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Modeling the deformation of Fayalite

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We are studying how the mineral fayalite deforms under stress while it is subject to high pressures and temperatures. Specifically, we are analyzing x-ray diffraction spectra obtained from experiments with the D-DIA apparatus at Brookhaven national labs. By fitting peaks to the diffraction spectra, we can calculate the spacing between lattice planes of fayalite and so we can observe how this spacing changes over time as the crystal structure deforms We hope to show that this deformation can be modeled using an Elastic Plastic Self Consistent model. In such a model, the material is treated as a cluster of independently oriented grains. When stress is applied to the material, deformation takes place because the lattice planes can slip by each other. A variety of slip systems are used to model the different ways these planes can move. The model allows us to calculate the aggregate properties of the material from the microscopic properties of the individual grains.

The goal of our project was to fit an Elastic Plastic Self Consistent (EPSC) model to experimental data on the deformation of the mineral fayalite (Fe_2SiO_4) which is the iron end member of olivine. In the past, Professor Burnley has successfully fit an EPSC model to experimental data on the deformation of quartz. If an EPSC model could be fit to data on fayalite, it would further support the use of these models to study the plastic deformation of minerals. Modeling the deformation of fayalite is of particular interest because olivine is an important component of the Earth's mantle and studying how it deforms at high temperatures and pressures can help us understand how the mantle moves over time.

The first step in our project was to analyze the experimental data set. We also explored some of the parameter space of the EPSC model before trying to fit the model to the data. Unfortunately, our attempts to fit the model to the experimental data have been unsuccessful, and this suggests that there may be another deformation mechanism involved in the deformation of fayalite.

Modeling the deformation of Fayalite

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Abstract

The goal of our project was to fit an Elastic Plastic Self Consistent (EPSC) model to experimental data on the deformation of the mineral fayalite (Fe_2SiO_4) which is the iron end member of olivine. In the past, Professor Burnley has successfully fit an EPSC model to experimental data on the deformation of quartz. If an EPSC model could be fit to data on fayalite, it would further support the use of these models to study the plastic deformation of minerals. Modeling the deformation of fayalite is of particular interest because olivine is an important component of the Earth's mantle and studying how it deforms at high temperatures and pressures can help us understand how the mantle moves over time.

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Analysis of the Experimental Data Set

The data set that we analyzed was produced using the D-DIA apparatus at Brookhaven National Laboratory. This apparatus uses six solid anvils to pressurize a sample and to deform it at a constant rate. While it is being deformed, the sample is exposed to an x-ray beam. The diffracted x-rays are monitored by four detectors that are arranged so that they pick up reflections from two different types of lattice planes. Two of the detectors pick up reflections from lattice planes perpendicular to the direction of compression while the other two detectors pick up reflections from lattice planes perpendicular to a plane that contains the x-ray beam and the compression direction.

By analyzing the spectra recorded by these detectors using the peak fitting program Plot85, we were able to calculate how the d-spacing of several lattice planes changed as the sample was deformed. By measuring photos of the sample taken during the deformation, we were able to calculate how the length of the sample changed during the deformation. Our results are summarized in figure 1.

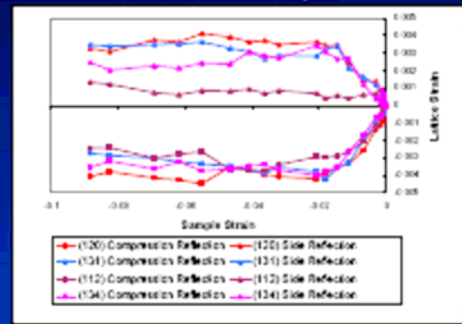


Fig 1. Plot of lattice strain vs. sample strain for the four planes that we observed. For each plane, the lattice strain increases linearly at small sample strains. This linear relationship indicates that the lattice is deforming elastically. As the sample strain increases, this relationship breaks down because the lattice yields and begins deforming plastically. In this plot and all the plots on this poster, negative strains correspond to compression.

Exploring the Parameter Space of the EPSC Model

Experiments have identified eight slip systems that may be involved in the plastic deformation of fayalite (Cordier, 2002). We studied an EPSC model provided to us by Carlos Tome from Los Alamos National Laboratory in which any combination of these eight slip systems could be simulated (Turner and Tome, 1994). In the model, the behavior of each slip systems is governed by two parameters, critical resolved shear stress (CRSS) and work hardening (H). The parameters for each slip system can be set independently. Once the parameters have been specified, the model simulates the deformation of a material by performing an iterative calculation. The model outputs lattice strains for planes perpendicular to three orthogonal directions.

Our analysis focused on characterizing how each slip system affected the model's output. We explored how changing the parameters CRSS and H changed the behavior of each slip system and compared the slip systems to each other. To describe the behavior of each slip system quantitatively, we looked at the percent change in slope of the plot of lattice strain vs. sample strain associated with the transition from elastic deformation to plastic deformation. We also calculated the sample strain at which that transition occurred. We estimated the slope associated with elastic deformation by fitting a linear trend line from 0-0.5% sample strain and we estimated the slope associated with plastic deformation by fitting a linear trend line from 7-8% sample strain. From these slope values, we calculated the percent change in slope. We estimated the yield point by finding the intersection of these two lines. Figure 2 provides a visualization of the method we used to calculate both the percent change in slope and the yield point and figures 3-8 provide a cross-section of our results.

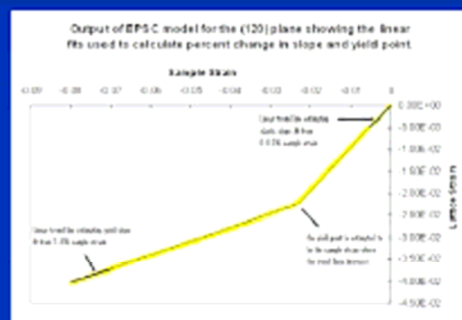
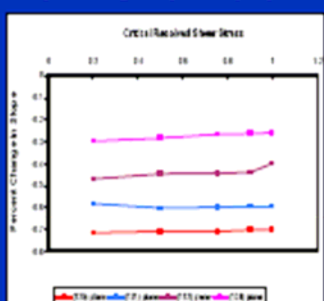


Fig 2. An example of the data produced by the EPSC model illustrating the linear trend lines that we fit to analyze the behavior of each slip system. From the trend lines, we calculate the percent change in slope associated with the transition from elastic deformation to plastic deformation and estimate the sample strain where the transition occurs.



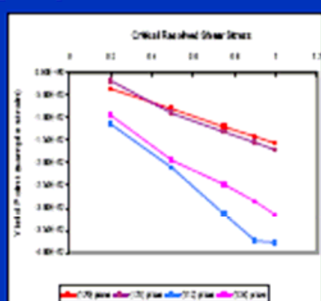
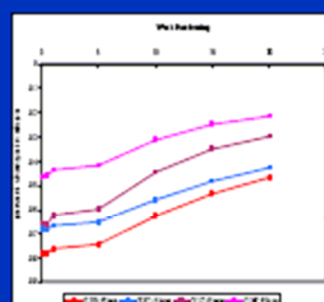
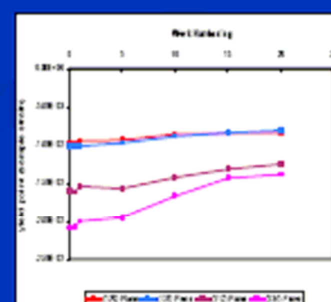
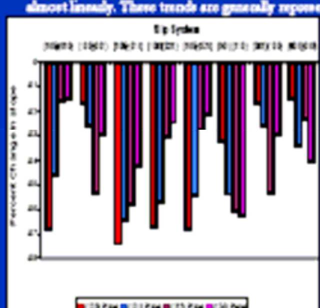


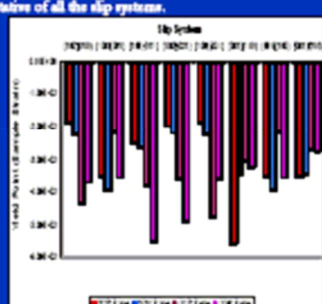
Fig 3 & 4. These plots shows how increasing CRSS affects the percent change in slope and the yield point for planes perpendicular to the compression direction when the [100]{021} slip system is activated with H=0.2. Note that percent change in slope is mostly unaffected by CRSS and the yield point decreases almost linearly. These trends are generally representative of all the slip systems.





Figs 4 & 5. These plots show how increasing H affects the percentage change in slope and the yield point for planes perpendicular to the compression direction when the [100]{011} slip system is activated with CRSS=0.5. Note that increasing H increases the percent change in slope and slightly increases the yield point. These trends are generally representative of all the slip systems.

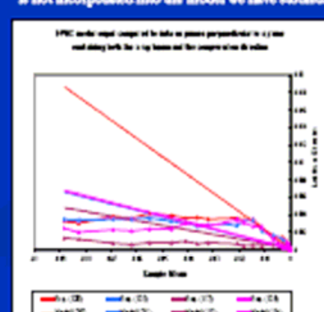




Figs 7 & 8. These plots compare the effect each slip system has on lattice planes perpendicular to the compression direction when CRSS=0.1 and H=1.5 The model shows similar trends for planes perpendicular to the other orthogonal axes although the magnitudes are somewhat different.

Fitting the Model to the Experimental Data

Figures 9 & 10 show our best attempt to fit the EPSC model to our data set. Clearly, we have not been able to fit the model to our data yet. We are beginning to study how the model behaves with multiple slip systems activated in hopes of obtaining a better fit, but the difficulty we have had in fitting the model to the data so far suggests that there may be a deformation mechanism involved in the deformation of fayalite that is not incorporated into the model we have studied.



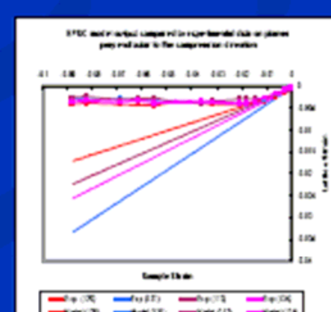


Fig 9 & 10. Our best attempt to fit the EPSC model to our data set. In this model all 8 slip systems were activated. The parameters for the [001]{110}, [001](100), and the [001](010) slip systems were CRSS=0.01, H=0.05. The parameters for the [100](010), [100](001), [100]{011}, [100]{021}, and the [100]{051} slip systems were CRSS=0.1, H=0.05.

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