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

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TWG meeting

Outline

Acknowledgments

Carlo Segre (IIT)
Yuri Shvyd'ko (APS)
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Jozef Maj (APS)
Xianrong Huang (APS)
Lahsen Assoufid (APS)
Chris Jacobsen (APS)

Kurt Goetze (APS)
Jeff Kirchman (APS)

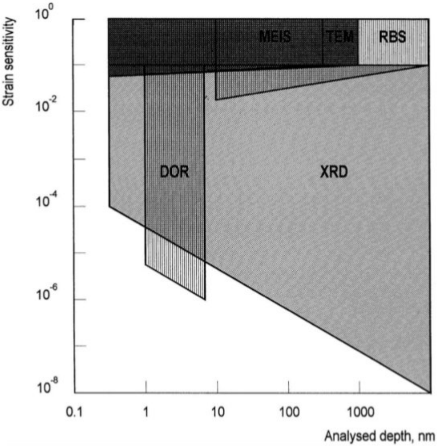
Overview

- **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"

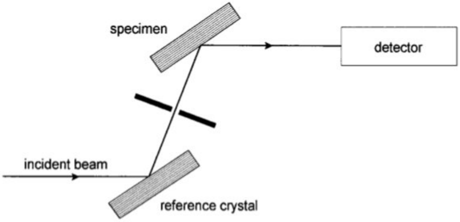


- science of crystal growth (studies of intrinsic defects)
- nondestructive evaluation and R&D in semiconductor industry
- characterization of x-ray crystal optics!

X-ray diffraction characterization of single crystals

X-ray diffraction characterization of single crystals

rocking curve measurement and analysis
example: double crystal (+,-) configuration (Bragg)



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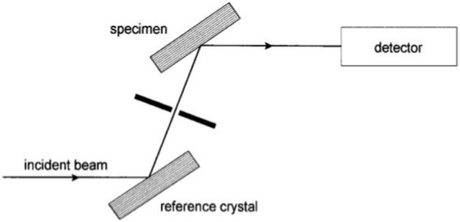

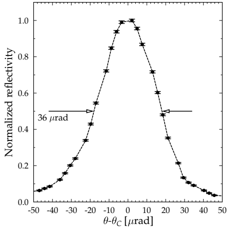

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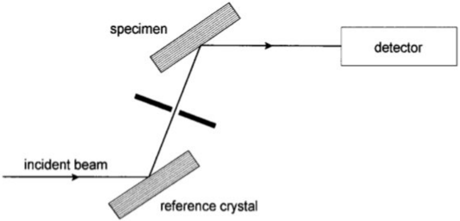
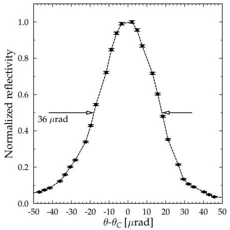
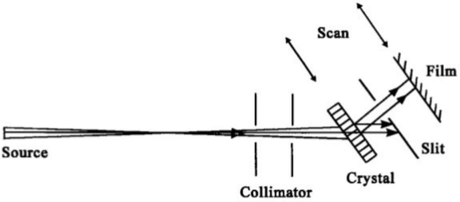




x-ray diffraction imaging
example: Lang projection topography (Laue)



X-ray diffraction characterization of single crystals

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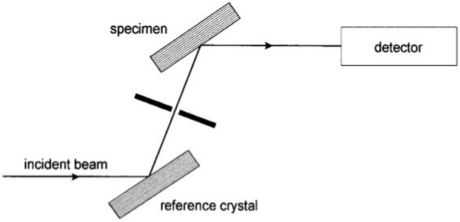

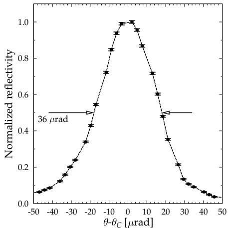

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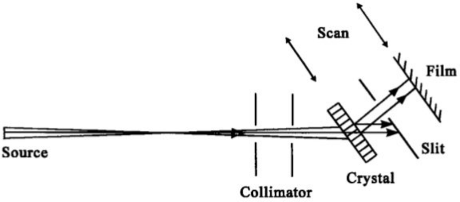
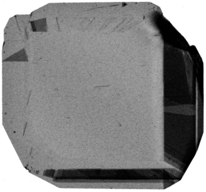
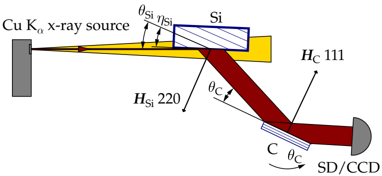




S. Krasnicki RSI 67, 3369 (1996)



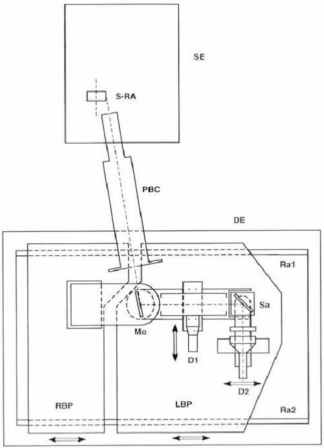


Fig. 1. General layout of the topography station.
SE - source enclosure, S-RA - source-rotating anode
PBC - primary beam collimator, DE - diffractometer enclosure
Ra1 - rail 1, Ra2 - rail 2, Mo - monochromator, Sa - sample
D1 - detector 1, D2 - detector 2,
RBP - right base plate, LBP - left base plate

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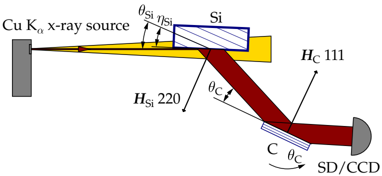
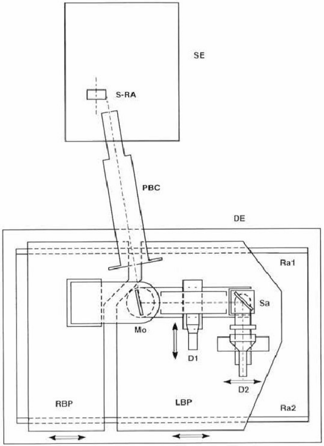


Recent improvements:

- ultraprecise angular stage for 2nd crystal
- control using EPICS and SPEC
- computer & OS upgrade



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Topography station at the APS

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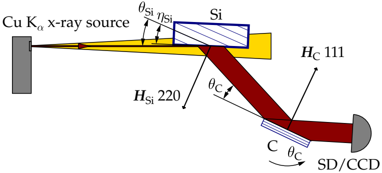

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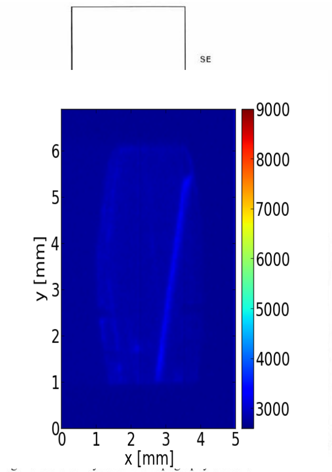

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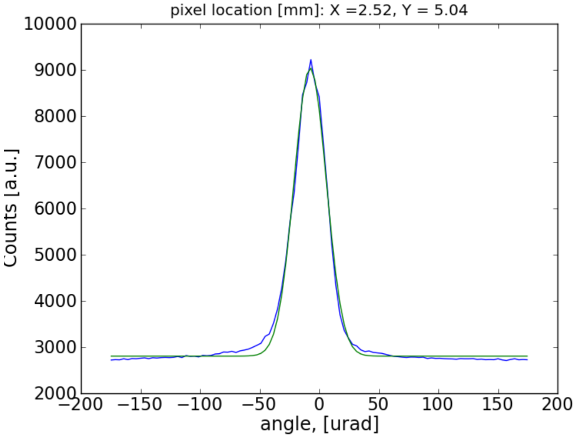
Rocking curve imaging

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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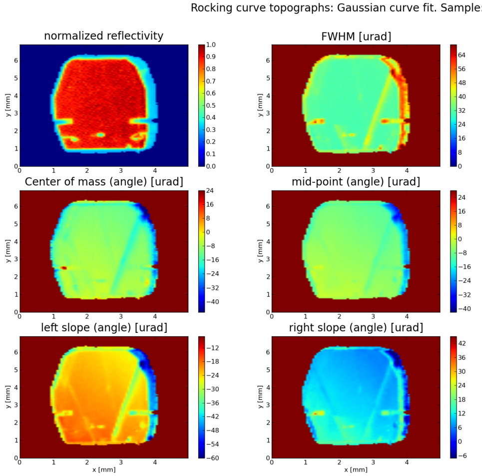

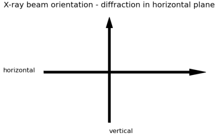

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FWHM_rms = 6.95020534694 urad
FWHM_pv = 51.6785457817 urad
Reflect_average = 0.776178037143
Reflect_rms = 0.224077790066
reflect_pv = 0.714037771251
COM_average = -11.0038862494 urad
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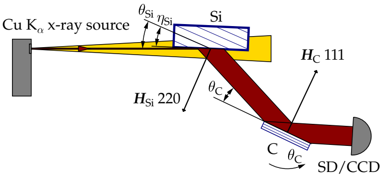
thneg_pv = 49.9673344658 urad
thpos_average = 10.2398947455 urad
thpos_rms = 3.62061021748 urad
thpos_pv = 47.6045335689 urad

rctopo: rocking curve imaging

- 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 μm) and wavefront resoluion (to 0.1 μrad).

Topo station at APS: possible improvements



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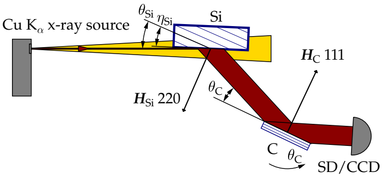

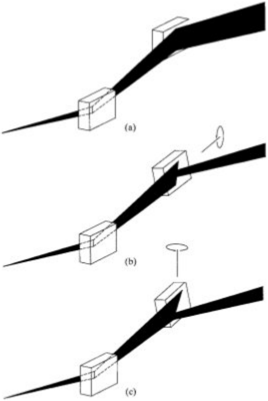

- upgrade CCD to achieve better spatial resolution (60 um -> 13 um pixel size is feasible)
- control all 3 angles for the sample - facilitate search of optimal condition
- use triple axis system with analyzer crystal in front of CCD - improve wavefront sensitivity

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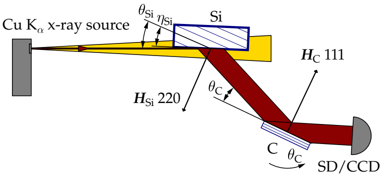

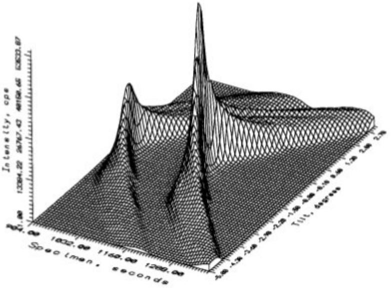

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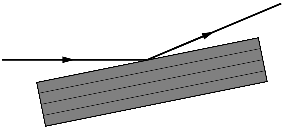
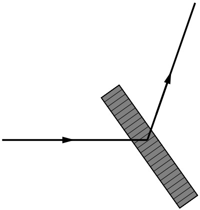
dtxrd: reflectivity and transmissivity (plane wave)

Bragg case



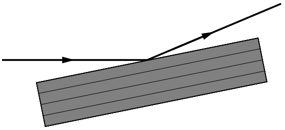
Laue case



dtxrd: reflectivity and transmissivity (plane wave)

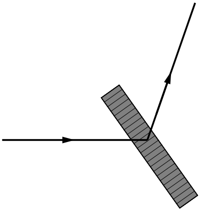
Bragg case

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



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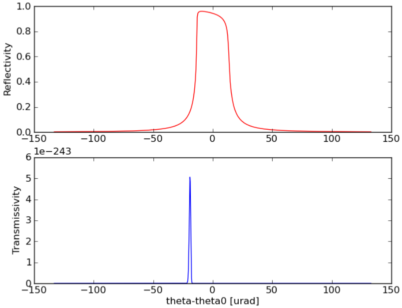
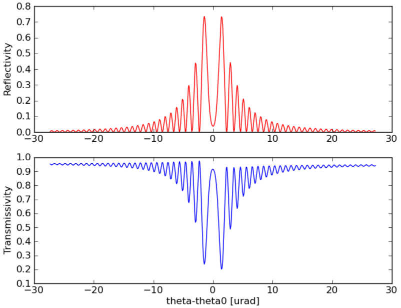


Laue case

```
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:

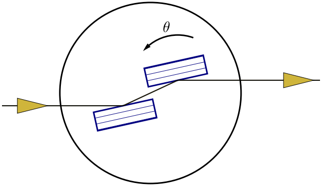
- only 2-beam Bragg or Laue case
- only perfect crystals
- only plane monochromatic wave
- grazing incidence and grazing emergence are not included

throughput: computational strategy

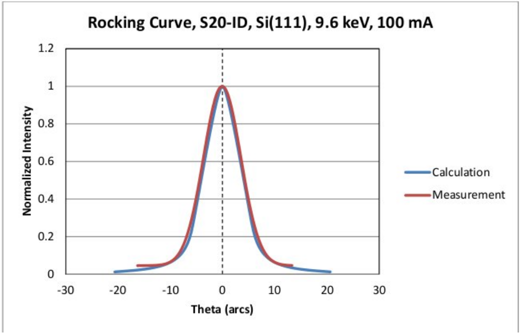
How to simulate a real case (multi-crystal configuration, source divergence and energy bandwidth)?

- 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)

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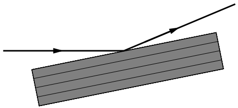
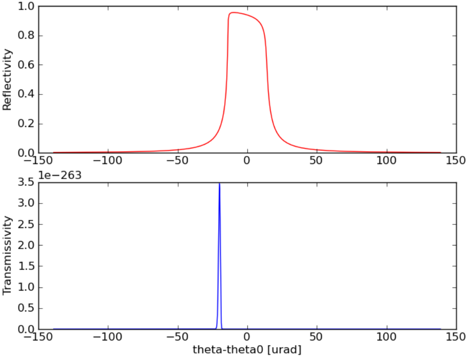
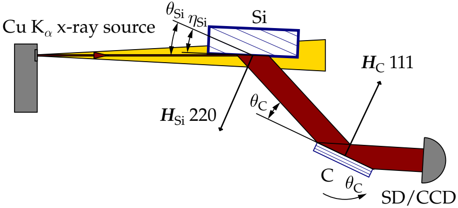
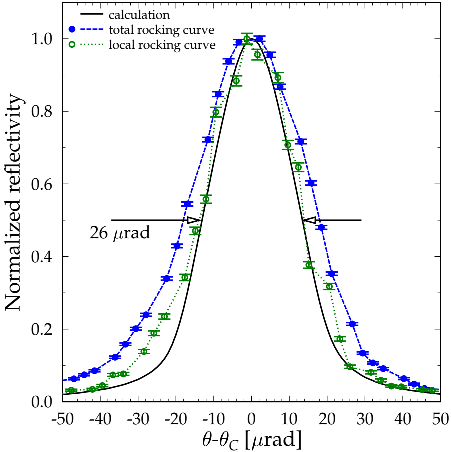




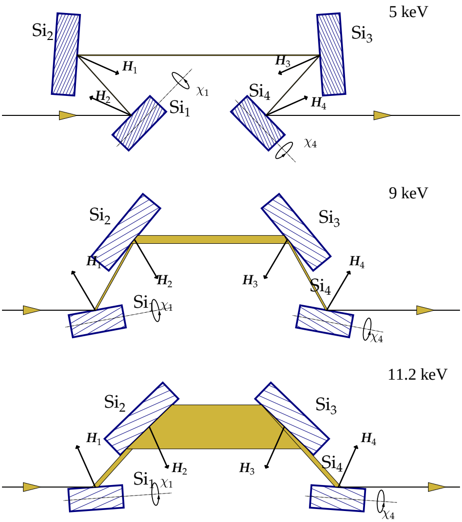
experiment: $\Delta\theta \simeq 8.5$ arcsec (FWHM)
theory (**dtxrd** calculation): $\Delta\theta \simeq 5.7$ arcsec (FWHM)

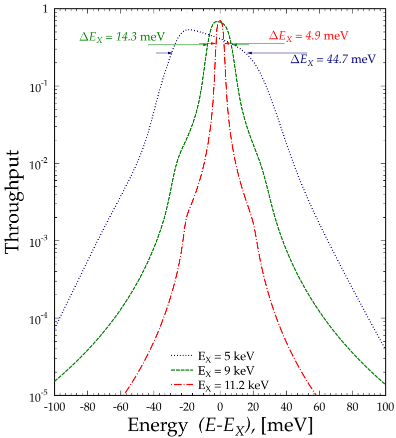
throughput: double-crystal topography





throughput: 4-bounce mono (MERIX)





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:

1. S. Stoupin, V. Blank, S. Terentyev, S. Polyakov, V. Denisov, M. Kuznetsov, Y. Shvyd'ko, D. Shu, P. Emma, J. Maj, et al., Diamond and Related Materials 33, 1 (2013)
2. S. Stoupin, Y. V. Shvyd'ko, D. Shu, V. D. Blank, S. A. Terentyev, S. N. Polyakov, M. S. Kuznetsov, I. Lemesh, K. Mundboth, S. P. Collins, et al., Opt. Express 21, 30932 (2013)
3. S. Stoupin, S. Terentyev, V. Blank, Y. Shvyd'ko, K. Goetze, L. Assoufid, S.N.Polyakov, M.S. Kuznetsov, N. Kornilov, J. Katsoudas, et al. (2014), submitted for publication, URL arXiv:1401.5879.

Great Stuff to Read!