FRIEDRICH-ALEXANDER
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FACULTY OF SCIENCES

Diffuse Scattering
Disordered Crystal Structures
Experimental Aspects

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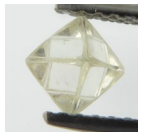
What ?

How ?

Where ?

What ?



1

What is your sample ?

- Single crystal
- Polycrystalline
- Nanocrystalline
- Composition — light / magnetic / isotopes

State of your sample ?

- Steady-state
- Changing (*in-situ* / *in-operando*)

You need to know what?

- Average structure
- **Disorder**
- Properties — Ionic conductivity
- **ETC**
- Dynamics — Vibrations / Diffusion
  - What time scale?
- Changes — Phase transitions
  - Nukleation **ETC**
  - What time scale?

Bragg scattering
Diffuse scattering

Inelastic neutron
Quasielastic

How ?

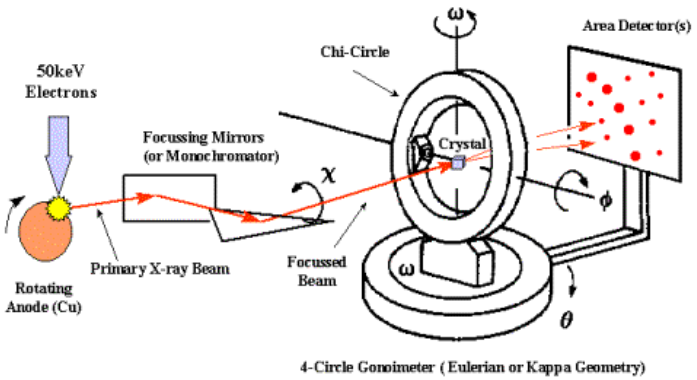
Where ?

1 Von Piotr Sosnowski - Eigenes Werk, CC BY-SA 4.0, https://commons.wikimedia.org/w/index.php?curid=4765104

Experimental aspects, introduction

What ?

Single crystal



4-Circle Goniometer (Eulerian or Kappa Geometry)

Rotate crystal around one / several axes

Many curved slices through reciprocal space

Transform onto regular 3D-grid

How ?

Laboratory source	few hours
Synchrotron source	few minutes
Neutron source	many minutes

Where ?

Experimental Aspects Radiation

The usual suspects

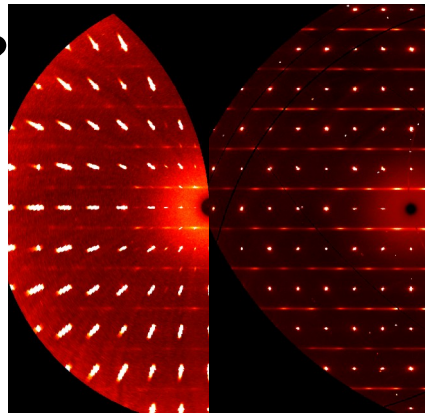
What ?

X-rays	neutrons	electrons
Super fast	Slow measurements	Sample preparation
Readily avaliable	Few sources	Sample stability
	D19 @ ILL SXD @ ISIS CORELLI @ SNS	Dynamic scattering
	Element contrast	Abundant instruments
	Energy discrimination	Very few experts
	Static / dynamic	
	Magnetism	

How ?

Image plate @ in-house

Pilatus @ ESRF

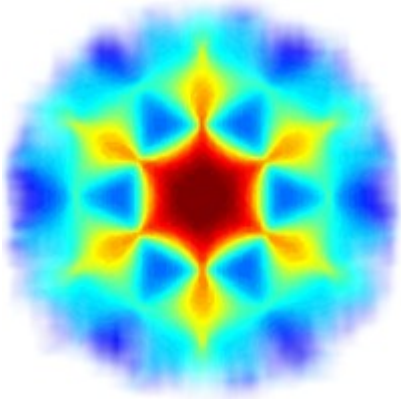


Where

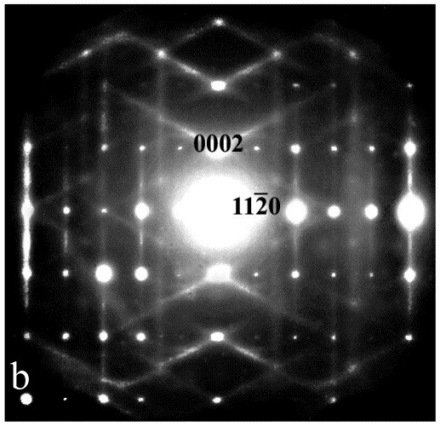
Kα1 / Kα2 / white radiation

mono-chromatic

Th. Weber ETH



Sendetskyi et al.
PRB **93**, 224413 (2016)



R.L. Withers et al.
Sol.StateSci. **5**, 427 (2003)

Choose your instrument **Powder diffraction**

What do you want to learn about the sample ?

Local structure over some 1 to 3 nm

- Instrumental resolution is not very relavant
  - Large area detector instrument, specialized PDF instrument
  - ID15, ID31 ESRF; 11-ID-B APS; XPDF Diamond

Domain structure over some 6 to 20 nm

- Instrumental resolution is decisive
  - Single counter high resolution instrument
  - ID22 ESRF; Mat. Sc. BL Swiss Light Source; P02 Petra III

Static structure

- Laboratory Instrument time about some 6 to 24 h
- Synchrotron Instrument time about 1/10th to 120 s
- Neutrons (SNS OakRidge) ~ half an hour

Time resolved stucture

- OK, WHAT time?
  - Large area detector instrument, specialized PDF instrument
  - ID15, ID31 ESRF; 11-ID-B APS; XPDF Diamond
  - Synchrotron Instrument time about 1/10th to 120 s
  - **XFEL time about 100 fs Dave Keen talk on Thursday**

What do you want to learn about the sample ?

Local structure over some 1 to 3 nm

- Instrumental resolution is not very relavant
  - Large area detector instrument, specialized PDF instrument
  - **ID23, Swiss-Norwegian beamline, generally single crystal**

Domain structure over some 6 to 20 nm

- Instrumental resolution is decisive
  - Single counter high resolution instrument
  - **ID23, Swiss Norwegian beamline, general single crystal**

Static structure

- Laboratory Instrument time about some 6 to 24 h
- Synchrotron Instrument time about a few minutes
- Neutrons (SNS OakRidge) ~ half an hour

Time resolved stucture

- OK, WHAT time?
  - Large area detector instrument, specialized PDF instrument
  - **ID23, Swiss Norwegian beamline, general single crystal**
  - Synchrotron Instrument time about a few minutes

What do you want to learn about the sample ?

Light atom structure

OK, light atoms only ? X-rays are just fine!

Hydrogen /Deuterium ????

Local environment around a particular element

Suitable absorption edges at 20 to 100 keV?

Instrumental with variable wave length

ID15, ID31, ID22 ESRF; Mat. Sc. BL Swiss Light Source

Isotope substitution with nice contrast ?

Neutron Instruments

GEM Polaris ISIS; Nomad SNS, Oak Ridge

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Neutron Instruments

D19 ILL; SXD ISIS; Topaz, Corelli SNS, Oak Ridge

What size is your sample ?

A few hundred nm to a micron?

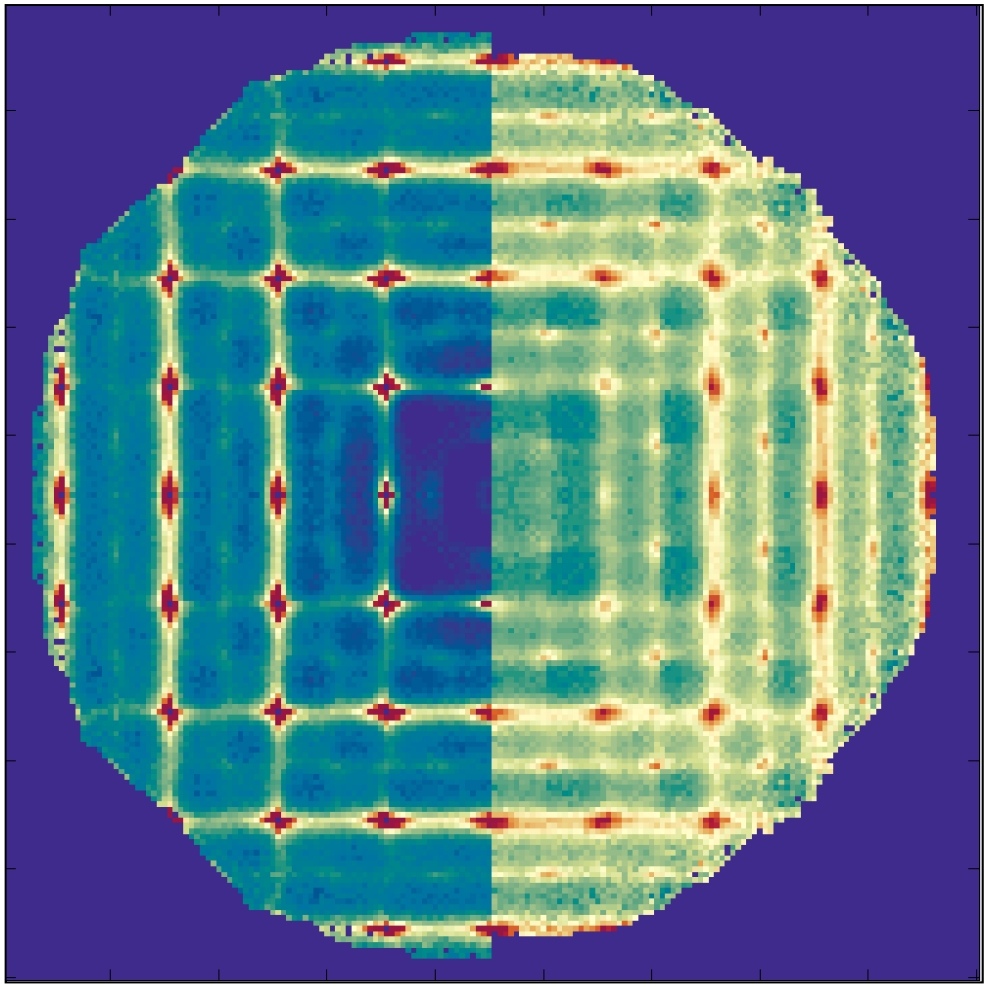
Single crystal X-ray diffraction is just fine
At ESRF Microfocus beam line

A few nm?

Single crystal electron diffraction

Ute Kolb, Univ. Mainz, Germany
Yoke Hadermann, Univ. Antwerp Belgium

Single crystal data collection **ADT** program
being coupled to DISCUS



Measurement and Reduction of Diffuse Scattering Data

Thomas Weber
ETH, Zürich

with kind permission

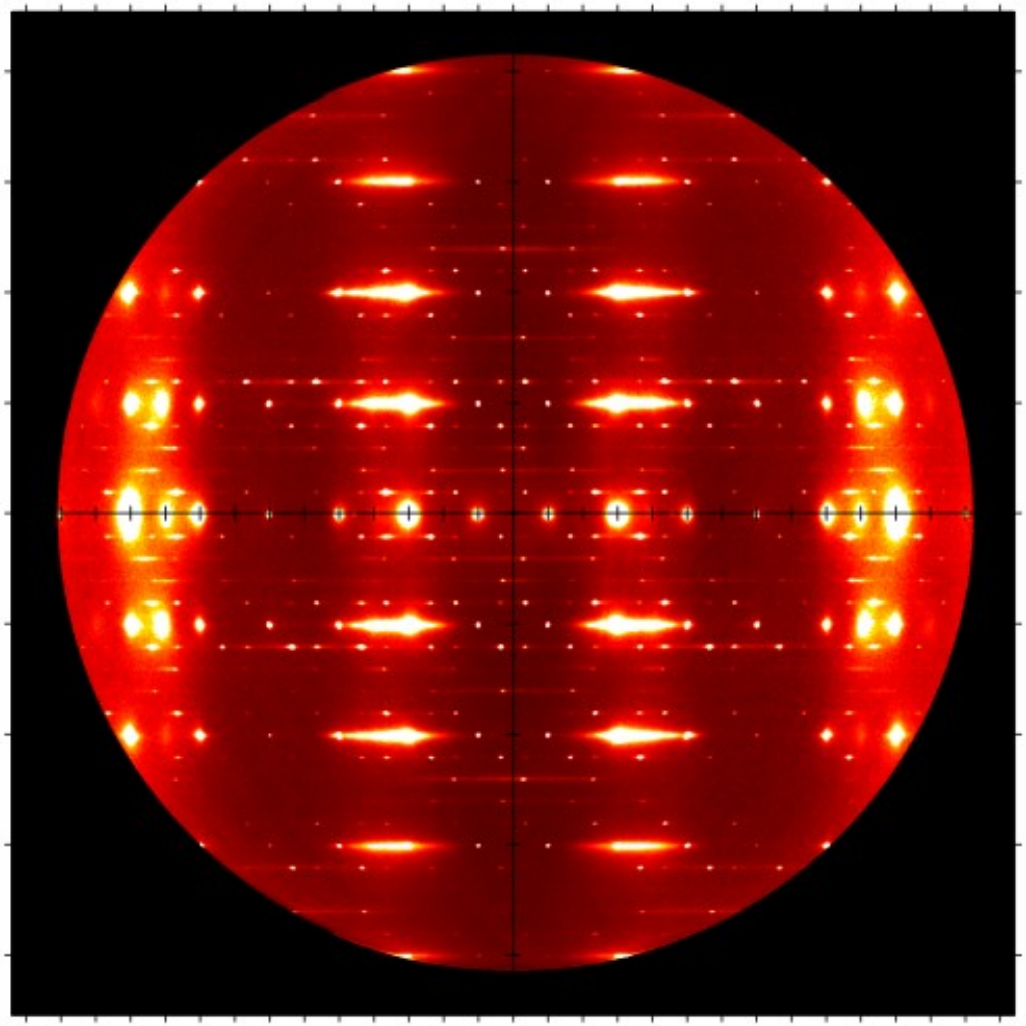
Same diffraction physics

Only the distribution of phonons differs

$I_{Bragg} > \sim 10^4 * I_{Diffuse}$

$\int I_{Bragg} \approx \int I_{Diffuse}$

$FWHM_{Bragg} <<< FWHM_{Diffuse}$



Experimental Aspects

Need to measure all of reciprocal space

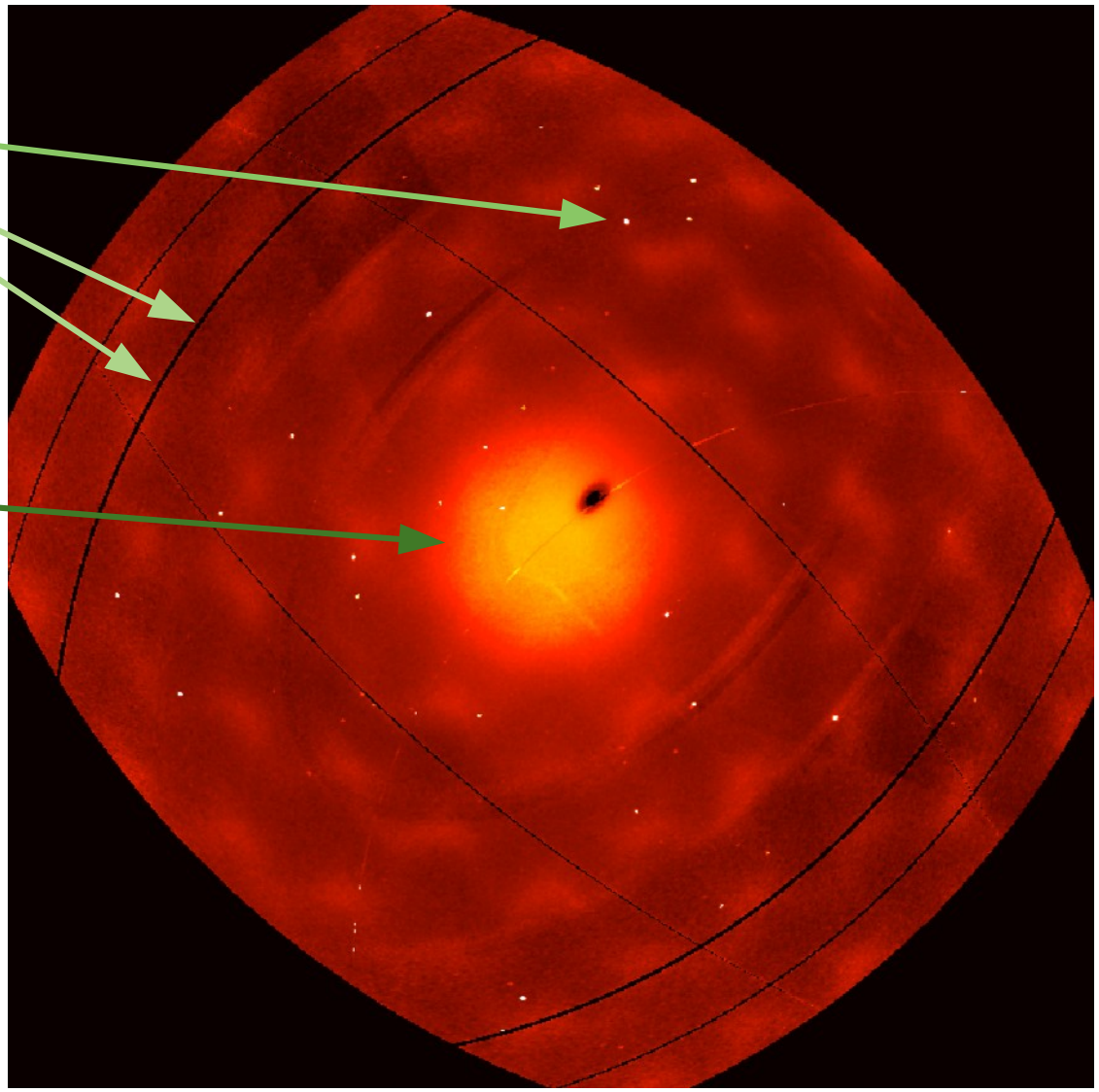
Everything will be measured

Detector glitches

Background

Sample ?

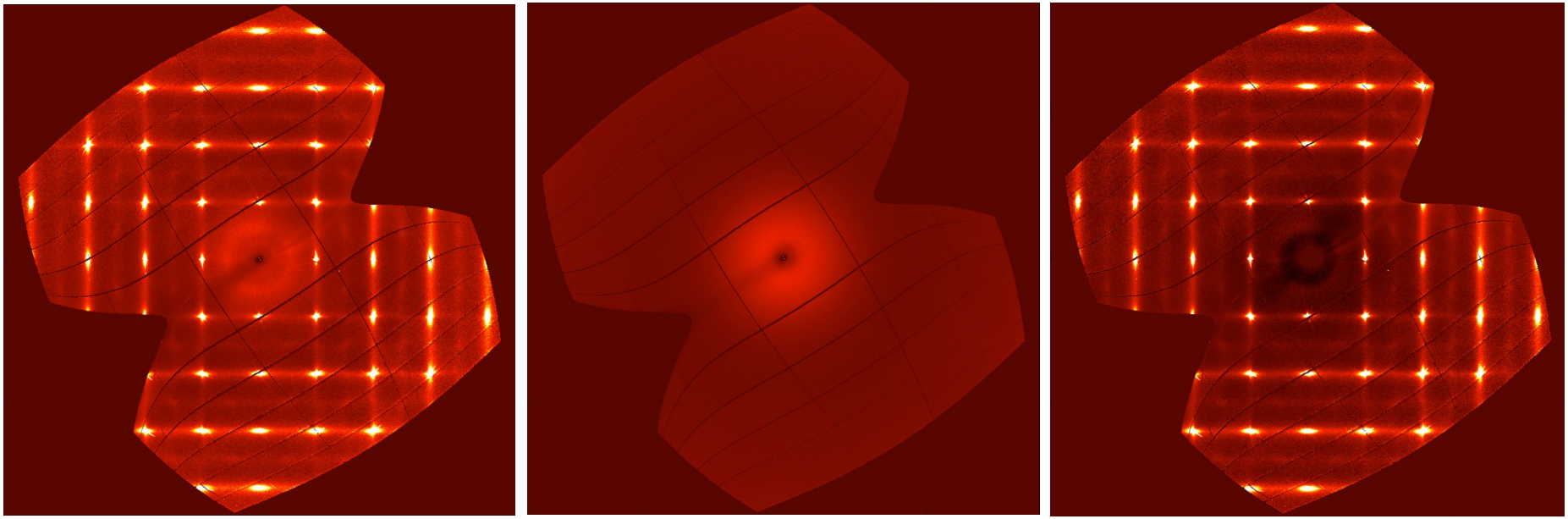
Experiment ?



Everything along the primary beam path does scatter !

Correct background scattering!

observed | measured background | corrected



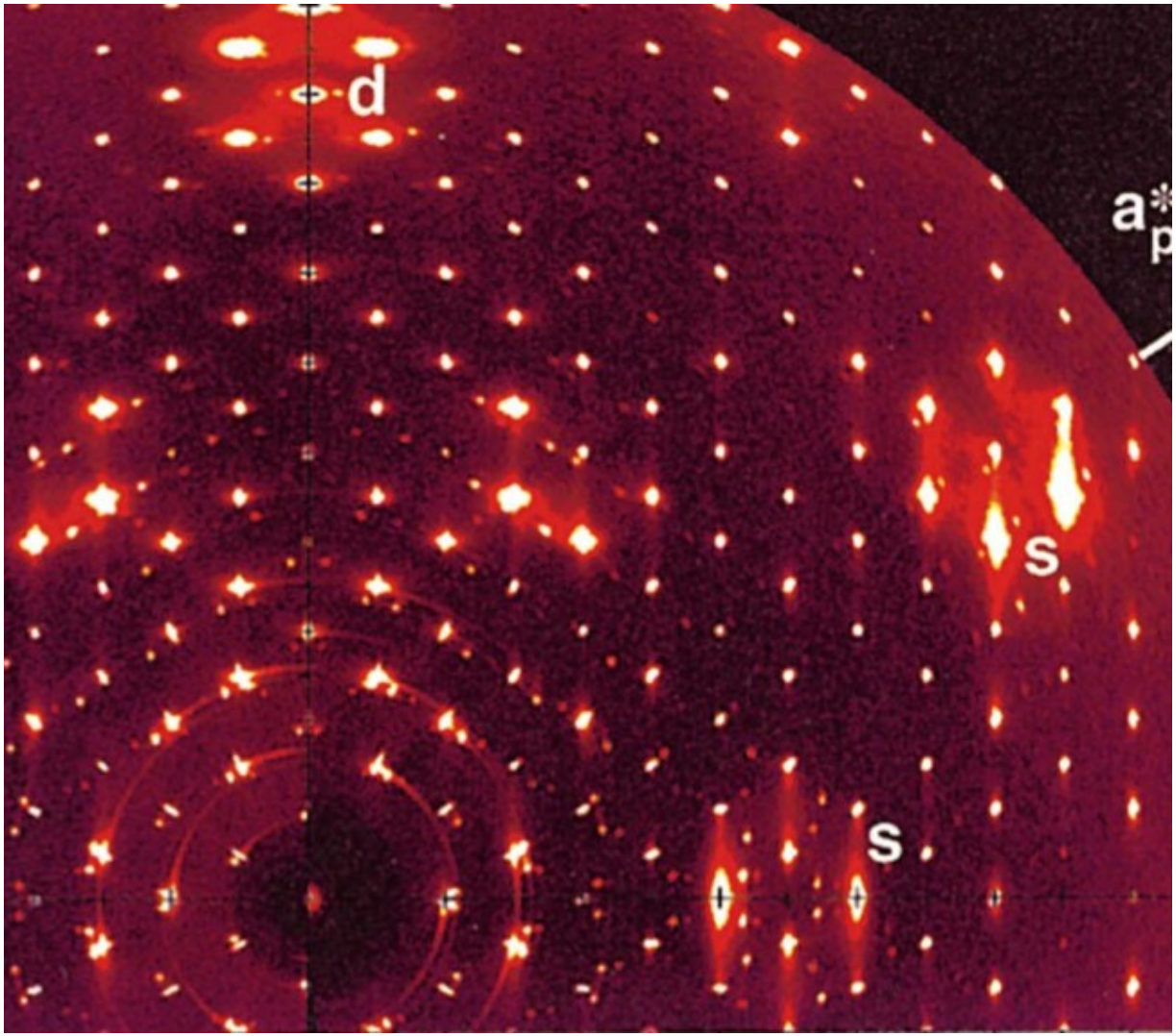
Pilatus @ Swiss Light Sourde, Sample: PbTe

Accurate background measurement with good counting time is a must!

Diffuse scattering is much weaker than Bragg reflections

Simultaneous measurement

- Detector dynamic range
- Radiation damage
  - Sample
  - Detector



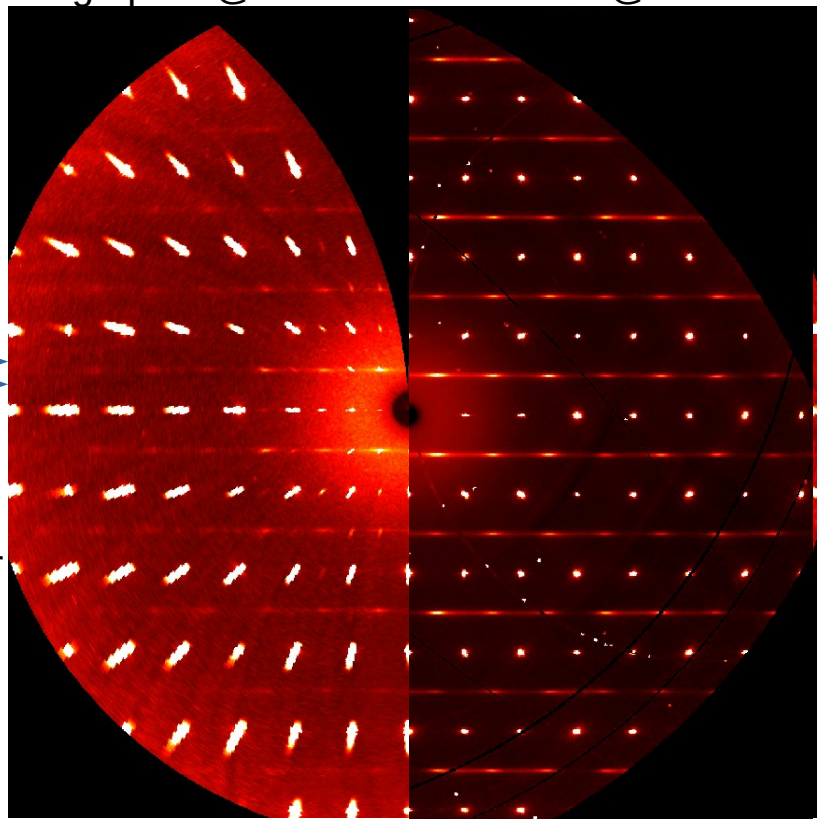
Experimental Aspects Background elimination

Diffuse streaks or layers ==> anything else is *background*

Image plate@in-house Pilatus@ESRF

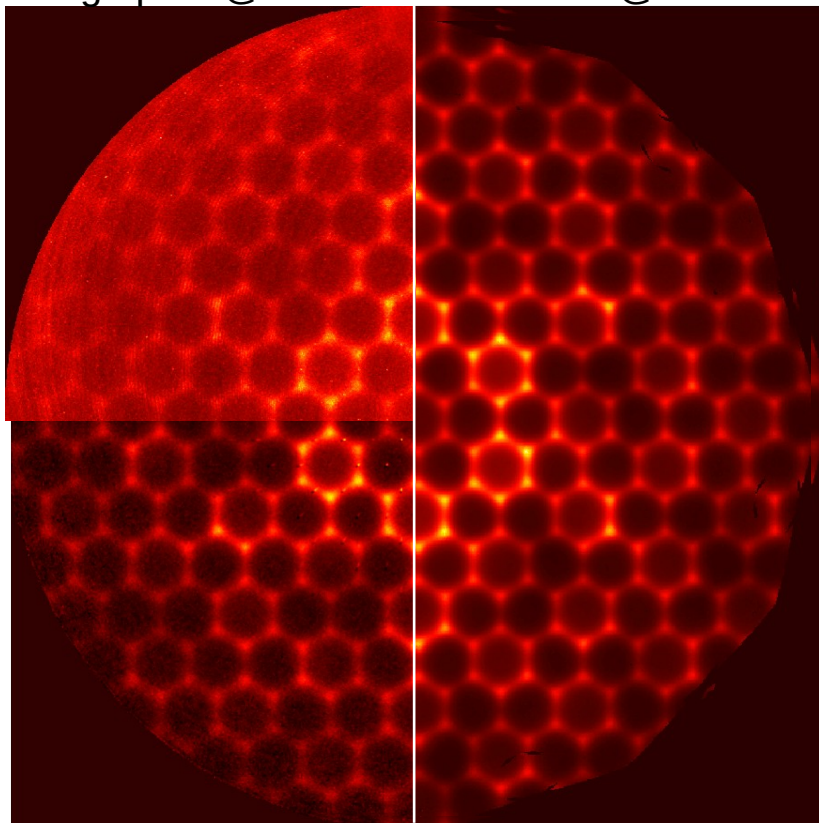
Background estimate

Intensity above / below diff. layer



uncorrected

Image plate@in-house Pilatus@ESRF



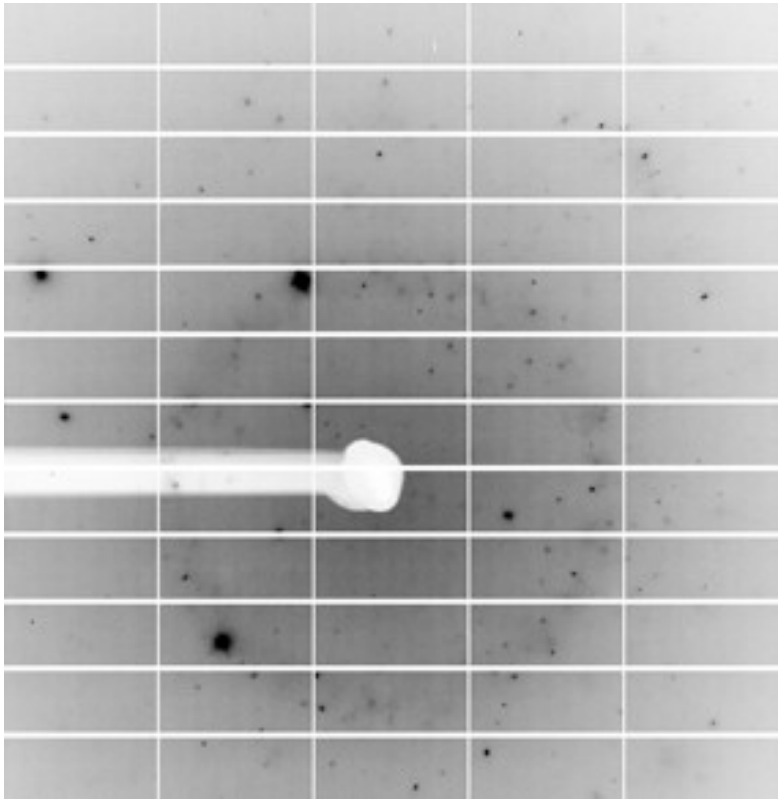
corrected

Experimental Aspects Parasitic Scattering

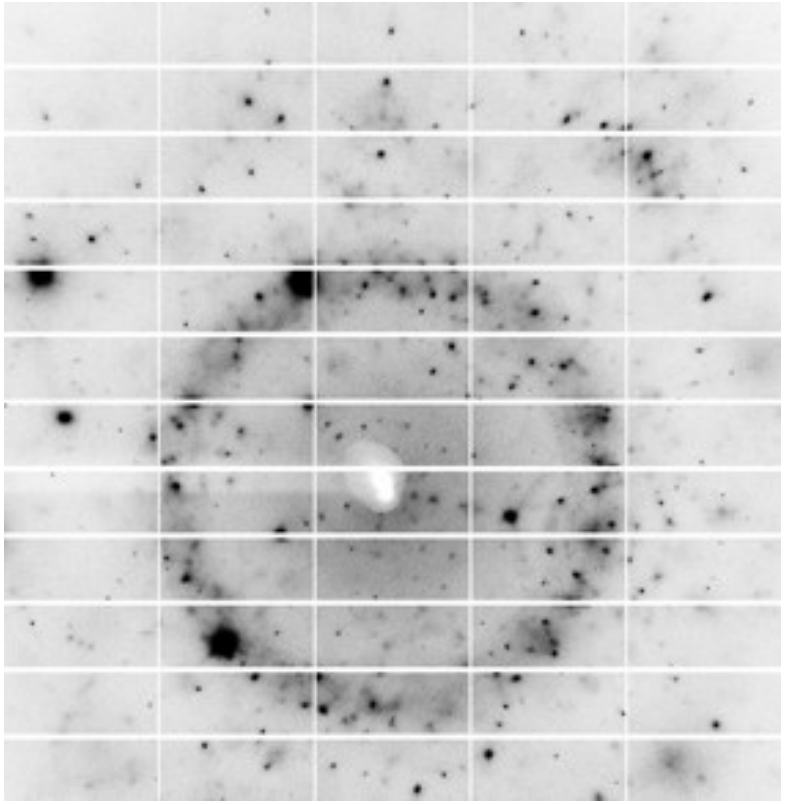
Everything along the primary beam path does scatter !

Correct fluorescence scattering by sample

E(primary) : 16 keV
E(threshold) : 8 keV



E(primary) : 16 keV
E(threshold) : 10 keV



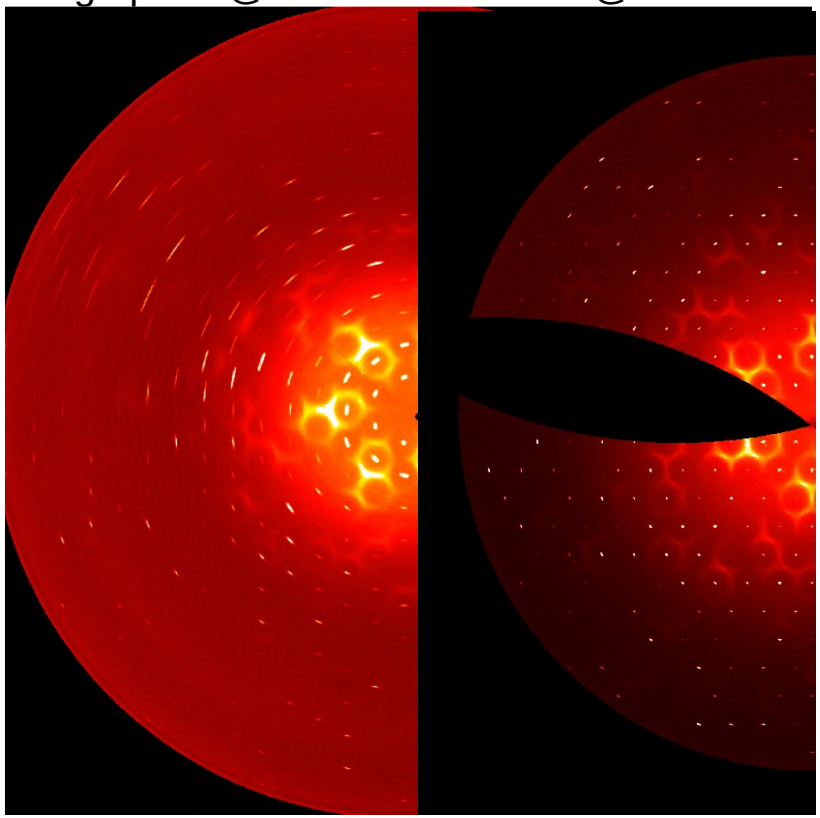
Pilatus @ Swiss Light Sourde, Sample: *i*-AlCuFe

Experimental Aspects Resolution function

Diffuse scattering profile carries structural information

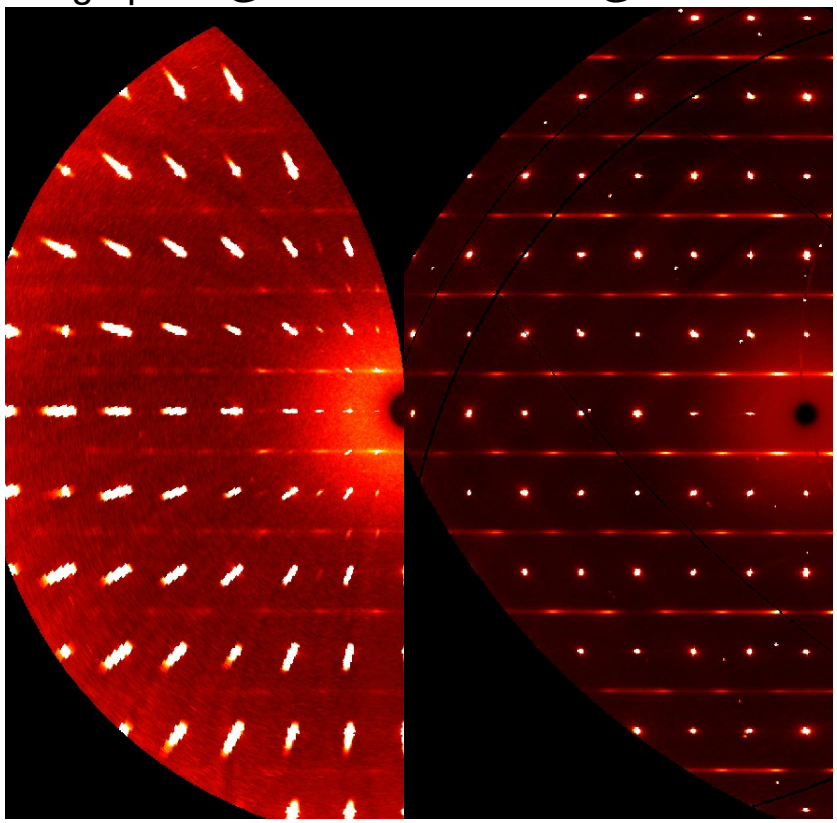
Optimize resolution function ==> choice of instrument

Image plate @ ESRF Pilatus @ ESRF



Large angular range

Image plate @ in-house Pilatus @ ESRF

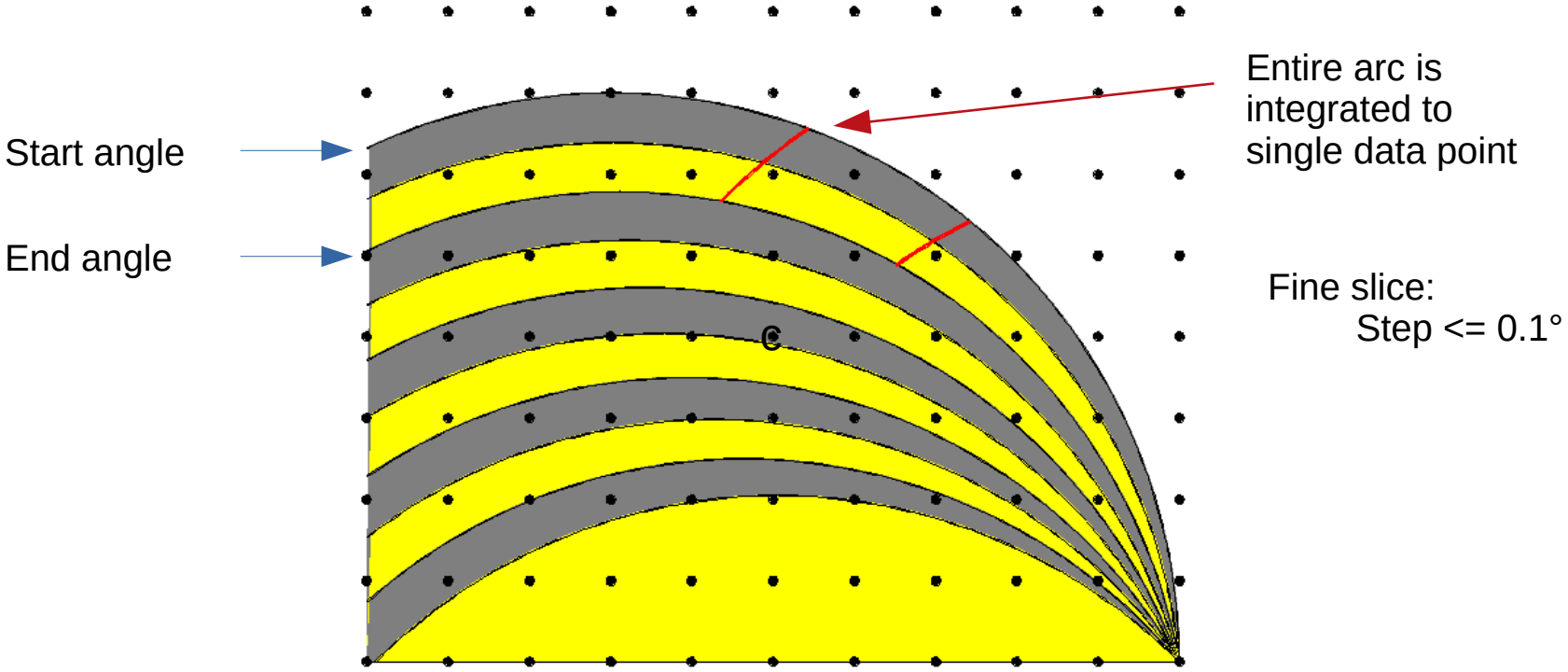


Kα1 / Kα2 / white radiation

Determine resolution function from **unsaturated** Bragg reflections

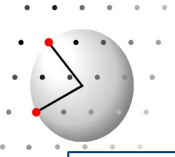
Experimental Aspects Measurement strategy

Diffuse scattering requires continuous scans over small angular range



Schematic image of reciprocal space
With sweeps of Ewald sphere

Fine slice with fast and noise-free detector



Experimental aspects