform serial sectioning of specimens, and then with interpolation create a full 3D model of
orientation data (Stoken et al., 2000). However, this technique is costly and time consuming, and the resulting data set is difficult to work with. In this work we hope to develop techniques for making a full microstructural characterization with a single OIM scan. This requires adopting certain assumptions; the most paramount is that a 2D cross section can in fact deliver a complete material characterization. Additionally, the two-dimensional statistics that are compiled must ultimately be extrapolated into a 3D representative volume element, so the statistics compiled must be tailored such that this translation is possible.

Two characterizations are often considered when analyzing OIM data, the orientation distribution function (texture) and the spatial correlation of crystal orientations. Texture is typically the most important microstructural characteristic in determining macroscopic plastic behavior. It is a relatively easy statistic to deal with, as it involves only the respective volume fractions of the crystal orientations present in the aggregate. It can be directly extrapolated from the 2D OIM scan into a 3D representative volume by using the stereological assumption that area fractions are equal to volume fractions. Texture can be determined with traditional x-ray diffraction techniques; however, OIM provides additional statistical information in the form of spatial correlations. It is this information that makes the OIM technique uniquely powerful as compared to x-ray diffraction techniques.

There is ample evidence that the spatial arrangements of grains should be important in determining the macroscopic behavior of a polycrystalline material. Mika and Dawson showed that in finite element simulations of polycrystalline plasticity in which each grain was represented by a single element, the spatial arrangement of the orientations changed the response of the simulation (Mika and Dawson, 1998).

In a real polycrystalline aggregate, the importance of the spatial information comes from the physical processes involved in plastic deformation. The misorientation of neighboring grains is important in the
role it plays in constraining the deformation of grains and creating local stress concentrations. Relative orientations of neighboring grains also play an important role in shear localization (Anand and Kalidindi, 1994). However, the spatial information is considerably more difficult to deal with than the texture, both because of its complexity and the need to extrapolate from two to three dimensions.

2.2 Calculating Microstructure Statistics

2.2.1 Experimental Procedure

Specimens for OIM analysis were taken from a spin-formed copper shaped charge liner at multiple locations along the length. Specimens were polished, and OIM data was collected using a TSL (TexSEM) orientation imaging microscope. Prior to any analysis, the data was run through a clean-up procedure available in the TSL software (TSL, 1999) to eliminate points with low confidence indices.

Figure 2-3(a) shows the OIM data set that was used in this work, which was taken from a sample near the apex of the shaped charge liner, as indicated in Figure 2-3(b). Figure 2-4 shows a pole figure for the OIM data represented in Figure 2-3. The (111) pole figure reveals that the strongest texture component is aligned 45 degrees to the axis that runs from the apex of the cone to the base.

The data set was sampled at a resolution of 479 points in the x-axis and 312 points in the y-axis. The data was scanned on a hexagonal grid, with a spacing of 0.45 μm in the x-direction and 0.78 μm in the y-direction. The average grain size in the sample is approximately 20 μm, while the thickness of the liner is nominally 2 mm. There could be considerable variation in the microstructure through the thickness, but additional experimental data is needed to evaluate this possibility.
2.2.2 Analysis of OIM Data

The data set resulting from an OIM scan is crystal orientation sampled over a set of data points on a hexagonal grid. The crystal orientation data is in the form of Euler angles, which define the rotation of the crystal relative to a reference frame. To translate this data into a form useful in creation of a 3D representative volume, statistics relating to the polycrystalline grains must be collected.

The first step in compiling the grain statistics is to make a point-by-point comparison of the data points and assign each point to an appropriate "grain". Figure 2-6 shows a schematic of this grain searching procedure. Beginning at the top left of the OIM file, each data point is progressively assigned to a grain. To determine which grain a point is assigned to, the orientation of the point is compared to the orientations of all grains within some distance of the point (indicated as a dashed box in Figure 2-6). This distance, typically a spacing of 5 to 10 data points, is enforced so that only contiguous regions of data points are assigned to the same grain. The orientation of the data point is considered to "match" the orientation of a grain if all of the Euler angles are within some tolerance angle. A tolerance value of 15 degrees typically gives good results, though there is little sensitivity to this value in the final result, as long as it is over a few degrees. If the orientations match, then the data point is assigned to the grain. The orientations of grains are determined as a running average of the data points added to each grain. If a data point does not match any of the grains it is compared to, then it is assigned to a new grain.

In addition to assigning each data point to a grain, nearest neighbor statistics are also collected when the OIM data is analyzed. Because the data is sampled on a hexagonal grid, two possible neighbor relationships are considered for each data point (indicated as two dashed lines in Figure 2-6). After each data point is assigned to a grain, it is compared to the data points
to the left and upper left. If either of these points is part of a different grain, then this “neighbor” is recorded. By only comparing each point to these two neighbors, it is insured that each possible neighbor relationship is tested only once.

Two additional steps must be taken to ensure the accuracy of the sampled set of grains. Because the grain search algorithm scans progressively through the data, it is possible for a concave shaped grain to be misinterpreted as two or more separate grains. To solve this problem, all grains are compared based on their orientation. If the grains have the same orientation (to within a few degrees in each Euler angle) and are adjacent, then the statistics of the two grains are combined. Also, noise, or bad data points in the OIM scan can result in grains consisting of one, or only a few data points. These grains are removed by setting a minimum grain size (generally about 5 points) and removing all grains with area smaller than this minimum. This procedure has a negligible effect on the total amount of data (less than 1%), but dramatically reduces the number of grains recorded.

For the OIM data in Figure 2-3, the grain search procedure initially finds 957 grains. Merging misinterpreted grains eliminates 182 of these, and the size cutoff eliminates 202 grains accounting for 521 data points. This leaves a final total of 573 grains for which grain statistics were compiled.

2.2.3 Grain Statistics

The point-by-point analysis of the OIM data yields a list of grain orientations, along with the number of data points in each grain. These two measures define the “grain texture”, a discrete set of orientations and respective weightings. For each of the \( n \) grains, the grain texture \((T, g)\) gives the orientation \( g \), in the form of three Euler angles, and
\[ T_i = \frac{N_i}{N_0} \] (2.1)
gives the volume fraction for grain \( i \), where \( N_i \) is the number of data points in grain \( i \), and \( N_0 \) is the total number of data points in the OIM file. The stereological assumption that area fraction and volume fraction are equal allows the direct translation of this quantity into three dimensions for use in creation of the representative volume.

Within any single grain, the orientation recorded at the OIM data points typically ranges by up to a few degrees in each Euler angle. This scatter is due to a combination of the error associated with the OIM measurement, and actual changes in local orientation over a grain. Non-uniform grain orientation can result from lattice strain caused by residual stresses or lattice rotation associated with geometrically necessary dislocations or subgrains. When each grain’s orientation is homogenized as the average of the points within it, there is a slight loss of texture information as compared to the original OIM data set.

The point-by-point analysis of the OIM data also yields a list of the nearest neighbor relationships for each grain. For each grain, \( i \), the computed matrix \( N_{ij} \) gives the number of instances of a grain boundary segment with grain \( j \). This information characterizes both the neighbors that each grain has, and the length of the grain boundary shared with that neighbor.

### 2.2.4 Considerations for Creating a 3D Microstructure Characterization

The grain statistics compiled from the OIM data will ultimately be used to create a representative three-dimensional aggregate of grains. One fundamental problem is that for each grain present in the 2D cross section,
only a few of its neighbors are revealed. However, when the 3D aggregate is created, each “grain” may have twenty or more neighbors. To determine whether a 3D “grain” in the representative aggregate properly represents the true microstructure, it is necessary to generate a more complete description. The statistics for similarly oriented grains in the 2D scan are combined to create a statistical characterization for a single 3D grain that will appear in the 3D representative volume.

The grains identified in the OIM data are sorted into groups by orientation using an adaptive binning algorithm; each group will represent a 3D grain. A single orientation is computed for each group as the average of the orientations of the grains in the group, weighted by the volume of each individual grain. The grain texture and boundary area statistics are redefined in the reduced basis defined by this set of orientation groups. The grain texture volume fractions, $T$, are redefined for the discrete set of orientations as $T^*$, which is computed as the sum

$$T^*_a = \sum_{i \in a} T_i$$  \hspace{1cm} (2.2)

over all grains $i$ in orientation group $a$.

In similar fashion, the matrix of grain boundary lengths, $N$, is grouped into $N^*$, which now describes the boundary length shared by grains of orientation groups $i$ and $j$.

Forming the reduced basis of grain orientations solves another problem associated with the creation of the 3D representation. The OIM data yields statistics for a large number of grains, and it may not be desirable to include as many grains in the 3D representation. The reduced basis allows the information in the OIM data to be compressed into a small number of representative 3D grains while still preserving most of the statistical character.
2.3 The Neighbor Correlation

Spatial correlation in OIM data is often explored in the form of a 2-point correlation (Adams and Olson, 1998). While this correlation offers a thorough characterization of spatial aspects of a microstructure, it is complex and difficult to work with. In addition, the 2-point correlation offers more information than is most likely necessary. For this work, the most important aspect in the spatial ordering of grains in an aggregate is the set of adjacent neighbors possessed by each grain. While long-range order has been shown to exist in polycrystalline specimens (Lee, 1999; Wittridge and Knutsen, 1999), it is most noticeable at scales larger than the sample dimensions for the OIM data in this work. For a region of the size considered here (200 microns) the primary influence of spatial ordering on the macroscopic plastic response comes from constraints and stress concentrations produced by the interactions between grains and their direct neighbors.

In an effort to capture the simplest statistical measure of the spatial ordering, while retaining the salient aspects, a construct called the neighbor correlation is created. For an aggregate of grains (in two or three dimensions), the neighbor correlation, \( \eta \), is defined as

\[
\eta_g = \frac{1}{|B_i|} |B_i \cap B_j|
\]

where \( B_i \) represents a measure of the boundary of grain \( i \). Thus each scalar component of \( \eta \) describes the magnitude of the area of intersection between grains \( i \) and \( j \), scaled by the total boundary area of grain \( i \). In terms of the reduced grain orientation basis, each component describes the intersection between orientation groups \( i \) and \( j \).

The neighbor correlation can be interpreted as a probability distribution function, where \( \eta_g \) represents the probability of a unit area of a grain \( i \) being
part of a boundary with grain $j$. This form is particularly well suited for the necessary extrapolation from two to three dimensions. Because of the scaling, the correlation is not a function of the total area, or number of neighbors, that a grain may have in the 3D representation.

In the 2D OIM data, the boundaries consist of discreet line segments and the neighbor correlation can be computed directly from the grouped matrix of boundary lengths, $N^*$, as

$$\eta_{ij} = \frac{1}{N_j} \sum_{\rho=1}^{N^*} N_{ij}$$  \hspace{1cm} (2.4)

In translating the neighbor correlation from 2D to 3D, the assumption that line length is equal to area is employed. In the 3D RVE, grain boundaries are composed of element faces. The calculation of $\eta$ is identical, except that element faces are counted instead of line segments.

The neighbor correlation, in combination with the grain orientations, characterizes grain boundary misorientation, albeit in a reduced basis. It would be possible to consider only grain boundary misorientation as the spatial statistic to match in the 3D representative volume. However, using the neighbor correlation insures that not only the grain boundary misorientation distribution is correct, but the various boundaries are present constraining the correct grains; the “absolute” misorientation distribution is preserved.

Figure 2-5 shows a graphical representation of the components of $\eta$ as computed for the OIM data in Figure 2-3 with the 50 grain-orientation groups listed in Table 2.1. Note that the diagonal is non-zero. Because each component represents multiple similarly oriented grains from the OIM data, the diagonal component represents boundaries between discrete grains within the same group. In the physical specimen, these boundaries were low angle misorientation boundaries, likely between two subgrains. As a
consequence of the procedure for forming a fully representative \( \eta \), these boundaries are reduced to a boundary between two grains of the same orientation, or, in effect, to no boundary at all.
Figure 2-1: Schematic of OIM (Adams 1998).

Figure 2-2: Kikuchi pattern generated by ESBD.
Figure 2-3: Graphical representation of OIM data, with color representing crystal orientation (a) taken from liner with coordinate system and approximate location as indicated in (b).
Figure 2-4: Pole figure for OIM data (TD and RD are x- and y-direction, respectively).

Figure 2-5: Neighbor correlation determined for a 50-orientation group basis.
Figure 2-6: Schematic illustration of point-by point OIM data analysis, point $p$ is being queried.
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<th>θ</th>
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<th>Tᵢ*</th>
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Table 2.1: Orientations (Euler angles in Bunge notation) and volume weightings for the reduced grain orientation basis.
Chapter 3

Creating a Representative Volume Element

3.1 Finite Element Representation of a 3D Polycrystalline Aggregate

The model aggregate is created in a regular rectangular mesh of finite elements. A “grain” is represented simply as a contiguous region of elements with the same crystal orientation. The size of the mesh is constrained by computational resources; the other major choice in creating the RVE is the number of grains to represent. Two factors compete in determining the appropriate number of grains. The larger the collection of grains represented, the more closely the aggregate can represent the microstructural statistics gathered from the OIM data. However, an increased number of grains dictates that each grain will be resolved with fewer elements. Using a smaller number of grains allows more accurate modeling of the deformation occurring within individual grains.

The task of creating the 3D model aggregate ultimately becomes the choice of crystal orientation for every element in the finite element mesh. This task is complicated by the need to make these choices as consistently as possible with both the texture and neighbor correlation defined by the
experimental observations, as well as the large number of elements in the problem.

To simplify the construction of the representative aggregate, the task is separated into two distinct aspects, creation of the grain geometry and choosing orientations for the grains. The geometry of the grains is created using Voronoi tessellation. Then, with the grain geometry held constant, appropriate orientations are chosen for the grains to optimize the texture and neighbor correlation of the aggregate relative to the observed microstructure characterization.

### 3.2 Voronoi Tessellation

Voronoi tessellation creates “grains” based on the spatial configuration of seed points. The grain associated with each seed is mathematically defined as the region of space which is closer to that seed than any other. Since a regular rectangular mesh is used to represent the RVE, only the discreet form of the Voronoi tessellation needs to be considered. This eliminates the need to consider the geometry of Voronoi cells, and the problem reduces to finding the closest seed to each element. A periodic grain geometry is created by considering the periodic images of each seed as well.

When creating a grain aggregate using Voronoi tessellation, it is desirable to ensure that a minimum spacing is enforced between seeds. This technique offers two benefits. By setting a minimum radius for each seed, the pathological grains created when two seeds in a Voronoi tessellation are too close can be avoided. In addition, the radius parameter gives some control over the volume distribution for the 3D grains created by the tessellation. The volume distribution can be made to match the area distribution observed in the physical microstructure.

To achieve a minimum seed spacing, the seeds are distributed in the mesh box through a hard sphere Monte Carlo algorithm (Allen and Tildesley,
The desired number of seeds is placed in the box, initially in a regular grid, such that the minimum spacing is achieved. The seeds are then randomized by perturbing seed positions and accepting the perturbation only if it overlaps no other seeds. Figure 3-1 shows a 1000-grain RVE created in a mesh with 10^6 elements. The minimum spacing used for this aggregate was relatively large (5, with a mesh face length of 100), resulting in nearly uniform grain size.

3.3 Choosing Grain Orientations

Once the grain geometry has been created, all that remains to complete the microstructure is choosing appropriate orientations for each grain. The most desirable set of orientations minimizes the error of the texture and neighbor correlation of the representative aggregate with respect to the characterization of the OIM data.

The technique employed in this minimization is simulated annealing. Simulated annealing is a very general optimization algorithm that employs the link between statistical mechanics and combinatorial optimization (Kirkpatrick et al., 1983). It has been applied in fields ranging from design of pipe networks (Costa et al., 2000) to timber harvest planning (Chen and Von Gadow, 2002).

In basic function, it minimizes a given quantity by making perturbations to a system and then accepting perturbations based on how they affect the minimization quantity. It is similar to an atomistic Monte Carlo method (Allen and Tildesley, 1987), except perturbations are evaluated based on an artificial parameter rather than the potential energy of a physical system. In optimizing the RVE, the system is perturbed by selecting any of the grains at random, and changing the orientation of that grain from its current orientation, to another orientation in the discrete collection of grain textures. The perturbations are accepted with a probability
where $\Delta E$ is the change in error resulting from the perturbation, and $\theta$ is a combined scaling factor and “temperature” parameter. The “error” at any point during the simulated annealing is effectively the difference between the current state of the aggregate and the optimal state, or that state which exactly matches the microstructural statistics of the OIM data. The error is computed as

$$E = wE_T + (1-w)E_\eta$$  \hspace{1cm} (3.2)$$

where the weighting parameter $w$ can be used to tailor the relative importance of the error with respect to the grain texture and neighbor correlation, $E_T$ and $E_\eta$. The grain texture error

$$E_T = \sum_{i=1}^{N} |T_i^* - T_i^{**}|$$  \hspace{1cm} (3.3)$$

is the difference between the orientation volume fractions $T_i^{**}$ in the current iteration, number $n$, of the simulated annealing, and $T^*$, the volume fractions (in grouped form) observed in the OIM data. The neighbor correlation error is similarly defined as

$$E_\eta = \frac{1}{N} \sum_{i=1}^{N} \sum_{j=1}^{N} |\eta_{ij} - \eta_{ij}^{**}|$$  \hspace{1cm} (3.4)$$

for an aggregate of $N$ grains. Note that both error measures are scaled such that the maximum error is one.

The “temperature” parameter $\theta$ decreases during the course of the simulated annealing. The minimization begins with this temperature at a relatively high level. The change in error brought about by a perturbation is
dependent on the number of grains in the RVE, since the errors are scaled. An appropriate initial temperature is selected at a level such that the majority of perturbations are accepted. This results in randomization at the beginning of the optimization, making the end result relatively independent of the initial state. The temperature is iteratively reduced through $n_s$ discrete temperature steps, with $n_p$ perturbations evaluated at each step. Obtaining the "best" minimum requires tinkering with these values, but values of 100 and 10000, respectively, are good starting points.

As the temperature decreases, the system settles into a minimum, and the simulated annealing ends when the temperature drops to the point that no perturbations are being accepted, typically two orders of magnitude. The high temperature at the start of the annealing is meant to make the eventual minimum as global as possible.

### 3.4 Resulting Aggregates

Figure 3-2(a) shows an RVE containing 250 grains resolved on a 27000-element mesh. The texture and neighbor correlation for 50 grain groups was matched with errors of $E_T = 0.018$ and $E_\eta = 0.087$. To achieve this match, 2.5 million perturbations were evaluated over the course of the simulated annealing. Even this large number is still the tiniest fraction of the total number of possible aggregate configurations. With 50 possible orientations for each of the 250 grains, there are $50^{250}$ possible aggregates.

It was found through experimentation that in order to achieve a satisfactory match in the grain statistics, around five times as many grains needed to be present in the RVE as the number of grains for which statistics were gathered. This is necessary in the case of the grain texture because the probability that the volumes of 50 grains in the RVE would match exactly with the 50 volume fractions dictated by $T^*$ is nearly zero. Multiple instances
of each grain are also necessary to achieve a close match in the neighbor correlation.

Figures 3-3(a) and (b) show the neighbor correlation of the aggregate at the start and end of the simulated annealing optimization. Comparing Figure 3-3(b) to Figure 2-5 shows a close qualitative match between the neighbor correlation of the RVE and the reduced neighbor correlation observed in the OIM data. Quantitatively, the neighbor correlation error is initially $E_\eta = 0.49$, compared to the final error $E_\eta = 0.087$. Figure 3-2(b) shows a pole figure for the RVE, and comparing this to the pole figure for the OIM data (Figure 2-3) shows some error. The match with the group grain texture $T^*$ is correct to less than 2%. This error is due primarily to the distortion in texture from grouping the grains, and to a limited extent, the homogenization of orientations within grains.
Figure 3-1: A representative volume containing 1000 grains resolved on a million-element mesh.
Figure 3-2: Final state of 250 grain, 27000-element RVE after simulated annealing: mesh (a) pole figure (b).
Figure 3-3: Neighbor correlation of 250 grain, 27,000-element RVE at initial state (a); and after simulated annealing (b).
Chapter 4

Evaluation of Material Anisotropy

4.1 Crystal Simulations

The ultimate source of the anisotropic behavior of the shaped charge liner is the underlying anisotropy of the single crystal grains. We capture this at the local grain level through use of crystal elasticity and crystal plasticity constitutive laws. In creating the representative volume, emphasis was placed on matching the characteristics of the experimentally-observed shaped charge liner microstructure. This representative volume can now serve as a virtual test specimen, behaving as the real material would, at least to the extent that the behavior of the single crystal grains can be accurately modeled.

The information that needs to be extracted from the representative volume is how the material responds to various deformations. With the simulation of jet rotation in mind, particular interest is given to finding the magnitude of the various normal-shear couplings. To ensure that all potential deformation couplings are sampled when exercising the representative aggregate, six independent simulations are performed. These are isochoric extensions in the three coordinate directions and three pure shear deformations in orthogonal planes. The boundary conditions were
applied as velocity gradients on the RVE surfaces. The velocity of each surface node is determined as \( v(x) = L(x - 0) \) with \( v(0) = 0 \). The appropriate velocity gradient, \( L \), is used for each of the tensile and shear simulations. For example, tensile extension in the x-direction and shear in the x-y plane are prescribed by

\[
L = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -0.5 & 0 \\ 0 & 0 & -0.5 \end{bmatrix} \quad \text{and} \quad L = \begin{bmatrix} 0 & 0.5 & 0 \\ 0.5 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix},
\]

respectively.

The simulations were performed in the parallel finite element code ALE3D (Couch et al., 1993). The simulations were executed on the ASCI Blue parallel computer at Lawrence Livermore National Laboratory. Each simulation was executed on 32 processors, which allowed a mesh consisting of 27000 elements to be used. Figures 4-1 and 4-2 show two examples of deformed meshes for the tensile and shear boundary conditions, respectively. The examples are shown at approximately 10% strain.

### 4.2 Crystal Elasticity and Plasticity

The crystal constitutive model employed is based on the crystal kinematics described by Asaro (Asaro, 1983) and the rate-dependent formulation of Peirce et al. (Peirce et al., 1983). Here the equations are recast to work in the current configuration rather than the reference, an updated Lagrangian framework rather than the total Lagrangian (Becker, 1998).

The velocity gradient, \( L \), is additively decomposed into elastic and plastic components

\[
L = L' + L'' \quad (4.1)
\]
The two components are further decomposed into symmetric and antisymmetric parts representing the rate of deformation tensor, \( \mathbf{D} \), and the spin tensor, \( \boldsymbol{\omega} \).

\[
\mathbf{L} = \mathbf{D} + \boldsymbol{\omega}
\]
\[
\mathbf{L}^* = \mathbf{D}^* + \boldsymbol{\omega}^*
\]
\[
\mathbf{L}^p = \mathbf{D}^p + \boldsymbol{\omega}^p
\]  

The plastic part of the rate of deformation tensor and the plastic spin are expressed in terms of the slip rates, \( \dot{s}^\alpha \), along the slip direction \( s^\alpha \) and on crystallographic planes with normals \( m^\alpha \).

\[
\mathbf{D}^p = \frac{1}{2} \sum_{\alpha=1}^{N} \dot{s}^\alpha (s^\alpha \otimes m^\alpha + m^\alpha \otimes s^\alpha) = \sum_{\alpha=1}^{N} \dot{\gamma}^\alpha \mathbf{P}^\alpha
\]

\[
\boldsymbol{\omega}^p = \frac{1}{2} \sum_{\alpha=1}^{N} \dot{s}^\alpha (s^\alpha \otimes m^\alpha - m^\alpha \otimes s^\alpha) = \sum_{\alpha=1}^{N} \dot{\gamma}^\alpha \mathbf{W}^\alpha
\]

For the present simulations of copper, an FCC metal, deformation is assumed to occur on the twelve slip systems with \(<110>\) slip directions and \{111\} slip-plane normals. The stretch and rotation of the crystal lattice are captured by the elastic part of the velocity gradient. The slip vectors evolve during deformation according to

\[
\dot{s}^\alpha = \mathbf{L}^* \cdot s^\alpha \quad \text{and} \quad \dot{m}^\alpha = \mathbf{L}^* \cdot m^\alpha
\]

By assuming a stress potential in which the stress is related to the elastic distortion of the crystal lattice, the rate of Kirchhoff stress, \( \dot{\tau} \), is given by

\[
\dot{\tau} = \mathcal{C} : \mathbf{D}^* + \mathbf{D}^* \cdot \tau + \tau \cdot \mathbf{D}^* + \boldsymbol{\omega}^* \cdot \tau - \tau \cdot \boldsymbol{\omega}^*
\]

where \( \mathcal{C} \) is the fourth-order tensor of elastic moduli and \( \tau \) is the Kirchhoff stress measure. Using the additive decomposition of the rate of deformation tensor and the spin into elastic and plastic parts, and combining the second
and third terms of Equation 4.6 with the modulus to define a new fourth-order tensor, $\mathbf{K}$, the Jaumann rate of Kirchhoff stress rate can be written

$$\mathbf{\dot{\tau}} = \mathbf{\dot{\omega}} + \mathbf{\dot{\tau}} = \mathbf{K} : \mathbf{D} - \mathbf{K} : \mathbf{D}^{\sigma} - \mathbf{\omega}^{\sigma} \cdot \mathbf{\tau} + \mathbf{\tau} \cdot \mathbf{\omega}^{\sigma}$$  \hspace{1cm} (4.7)

The last three terms of Equation 4.7 involve plastic deformation. They can be expressed in terms of slip rates as

$$\sum_{\alpha=1}^{N} \dot{\gamma}^\alpha (\mathbf{K} : \mathbf{P}^\alpha + \mathbf{W}^\alpha \cdot \mathbf{\tau} - \mathbf{\tau} \cdot \mathbf{W}^\alpha) \equiv \sum_{\alpha=1}^{N} \dot{\gamma}^\alpha \mathbf{R}^\alpha$$  \hspace{1cm} (4.8)

where $\mathbf{P}^\alpha$ and $\mathbf{W}^\alpha$ are defined in Equations 4.3 and 4.4. Using Equation 4.8, the Jaumann stress rate is given by

$$\mathbf{\dot{\tau}} = \mathbf{K} : \mathbf{D} - \sum_{\alpha=1}^{N} \dot{\gamma}^\alpha \mathbf{R}^\alpha$$  \hspace{1cm} (4.9)

The tensor, $\mathbf{K}$, is known in terms of the crystal moduli and the current stress state. The tensors $\mathbf{R}^\alpha$ are functions of the stress state and the known crystal geometry.

What remains is to specify the slip rates, $\dot{\gamma}^\alpha$. In the rate-dependent constitutive formulation adopted here, the slip rate on a slip system is assumed to be related to the resolved shear stress, $\tau^\alpha = \mathbf{\tau} : \mathbf{P}^\alpha$, through a power law relation

$$\dot{\gamma}^\alpha (s^{-1}) = \dot{\gamma}_0^\alpha \left( \frac{\tau^\alpha}{g^\alpha} \right)^{m_{\tau}}$$  \hspace{1cm} (4.10)

where $g^\alpha$ is the slip system strength or resistance to shear, $m = 0.005$ is the strain rate sensitivity exponent and $\dot{\gamma}_0^\alpha = 0.002 (s^{-1})$ is a reference shear rate. The value of the strain rate sensitivity exponent is low, and the material is nearly rate independent.
With the slip rates given as an explicit function of the known resolved shear stresses, the rate-dependent method avoids the ambiguity in the selection of active slip systems which is encountered in many rate independent formulations. However, integration of the stress rate, Equation 4.9, with the slip rate defined by Equation 4.10 produces a system of equations which is numerically “stiff”. A fully implicit integration scheme for the slip rates is used to increase the stable time step (Becker, 1997).

For evolution of the slip system hardness, the Taylor hardening assumption, that all slip system strengths are equal at a material point, is employed. The hardening as a function of accumulated slip,

\[ \gamma = \sum_{\alpha=1}^{N} \gamma^{\alpha} dt' \]  

(4.11)

is assumed to follow the macroscopic hardening behavior, which is fit to a power law relationship

\[ g^{\alpha}(MPa) = C_1 (\gamma + C_2)^{C_3} \]  

(4.12)

The constants \( C_1 = 62.05 \), \( C_2 = 0.002 \), and \( C_3 = 0.1 \), were used in the simulations and are realistic for copper, but were not fit to the strain hardening of the particular copper in the shaped charge liner, for which this data was not available.

### 4.3 Generalized von Mises Yield Surface

The results of the crystal simulations are the stress response of the RVE to various deformations. This needs to be translated into a useful set of data that somehow represents the anisotropy of the material response. It is also necessary that this computed anisotropy be useable in a macroscale simulation. The goal of the multi-scale framework is that a macro-scale
simulation can be conducted wherein each element has the average
constitutive response of the RVE.

A constitutive model that can achieve this is a generalized quadratic yield
function, also called a generalized von Mises yield function. It is sufficiently
general to allow the normal-shear couplings that are critical to accurately
modeling the shaped charge liner collapse. This form of a yield function first
appears in work by Green and Naghdi (Green and Naghdi, 1965). The yield
surface is defined as

\[ \phi = 0 = \sqrt{\frac{3}{2}} \sigma' : K : \sigma' - \sigma_f \] (4.13)

where \( \sigma_f \) is the equivalent flow strength and \( K \) is a fourth-order tensor
mapping the deviatoric stress direction to the deviatoric strain rate direction.
The flow strength is determines if the material has yielded in the current
stress state \( \sigma' \), and, through a normality flow assumption, \( K \) determines the
direction of plastic flow if yield has occurred. Primary attention in this work
is given to the direction of plastic flow. In the collapse of a shaped charge
liner, the material undergoes huge strains (>> 1) and will yield very early in
the collapse. Determining the exact moment of yield is not as important as
accurately capturing the direction of subsequent plastic flow. As such,
primary attention is given to computing \( K \), while the flow strength is
approximated as constant. More accurate modeling would require
considering the evolution of flow strength.

\( K \) has the symmetries \( K_{ijkl} = K_{ijlk} = K_{klij} \), which leave only 21 independent
components. Because \( K \) is multiplying only the deviatoric stress, there are
actually only 15 independent components, but the full set of 21 components
will be computed. If \( K \) is equal to the identity tensor, the yield surface and
plastic flow model would be identical to classical J2-flow theory.
4.4 Determining Yield Function Parameters

4.4.1 Calculating K

The normality flow assumption, that plastic flow occurs in a direction normal to the yield surface, yields a flow rule defined as

\[
d^p = \dot{\lambda} \frac{\partial \phi}{\partial \sigma'} = \frac{3}{2} \frac{\dot{\varepsilon}^p}{\sigma'_f} K : \sigma'
\]  

(4.14)

where \( \dot{\varepsilon}^p \) is the plastic work rate.

The crystal simulations give the stress response to various strain rates. These stress results are averaged over the entire mesh to form a single set of six stresses, \( \{\bar{\sigma}\} \), that characterize the response of the RVE. Thus each simulation provides a set of six equations for the components of \( K \),

\[
\{d^p\} = \frac{3}{2} \frac{\dot{\varepsilon}^p}{\sigma'_f} K \{\bar{\sigma}\} = \chi K \{\bar{\sigma}\}
\]  

(4.15)

The plastic strain rate of the RVE, \( \{d^p\} \), is determined based on the boundary conditions of the simulations and the initial elastic response, an exercise left for Section 4.4.2. The average value of the von Mises equivalent stress is used as the RVE flow stress. The plastic work rate could also be averaged over the mesh, but for the calculations in this work, the values of plastic work were not available due to post-processing limitations. Hence, the average total strain energy rate, \( \bar{\varepsilon} \), is used in its place. This approximation should result in a negligible effect for results in the fully plastic range.

To solve these equations for the components of \( K \), Equation 4.15 is recast as

\[
[\sigma] \{K\} = \frac{1}{\chi} \{d^p\}
\]  

(4.16)
with $\mathbf{K}$ expressed as a vector of 21 components, $\mathbf{d}^p$ a vector of six components, and \{\overline{\sigma}\} as the matrix $[\sigma]$ with dimensions of 6 by 21 containing the average stress components as defined in Table 4.1. By combining the results from the six simulations, with data taken at the same average strain energy in each simulation, a set of thirty-six equations can be formed. This system is overdetermined, but the use of all six simulations ensures that all possible deformation couplings are represented.

The combination of the results from the six simulations yields the system of equations

$$
[\sigma]_{6x21} \{K\}_{21x1} = \left\{ \begin{array}{c} 
\mathbf{d}^p \\
\mathbf{X}
\end{array} \right\}_{36x1} 
$$

(4.17)

which is solved by employing a singular value decomposition (SVD). The matrix $[\sigma]$ is decomposed as

$$
[\sigma]_{6x21} = [U]_{6x21} [S]_{21x21} [V]^T_{21x21} 
$$

(4.18)

where $[U]$ and $[V]$ are orthogonal matrices and $[S]$ is diagonal. This decomposition allows the pseudo-inverse to be formed as

$$
[\sigma]^{-1}_{21x36} = [V][S]^{-1}[U]^T 
$$

(4.19)

The pseudo inverse allows the direct solution, in a least squares sense, of Equation 4.17. In solving for $\mathbf{K}$, stress results from the six crystal simulations can be chosen at any value of strain energy after the elastic-plastic transition. Table 4.2 shows the components of $\mathbf{K}$ as determined for the RVE shown in Figure 3-3(a) with the results of the crystal simulations taken at strain energies corresponding to strain levels of approximately 1% and 10%. 

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This entire tensor represents the anisotropic behavior of the RVE, but for the simulation of the shaped charge liner, the lower-left block of nine components is the most significant. These are the components that describe the couplings between normal stress and shear strain that mainly are responsible for jet rotation. These components would be zero for an isotropic material. There is also a considerable change in these components at the two strain energy levels. These values evolve with strain as the texture and slip system strengths change.

### 4.4.2 Calculating Elastic Compliance of RVE

The procedure for calculating \( K \) relies on knowledge of the plastic strain rate occurring in the RVE. However, the boundary conditions of the crystal simulations specify a total strain rate. The strain rate can be additively decomposed into plastic and elastic components

\[
d = d^e + d^p
\]

In the absence of macroscopic spin, the elastic strain rate relates to the stress rate by

\[
d^e = C\dot{\sigma},
\]

where \( C \) is the elastic compliance tensor, yielding the expression for the plastic strain rate

\[
d^p = d - C\dot{\sigma}
\]

Strictly speaking, an objective stress rate should be used, but since the simulations were all performed with boundary conditions that result in no macroscopic spin, this approximation is sufficient.

The effective elastic compliance tensor, \( C \), for the RVE can be obtained from the stress response prior to the onset of plasticity, where the total strain
rate is equal to the elastic strain rate. To solve for \( C \), the procedure employed for determining \( K \) (Equations 4.16 thru 4.19), is employed with the relation

\[
\begin{bmatrix}
\ddot{\sigma}
\end{bmatrix} \begin{bmatrix}
\{C\}
\end{bmatrix} = \begin{bmatrix}
\{\dot{q}\}
\end{bmatrix}
\]

(4.23)

in place of Equation 4.16. The resulting system of equations

\[
\begin{bmatrix}
\sigma_{ij}\end{bmatrix}_{6x21} \begin{bmatrix}
\{C\}_{21x1}
\end{bmatrix} = \begin{bmatrix}
\{\dot{q}\}_{6x1}
\end{bmatrix}
\]

(4.24)

is again solved by singular value decomposition. Strictly speaking six simulations do not need to be used to calculate \( C \). However, this method is used as a convenience.

The flaw in this method is that all of the simulation data is for isochoric strains, so the system of equations has no information about the bulk modulus. The computed result for \( C \), is correct, except that the SVD algorithm sets the bulk modulus to an arbitrary value. This can be accounted for by subtracting the arbitrary shift in the upper left block of nine components. The value corresponding to the correct bulk modulus can then be added. The true value is known, because it is the same as the single crystal value.
\[
[\sigma] = \begin{bmatrix}
\sigma_1 & \sigma_2 & \sigma_3 & 2\sigma_3 & 2\sigma_3 & 2\sigma_3 \\
\sigma_1 & \sigma_2 & \sigma_3 & 2\sigma_3 & 2\sigma_3 & 2\sigma_3 \\
\sigma_1 & \sigma_2 & \sigma_3 & 2\sigma_3 & 2\sigma_3 & 2\sigma_3 \\
\sigma_1 & \sigma_2 & \sigma_3 & 2\sigma_3 & 2\sigma_3 & 2\sigma_3 \\
\sigma_1 & \sigma_2 & \sigma_3 & 2\sigma_3 & 2\sigma_3 & 2\sigma_3 \\
\sigma_1 & \sigma_2 & \sigma_3 & 2\sigma_3 & 2\sigma_3 & 2\sigma_3 \\
\end{bmatrix}
\]

Table 4.1: Definition of \([\sigma]\).
Table 4.2: \( \mathbf{K} \) tensor at strain energies corresponding to strains of approximately 1\% (a) and 10\% (b) and values for an isotropic material (c).
Figure 4-1: Deformed mesh for x-axis tensile boundary condition.
Figure 4-2: Deformed mesh for xy-shear boundary condition.
Chapter 5

Results and Discussion

5.1 Macro-scale Simulations

The final use of the $K$ tensor calculated in Chapter 4 would be a full-scale simulation of a shaped charge liner collapse, in which spin compensation could be captured. Such a full scale simulation is beyond the scope of this work, but a simplified prototype simulation was undertaken. This simulation consists of a thin ring collapsing under an external pressure load. The ring has a diameter of 40 mm and a thickness of 2 mm, approximating the dimensions of a shaped charge liner. The ends of the ring are constrained in the $z$-direction, holding the length constant.

The simulation was conducted using an implementation of the generalized von Mises yield function in the finite element code ALE3D. The yield surface was assumed to be constant throughout the simulation (anisotropic, non-hardening. In the real material, the hardening of the material could be captured by evolution of the flow strength, which was neglected in this simulation. The $K$ tensor is mapped around the cylinder's axis such that in each element, $K$ is in the local coordinate system defined by normal and tangent directions (as indicated in Figure 5-1).

Figure 5-1 shows the initial mesh and the collapsed mesh, with magnified views of the final mesh as computed for isotropic values of $K$ and the values
listed in Table 4.2(a). As expected, the isotropic case exhibits no longitudinal twist, while the anisotropic case exhibits a longitudinal twist of 4.38 degrees.

### 5.2 Texture Distortion

The prototypical simulation can also be used to gauge the relative importance of changes in $K$ brought about by variations in the multi-scale procedure. One significant error that arises during the creation of the RVE is the difference between the grain texture represented and the actual texture in the OIM data. This error is a consequence of the representation of statistics for only 50 3D grains in the RVE, which inevitably leads to an averaged and distorted texture.

One of the most important choices in creation of the RVE is the number of grains to represent, which dictates the number of orientation groups by which the OIM data is represented. Representing a smaller number of grains allows a greater number of elements to resolve each grain. However, the cost of this element resolution is that the grain statistics observed in the OIM data are represented with less fidelity.

It is difficult to say where the optimum position in this trade off lies, but the relative importance of the texture distortion can be investigated. By creating an RVE with a sufficiently large number of grains, the texture in the OIM data can be almost exactly matched. Figure 5-2(a) shows a RVE containing 2500 grains that was constructed using the ungrouped set of grain statistics taken from the OIM data. Thus the only change in texture from the OIM data is the averaging that occurs within the OIM grains, and the grain texture error, $E_T$, which was 0.014 for this RVE.

Table 5.1 shows the shear-normal components of the $K$ tensor computed for this RVE, along with the components calculated for the 250 grain RVE, both at strain energies corresponding to approximately 1% strain. The most relevant terms for the macro-scale simulation are the terms that couple to a
23-shear, which causes the longitudinal rotation. Comparing these terms for the two RVE reveals an average change of 42%, indicating that the texture distortion is likely a significant factor. Just how much of this 42% change is a result of the texture change is difficult to determine, since the change is the result of more than one difference in the two RVE's. The change in texture, the change in element resolution per grain, and the change in neighbor correlation all likely play a role in the change in $K$, but it is difficult to separate these effects without performing additional simulations.

Figure 5-2(b) shows the result of the macro-scale twist simulation for the $K$ tensor computed using the 2500 grain RVE. The total longitudinal twist is 2.83 degrees, compared to 4.75 degrees for the 250 grain RVE, or a 40% difference.

5.3 Neighbor Effects

The motivation for grouping the grains observed in the OIM data was primarily to enable a complete description of a 3D neighbor correlation. The 2500 grain RVE demonstrated that the texture error caused by this grouping may result in a significant error in the behavior of the RVE. To gauge the relative importance of the neighbor correlation as compared to the texture an additional 250 grain RVE was created with the same texture and grain geometry as the first 250 grain RVE, but with a random neighbor correlation (i.e., the same Voronoi tessellation was used, but the grain orientations were switched).

Comparing the two RVEs with the error measures defined by Equations 3.2 and 3.3 yields values of $E_T = 0.013$ and $E_\eta = 0.48$. The textures are almost identical, while the neighbor correlations are quite different. Table 5.2 gives the resulting shear-normal components of $K$ for the two RVEs at two different strain energies. At a strain of 1%, there is an average difference of 17.8% in the 23 shear terms. This difference increases to 30.6% at 10%
strain. The twist in the macro-scale simulation for the K tensors computed at 1% and 10% strain were 4.38 and 3.67 degrees respectively for the RVE with a random neighbor correlation, compared to 4.75 and 4.23 degrees for the RVE with the OIM derived neighbor correlation. The relative effect of the neighbor correlation clearly increases at larger strains.

Figures 5-4 and 5-5 compare total plastic slip in two deformed meshes for the physical η RVE and random η RVE. Comparing the distribution of slip in the two sets of plots reveals that the plastic deformation is more uniformly distributed in the physical η RVE. The difference is not drastic, and the results for the macroscopic behavior (a 13% change in twist) do not suggest that there should be dramatic differences at the local level. However, they are suggestive of how the neighbor correlation can affect the distribution of plastic strain, and thus the macroscopic behavior of the material. The mesh used is still too coarse to fully resolve shear localization within grains, and the neighbor correlation would likely play an even more significant role if the mesh were finer.
Table 5.1: Normal-shear components of $\mathbf{K}$ tensors at 1% strain

(a)  
\[
\begin{array}{ccc}
0.0337 & -0.0260 & -0.0078 \\
0.0032 & -0.0245 & 0.0213 \\
-0.0090 & 0.0086 & 0.0004 \\
\end{array}
\]

(b)  
\[
\begin{array}{ccc}
0.0221 & -0.0116 & -0.0106 \\
0.0031 & -0.0187 & 0.0156 \\
-0.0024 & 0.0022 & 0.0001 \\
\end{array}
\]

(c)  
\[
\begin{array}{ccc}
11-23 & 22-23 & 33-23 \\
11-13 & 22-13 & 33-13 \\
11-12 & 22-12 & 33-12 \\
\end{array}
\]

Table 5.1: Normal-shear components of $\mathbf{K}$ tensors at 1% strain (a) 250 grain RVE (b) 2500 grain RVE (c) couplings represented by each component.
<p>| | | | |</p>
<table>
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<tbody>
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<td></td>
<td>0.0337</td>
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<tr>
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<td>0.0032</td>
<td>-0.0245</td>
<td>0.0213</td>
</tr>
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<td>-0.0090</td>
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<td></td>
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<tr>
<td></td>
<td>0.0338</td>
<td>-0.0228</td>
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<td></td>
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<tr>
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<td>-0.0097</td>
<td>0.0099</td>
<td>-0.0002</td>
</tr>
<tr>
<td>(b)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.0307</td>
<td>-0.0246</td>
<td>-0.0060</td>
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<tr>
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<tr>
<td></td>
<td>-0.0163</td>
<td>0.0158</td>
<td>0.0006</td>
</tr>
<tr>
<td>(c)</td>
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<tr>
<td></td>
<td>-0.0151</td>
<td>0.0138</td>
<td>0.0013</td>
</tr>
<tr>
<td>(d)</td>
<td></td>
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Table 5.2: Normal-shear components of $K$ tensors (a) physical $\eta$ RVE at 1% strain (b) random $\eta$ RVE at 1% strain (c) physical $\eta$ RVE at 10% strain (d) random $\eta$ RVE at 10% strain.
Figure 5-1: Simulation of collapsing ring (a) original mesh (b) deformed mesh (c) magnified view for response with isotropic $K$ (d) magnified view for response with $K$ from Table 4.2(a).
Figure 5-2: Mesh for 2500-grain RVE (a) and resulting ring collapse with $K$ computed at 1% strain (b).

Figure 5-3: Mesh for random $\eta$ RVE (a) and resulting ring collapse with $K$ computed at 1% strain (b).
Figure 5-4: Comparison of deformation in RVE with OIM defined $\eta$, grain orientations (a) and total slip (b) with RVE with random $\eta$, grain orientations (c) and total slip (d).
Figure 5-5: Comparison of deformation in RVE with OIM defined $\eta$, grain orientations (a) and total slip (b) with RVE with random $\eta$, grain orientations (c) and total slip (d).
Chapter 6

Conclusions and Future Work

6.1 Conclusions

This work has outlined a multi-scale framework for calculating the plastic anisotropy of a shaped charge liner. Orientation imaging microscopy was utilized to make a statistical characterization of the liner's microstructure, and this characterization was used to generate a three dimensional representative volume element. The RVE was subsequently used in crystal plasticity simulations, the results of which were used to calculate the plastic anisotropy. A successful implementation has been demonstrated, insofar as the prototypical macro-scale simulations exhibited a rotation. Determination of the extent of this success (if the predicted rotation is correct) requires further validation.

The basic philosophy of this work is that the statistical character of polycrystalline microstructure is at the root of the macroscopic plastic anisotropy observed in shaped charge liners. Two statistics were considered, the grain texture and the neighbor correlation. A preliminary effort was made at determining the relative importance of these two statistics. As might have been expected the grain texture seemed to have a more significant effect on the final result, but the neighbor correlation was shown to be a significant secondary effect.
The most serious flaw of the framework as demonstrated was the need to compromise between accurately representing the texture and the neighbor correlation in the representative volume. Some improvement can be made in this regard by implementing improved methods of sorting grain orientations into the reduced orientation basis, thus reducing resulting distortion of texture.

Ultimately, a balance must be found between the desire to resolve each of the grains in the representative aggregate with a large number of elements, and the need to model a large set of grains to accurately reproduce the experimentally determined grain statistics. Two extreme cases were examined in this work, and the best balance may lie somewhere in the middle ground. Again, further investigation requires some determination of the “right” answer for the macro-scale anisotropy.

The multi-scale framework that has been outlined may be useful beyond modeling of shaped charge liners. It could be utilized in any application where plastic anisotropy is significant. The techniques for creating a 3D representative polycrystalline aggregate based on 2D OIM data may prove useful in other areas of research. This work used the RVE only to determine the average macroscopic response of a polycrystalline aggregate, but a model aggregate could also be used in more detailed studies of the mechanisms of polycrystalline plasticity.

6.2 Future Work

The next step in this work is to validate the predicted anisotropy parameters. This validation can take two forms; the more ambitious validation would be a full-scale simulation of a shape charge liner collapse. A number of aspects remain to be resolved before a full-scale simulation could be undertaken. The prototypical simulation in this work approximated the anisotropy of the liner as constant circumferentially. In the actual liner, the
microstructure results from a combination of the rolling texture of the original sheet and the shearing associated with the spin forming. The rolling texture is wrapped around the cone and superposed with a shear texture, resulting in anisotropy that varies both circumferentially and longitudinally. Variation in the microstructure through the thickness of the liner may also prove to be important. Additional data needs to be collected to create a more complete map of anisotropy in the liner.

A simpler form of validation can be achieved through experiments that are currently underway at Lawrence Livermore National Laboratory. Small coupon specimens were taken from a liner for use in simple compression experiments. Additional adjacent coupons were prepared for OIM scans, and data will be taken on both sides to gauge through-thickness variation. The collected OIM data can be used to compute anisotropic parameters for simulations of the compression tests.

There are a number of future improvements that can be made in the multi-scale framework. In terms of creation of the RVE, additional grain statistics could be employed, for example, grain shape. Also, the grain geometry is currently held constant, but this could potentially be changed over the course of the simulated annealing, along with grain orientations.

This work considered only nearest neighbor spatial correlations. Longer-range correlations could be incorporated and may be important. Also, the nearest neighbor correlation employed was still not a “complete” description of neighbor relationships, since it carries no information about the absolute position of neighbors. The orientations of neighbors are correctly matched, but whether a given neighbor should be appearing “to the left of” or “above” a grain is not captured. This spatial arrangement may prove to be significant.

Also, the neighbor correlation employed in this work would benefit by being rephrased into a form that carries some absolute meaning. As it is currently used, the neighbor correlation is useful only for determining the match between two microstructures with the same set of grain orientations.
Ideally, a form could be created that allows comparison between two different microstructures.

Another aspect that needs improvement is the formation of a reduced grain basis. Currently, an adaptive binning algorithm is used to sort grain orientations into groups. This technique does not provide an optimal reduced basis, and employing a better algorithm could eliminate a great deal of the texture distortion associated with forming the reduced basis.

The crystal simulations could be improved by going to larger strains, and capturing the changing texture and microstructure of the RVE in an evolving $K$ tensor. Employing periodic boundary conditions, and using more robust slip hardening relations could also make the results of the crystal simulations more accurate.

A number of basic questions about the multi-scale framework also remain to be answered. One important issue is the question of how big a RVE needs to be, both in terms of the number of grains it contains and the amount of OIM data used to create it, before it is truly “representative.” Another issue is the choice of yield surface, and it would be possible to fit the RVE response to other yield surface forms.

Of course the most fundamental assumption in this work was that a single 2D OIM scan could fully capture the relevant microstructure statistics responsible for macro-scale anisotropy. This remains to be proven, and in fact it may be necessary to examine two or more orthogonal OIM scans to fully capture any directionality of the neighbor correlation.
Bibliography


