A Program For Analysis of Two Dimensional Powder Diffraction Data

By Joshua Lande, Marlboro College

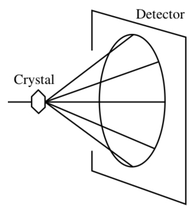
Introduction

X-ray diffraction is a technique used to analyze the structure of crystals. It records the interference pattern created when x-rays travel through a crystal. Three dimensional structure can be inferred from these two dimensional diffraction patterns. Powder diffraction is done by imaging a microcrystalline sample.

A compute program called the Area Diffraction Machine was written to facilitate in the analysis of powder diffraction data. This program can perform detector calibration, polygon masking of diffraction data, and intensity integration of diffraction data. The entire program can be fully automated with macros.

Powder Diffraction

- X-rays are generated at a Synchrotron.
- High energy X-rays are sent through a crystal.
- X-rays preferentially scatter in cones of light.
- The detector records conic sections.
- The scattering angles can be used to infer crystalline properties.

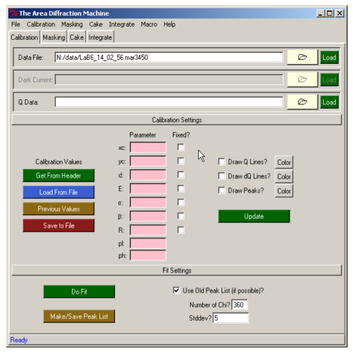


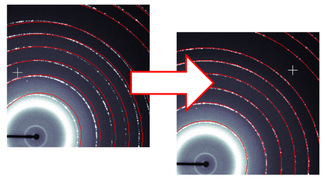
Code

- Mostly written in Python.
- Numerical algorithms written in C and wrapped with Python extensions.
- The Python package Numeric was used to handle data arrays.
- Tkinter was used for the GUI.
- The software is released under the GPL.
- The manual was written in LaTeX.
- AreaDiffractionMachine.googlecode.com.

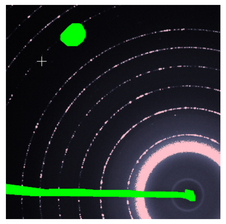
Area Diffraction Machine

Calibration



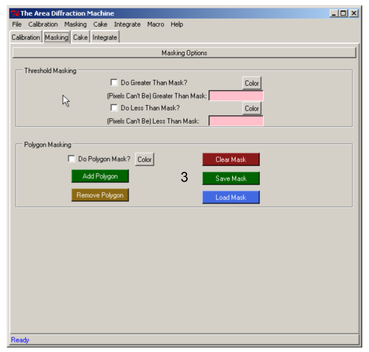


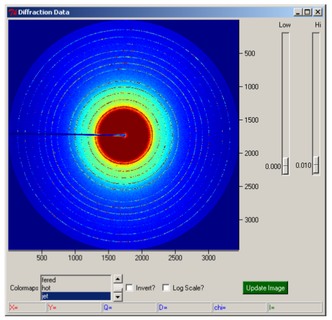
Determine experimental parameters



Mask parts of the image

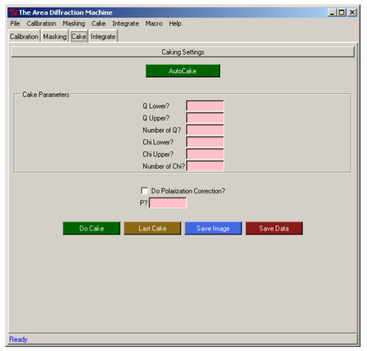
Masking

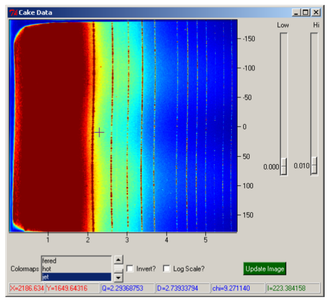




Display diffraction data

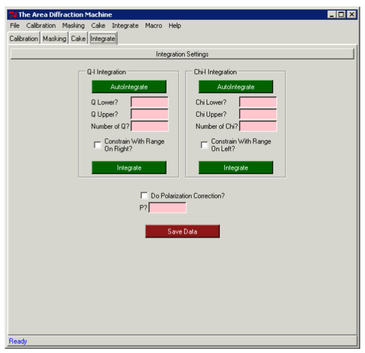
Caking

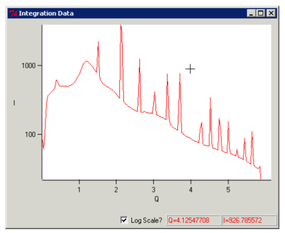




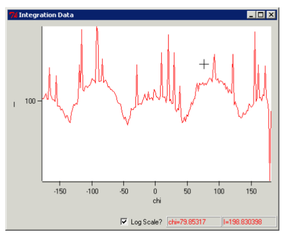
Display caked data

Integration





Q-I Integration



X-I Integration

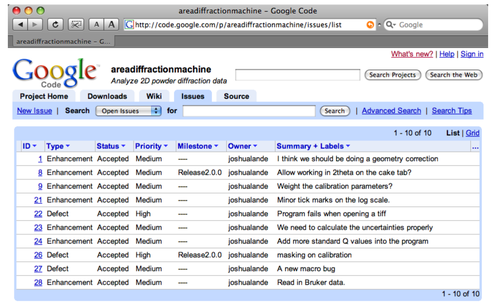
Macro

```
# Macro recorded Wed Jan 30, 2008
Data File:
   C:/Data/
Q Data:
   C:/data/Qdata_TiO2.dat
Do Fit
Save Calibration
   C:/data/cal/FILENAME_cal.dat
Q Data:
   C:/data/Qdata_SS.dat
Make/Save Peak List
   PATHNAME/FILENAME_peaks.dat
AutoCake
Save Cake Data
   PATHNAME/FILENAME_cake.dat
Save Cake Image
   PATHNAME/FILENAME_cake.jpg
```

Project Hosting

- Google Code was used for project hosting.
- Subversion was used for version control.
- Google Code was used for issue tracking.
- Google Groups was used for collaboration.

Issue Tracking


areadiffractionmachine – Google Code

Google Code areadiffractionmachine — Analyze 2D powder diffraction data

Project Home | Downloads | Wiki | Issues | Source

New Issue | Search | Open Issues | for | Search | Advanced Search | Search Tips

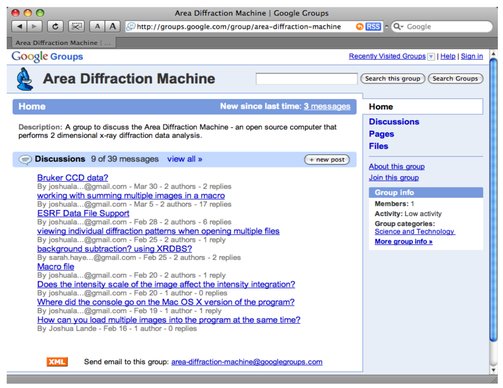
1 - 10 of 10 List | Grid

ID	Type	Status	Priority	Milestone	Owner	Summary + Labels
1	Enhancement	Accepted	Medium	---	joshualande	I think we should be doing a geometry correction
8	Enhancement	Accepted	Medium	Release2.0.0	joshualande	Allow working in 2theta on the cake tab?
9	Enhancement	Accepted	Medium	---	joshualande	Weight the calibration parameters?
21	Enhancement	Accepted	Medium	---	joshualande	Minor tick marks on the log scale.
22	Defect	Accepted	High	---	joshualande	Program fails when opening a tiff
23	Enhancement	Accepted	Medium	---	joshualande	We need to calculate the uncertainties properly
24	Enhancement	Accepted	Medium	---	joshualande	Add more standard Q values into the program
26	Defect	Accepted	High	Release2.0.0	joshualande	masking on calibration
27	Defect	Accepted	Medium	---	joshualande	A new macro bug
28	Enhancement	Accepted	Medium	---	joshualande	Read in Bruker data.

1 - 10 of 10

©2008 Google - Code Home - Terms of Service - Privacy Policy - Site Directory

Discussion Group


Area Diffraction Machine | Google Groups

Google Groups — Area Diffraction Machine

Home — New since last time: 3 messages

Description: A group to discuss the Area Diffraction Machine - an open source computer that performs 2 dimensional x-ray diffraction data analysis.

Discussions 9 of 39 messages view all » + new post

Bruker CCD data?
By joshuala...@gmail.com - Mar 30 - 2 authors - 2 replies
working with summing multiple images in a macro
By joshuala...@gmail.com - Mar 5 - 2 authors - 17 replies
ESRF Data File Support
By joshuala...@gmail.com - Feb 28 - 2 authors - 6 replies
viewing individual diffraction patterns when opening multiple files
By joshuala...@gmail.com - Feb 25 - 2 authors - 1 reply
background subtraction? using XRDBS?
By sarah.haye...@gmail.com - Feb 25 - 2 authors - 2 replies
Macro file
By joshuala...@gmail.com - Feb 20 - 2 authors - 1 reply
Does the intensity scale of the image affect the intensity integration?
By joshuala...@gmail.com - Feb 20 - 1 author - 0 replies
Where did the console go on the Mac OS X version of the program?
By joshuala...@gmail.com - Feb 19 - 1 author - 1 reply
How can you load multiple images into the program at the same time?
By Joshua Lande - Feb 16 - 1 author - 0 replies

Home | Discussions | Pages | Files | About this group | Join this group | Group Info | Members: 1 | Activity: Low activity | Group categories: Science and Technology | More group info »

Send email to this group: area-diffraction-machine@googlegroups.com

Acknowledgements

This project began during a Department of Energy Science Undergraduate Laboratory Internships I participated in at the Stanford Linear Accelerator Center during the summer of 2007. This research was done in collaboration with Dr. Apurva Mehta, Dr. Samuel Webb, and David Bronfenbrenner at the Stanford Synchrotron Radiation Laboratory. Thanks also to my advisers Travis Norsen and Jim Mahoney at Marlboro College.