DTXRD - software for evaluation of single crystals using x-ray diffraction

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TWG meeting
Outline

1. Overview
2. X-ray diffraction characterization of single crystals
3. Rocking curve imaging
4. Dynamical diffraction calculations for a plane wave
5. Throughput and rocking curves of multi-crystal configurations
6. Summary
Acknowledgments

Carlo Segre (IIT)
Yuri Shvyd’ko (APS)
Pete Jemian (APS)

Jozef Maj (APS)
Xianrong Huang (APS)
Lahsen Assoufid (APS)
Chris Jacobsen (APS)

Kurt Goetze (APS)
Jeff Kirchman (APS)
Overview

- **dtxrd**: calculations of reflectivity/transmissivity using the dynamical theory of x-ray diffraction for monochromatic wave
- **rcpeak**: plotting and calculations of parameters of a reflectivity curve
- **rctopo**: calculations of x-ray rocking curve images (for a series of hdf4 CCD snapshots)
- **seehdf**: hdf4 image data viewer
- **specscan**: extraction of individual scans from a file generated by SPEC
- **throughput**: calculations of a throughput and rocking curves of a multicrystal configuration

**online documentation:**
http://python-dtxrd.readthedocs.org
Single crystal x-ray diffraction: Applications

Comparison of application ranges. (from D.K. Bowen, B.K. Tanner, "High Resolution X-ray Diffractometry and Topography"

- science of crystal growth (studies of intrinsic defects)
- nondestructive evaluation and R&D in semiconductor industry
- characterization of x-ray crystal optics!
X-ray diffraction characterization of single crystals

rocking curve measurement and analysis

example: double crystal (+,-) configuration (Bragg)

x-ray diffraction imaging
example: Lang projection topography (Laue)
rocking curve measurement and analysis
example: double crystal (+,-) configuration (Bragg)
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example: double crystal (+, -) configuration (Bragg)
X-ray diffraction characterization of single crystals

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example: Lang projection topography (Laue)
Recent improvements:
- ultraprecise angular stage for 2nd crystal control using EPICS and SPEC computer & OS upgrade

Stanislav Stoupin (APS, ANL)

Fig. 1. General layout of the topography station.
SE - source enclosure, S-RA - source-rotating anode
PBC - primary beam collimator, DE - diffractometer enclosure
Ra1 - rail 1, Ra2 - rail 2, Mo - monochromator, Sa - sample
D1 - detector 1, D2 - detector 2,
RBP - right base plate, LBP - left base plate
Topography station at the APS

S. Krasnicki RSI 67, 3369 (1996)

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**Rocking curve imaging**

**rctopo**: Sort sequence of diffraction images on per-pixel basis to generate local rocking curves. First demonstrated by Lübbert et al., NIM B, 160 (2000).
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brings spatial resolution to rocking curve analysis
ultraprecise evaluation of strain and lattice tilt for single crystals
a starting point to explore wavefront preservation properties of diffracting optics
use of a synchrotron source would improve spatial resolution (to 1 \( \mu \text{m} \)) and wavefront resolution (to 0.1 \( \mu \text{rad} \)).
Topo station at APS: possible improvements

Cu Kα x-ray source

SD/CCD

Si

Si, C

H₁ 111

C

H₂ 220

θₜ, ηₜ

upgrade CCD to achieve better spatial resolution (60 um ~ 13 um pixel size is feasible)

control all 3 angles for the sample - facilitate search of optimal condition

use triple axis system with analyzer crystal in front of CCD - improve wavefront sensitivity
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**dtxrd**: reflectivity and transmissivity (plane wave)

Bragg case

Laue case
**dtxrd**: reflectivity and transmissivity (plane wave)

**Bragg case**

```plaintext
dtxrd Si 1 1 1 0 0 300 20 e 10
```

**Laue case**

```plaintext
dtxrd C 0 0 4 90 0 300 0.1 e 12
```
**dtxrd**: reflectivity and transmissivity (plane wave)

**Bragg case**

```
dtxrd Si 1 1 1 0 0 300 20 e 10
```

**Laue case**

```
dtxrd C 0 0 4 90 0 300 0.1 e 12
```
**dtxrd**: dynamical diffraction calculations for plane wave

- calculates reflectivity/transmissivity and various parameters of a given reflection in arbitrary geometry for a given energy or angle of incidence.
- includes backscattering cases
- crystal thickness and temperature are input parameters
- available crystal models: Si, C (diamond), Ge, Al2O3 (sapphire)

Limitations:

- only 2-beam Bragg or Laue case
- only perfect crystals
- only plane monochromatic wave
- grazing incidence and grazing emergence are not included
How to simulate a real case (multi-crystal configuration, source divergence and energy bandwidth)?

- introduce a regular 2D grid that will cover angular and energy acceptance of the first crystal in a multi-crystal configuration
- introduce energy and angular distribution of the source in this region
- propagate each ray through analytical formulas of 2-beam diffraction for a sequence of reflections
- for calculations of a rocking curve - perform this procedure for a sequence of angular positions of the crystal of interest
throughput: double-crystal high heat load mono

courtesy of Z. Liu, S. Heald et al.

experiment: $\Delta \theta \simeq 8.5$ arcsec (FWHM)
theory (throughput calculation): $\Delta \theta \simeq 8.0$ arcsec (FWHM)
throughput: double-crystal high heat load mono

experiment: $\Delta \theta \approx 8.5$ arcsec (FWHM)
theory (dtxrd calculation): $\Delta \theta \approx 5.7$ arcsec (FWHM)
throughput: double-crystal topography

Cu Kα x-ray source

$H_{Si} 220$

$H_C 111$

$\theta_{Si}$, $\eta_{Si}$

$\theta_C$

SD/CCD
throughput: 4-bounce mono (MERIX)

![Diagram of 4-bounce mono (MERIX) setup with energy levels 5 keV, 9 keV, and 11.2 keV]

Throughput

Energy $(E - E_X)$, [meV]

- $E_X = 5$ keV
- $E_X = 9$ keV
- $E_X = 11.2$ keV

Throughput

- $\Delta E_X = 4.9$ meV
- $\Delta E_X = 14.3$ meV
- $\Delta E_X = 44.7$ meV
throughput: multi-crystal configurations

- calculates throughput and rocking curves for divergent incident beam with finite energy bandwidth
- includes backscattering cases
- source energy distribution can be assigned
- available crystal models: Si, C (diamond), Ge, Al2O3 (sapphire)

Limitations:

- only 2-beam Bragg or Laue case
- only perfect crystals
- angular spread only in scattering plane
- grazing incidence and grazing emergence are not included
- infinite wavefront
Summary

- documentation: http://python-dtxrd.readthedocs.org
- availability (APS Linux): /APSshare/epd/rh6-x86_64/bin
- source: https://subversion.xray.aps.anl.gov/dtxrd
- a goal to improve and make more user-friendly!

references:

Great Stuff to Read!

X-Ray Optics
Yu. Shvyd’ko
High-Energy-Resolution Applications

High Resolution X-ray Diffractometry and Topography
D. Keith Bowen
and Brian K. Tanner