Aug 9th, 10:15 AM - 12:00 PM

Correlation between grain dislocation density and orientation for naturally deformed mantle xenolith from Jagersfontein Mine

Quinton Guerrero
Monmouth College

Quinlan Smith
California Lutheran University

Correlation Between Grain Dislocation Density and Orientation for Naturally Deformed Mantle Xenolith from the Jagersfontein Mine

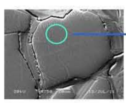
Quinton Guerrero (Monmouth College) and Quinlan Smith (California Lutheran University)
UNLV Physics REU Advisor: Pamela Burnley
Dept. of Physics, University of Nevada Las Vegas, Las Vegas NV 89119

Abstract

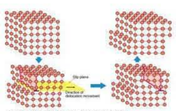
Determining the reaction of poly-crystalline structures to induced stress is an extremely difficult problem in contemporary engineering and geology. The main challenge lies in the inhomogeneity of the grains inside of the poly-crystalline structures. To predict the response of a certain polycrystalline structure to a specific stress, you must resort to one of two views on grain interaction, an orientation or propagation based model. For every material there may be certain correlations between the prediction model used and the actual deformation that occurred. Our work centers around describing the correlation of these prediction models with a sample of naturally deformed mantle xenolith from the Jagersfontein Mine in South Africa. In order to correlate the models with the sample, we needed to calculate the orientation and dislocation density of the individual grains. To measure the dislocation density, the ratio of the area of the dislocations to the total area of the grain itself, the sample needed to go through a decoration process. The sample was heated to accelerate oxidization and highlight the sample's dislocations. This "decorating" process allows us to easily discern the dislocations on the surface of the sample using a Scanning Electron Microscope (SEM). Dislocation density can then be calculated by using an open-source image analysis software called ImageJ on the image of the grain. Additionally, the other calculation, the orientation of the grain, is measured by an Electron Backscatter Diffraction (EBSD) analysis of the sample. The EBSD is a process of firing electrons at the sample and reading the diffractions produced. These diffractions create a "picture" of Kikuchi Bands, simply the diffraction lines produced by the electrons, which can be analyzed by proprietary software resulting in a calculation of the orientation of each grain. We were then able to look for correlations between the dislocation density and the orientation of each grain and identify which model describes the deformation results most accurately.

Introduction

Our sample rock is a piece of Kimberlite, a poly-crystalline rock which is usually created in the upper mantle of the earth's core. This rock, being poly-crystalline, is composed of many grains of crystals. In a deformation process, such as one that occurs naturally in the Earth's upper mantle, the grains of the poly-crystalline rock are subjected to pressures and forces that are great enough to displace and move atoms in the crystal structures of the grains. The results of these movements and displacements of atoms in the crystals are what we refer to as dislocations. There are two major types of dislocations, edge dislocations and screw dislocations. Both of these types can be highlighted through an oxidation process, which can occur because of iron naturally present in the rock. The iron can be oxidized by subjecting it to extremely high temperatures for an extended period of time. This oxidation process creates a visible contrast between the dislocations and the grain itself. This contrast is what we are examining in our SEM images.



Picture of Grain 13 with a few dislocations circled



This is a diagram showing how dislocations can occur on the atomic level

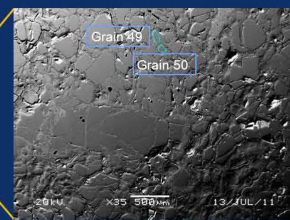
The orientation of a grain is the calculated orientation of the plane of the atoms of the crystalline structure. For poly-crystalline rocks every grain has its own orientation, and these orientations affect the way that a stress field is transferred through the rock. Different orientations cause different reactions to a specific stress field. Every orientation has a slip system which can be conducive to a stress field or non-conducive. If the orientation is conducive to a stress field, then the slip system will be aligned with the stress field and a dislocation can be formed and propagated through the crystal. If the orientation is non-conducive, then the slip system will not be aligned with the stress field and no dislocations can be formed. In essence, orientation is the basis for the formation of dislocations, and attempting to combine these two ideas experimentally is the basis of our research.

Experiment

- A thorough polishing of our sample was done, ranging from 400 grit down to ¼ micron.
- The sample was then decorated (oxidized) in a lab furnace at 900 degrees Fahrenheit for 45 minutes.
- Dislocation density data was collected by using the SEM to take photographs of the grains.
- Orientation data was collected by using the EBSD function of the SEM.
- EBSD data was taken by hand using optical and SEM images of the sample's surface to locate our SEM grains.
- Orientation data was converted into pole figures, allowing a visual display of orientation for all the grains.
- The SEM pictures were analyzed using the open source image analysis software, ImageJ, which allowed us to calculate both dislocation density area and total area of every grain.
- The dislocation density was divided into ranges, then colored, and finally mapped to the pole figures, allowing for a qualitative analysis of correlation.

SEM Results

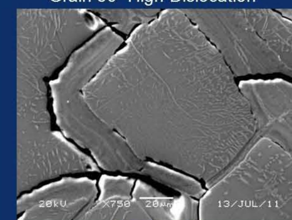
Mantle Xenolith scan 1x



SEM Scan of Xenolith x35

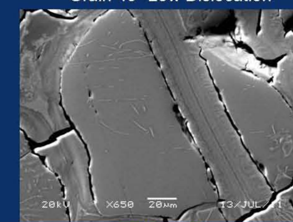
In total 50 grains were photographed at high magnification.

Grain 50- High Dislocation



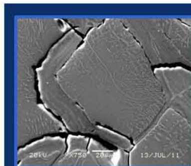
SEM Scan x750

Grain 49- Low Dislocation



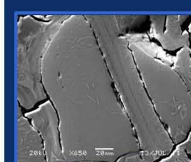
SEM Scan x650

Image Analysis

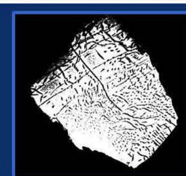


Process for ImageJ analysis:

1. Cut out grain
2. Measure total area
3. Adjust threshold

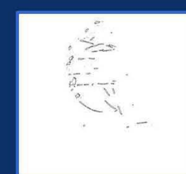


4. Remove outliers (dark spots smaller than 2 pixels)



5. Measure amount and properties of dislocations
6. Record total dislocation area

7. Divide total dislocation area by total area to get dislocation density



ImageJ was used to measure areas of the grains and dislocations. Those numbers where then used to find the dislocation density of a grain.

EBSD Analysis

Electron Back Scatter Diffraction was used to determine the crystal orientation in all 50 grains.

EBSD Map 4 85x

Kikuchi Band Image used to find Euler Angles (crystal orientation)

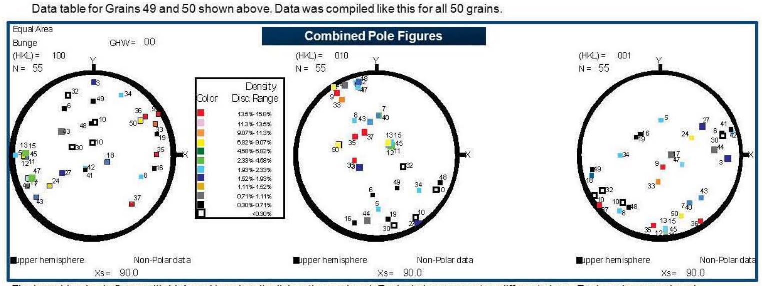
Test Pt.	Euler1(°)	Euler2(°)	Euler3(°)
11	101.8462	105.1199	36.14105
12	125.6644	117.2289	30.28106

Euler Angles produced by software processing of he Kikuchi Bands

Results

Grain	EBSD Map	Test Point	Euler1(°)	Euler2(°)	Euler3(°)	Dislocation Type	Total Area	Total Dis. area	Dis. Density
49	4	12	101.8462	105.1199	36.14105	Low	5.653	.044	0.78%
50	4	11	125.6644	117.2289	30.28106	High	5.49	0.517	9.4%

Data table for Grains 49 and 50 shown above. Data was compiled like this for all 50 grains.



Final combined pole figure with high and low density dislocations colored. Each circle represents a different plane. Each grain we analyzed Has three different Euler angles describing its orientation. As can be seen in the above diagram grains with similar dislocation densities seem to cluster around the same areas in the plane.

Conclusions

- Evaluation of the pole figures revealed a noticeable trend between orientation and dislocation density
- High dislocation dense grains clustered on the right side of the 100 direction and they clustered on the top of the 010 direction.
- Low dislocation dense grains clustered in the middle of the 100 direction and the bottom of the 010 direction.
- In the end its easy to see a trend between dislocation density and orientation, but, because of systematic error in the image analysis of ImageJ, definite conclusions cannot be drawn.

Acknowledgements

Support from the REU program of the National Science Foundation under grant DMR-1005247, and support from the High Pressure Science and Engineering Center (HPSEC), funded by the US Department of Energy, is gratefully acknowledged. Thanks would like to be extended to the SEM Lab and to the Rock Deformation Lab, for the use of their equipment, and a special thank you to our research advisor, Dr. Pamela Burnley.