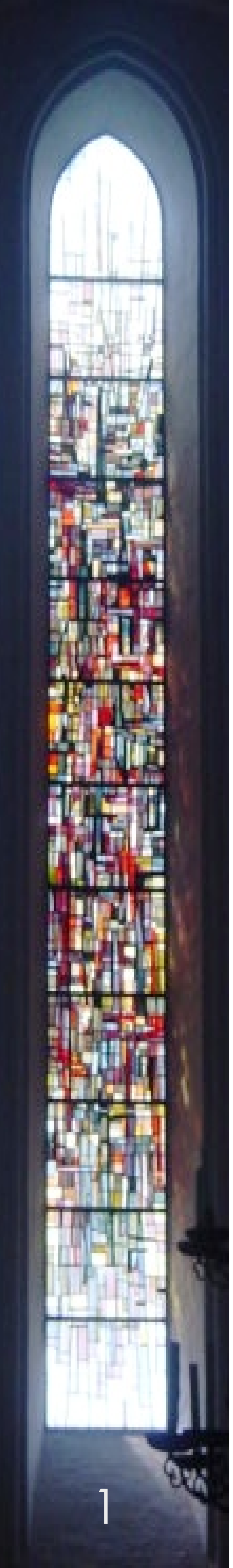
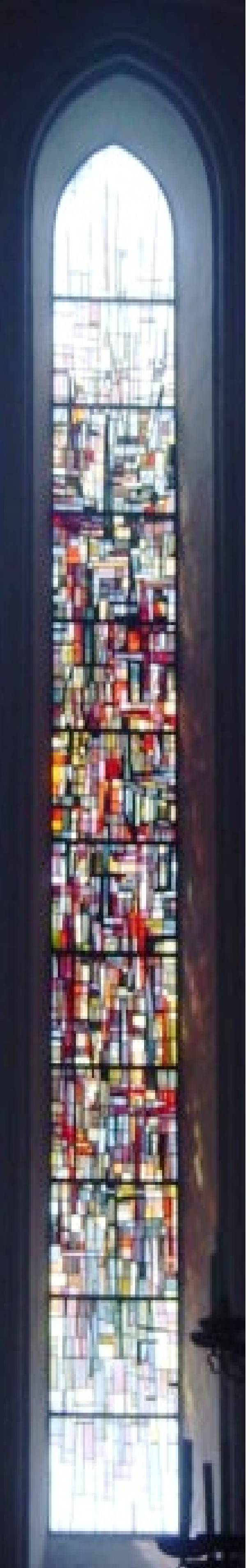


Total scattering data from ISIS

Martin Dove
University of Cambridge



The team

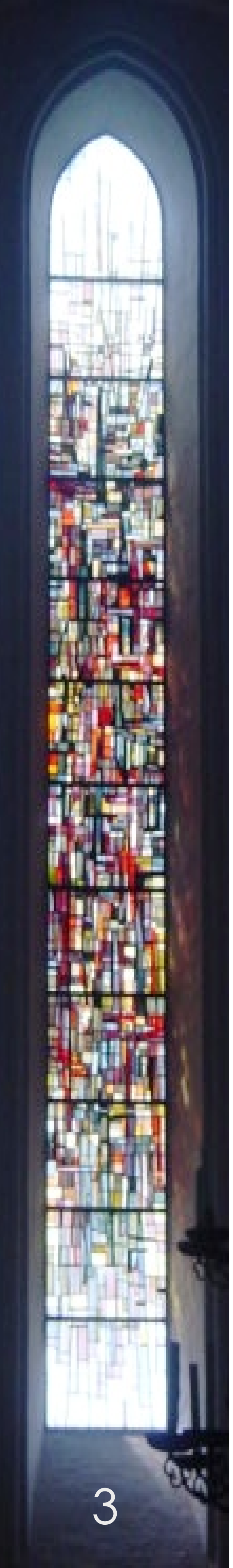
The work I describe here is carried out in collaboration with:

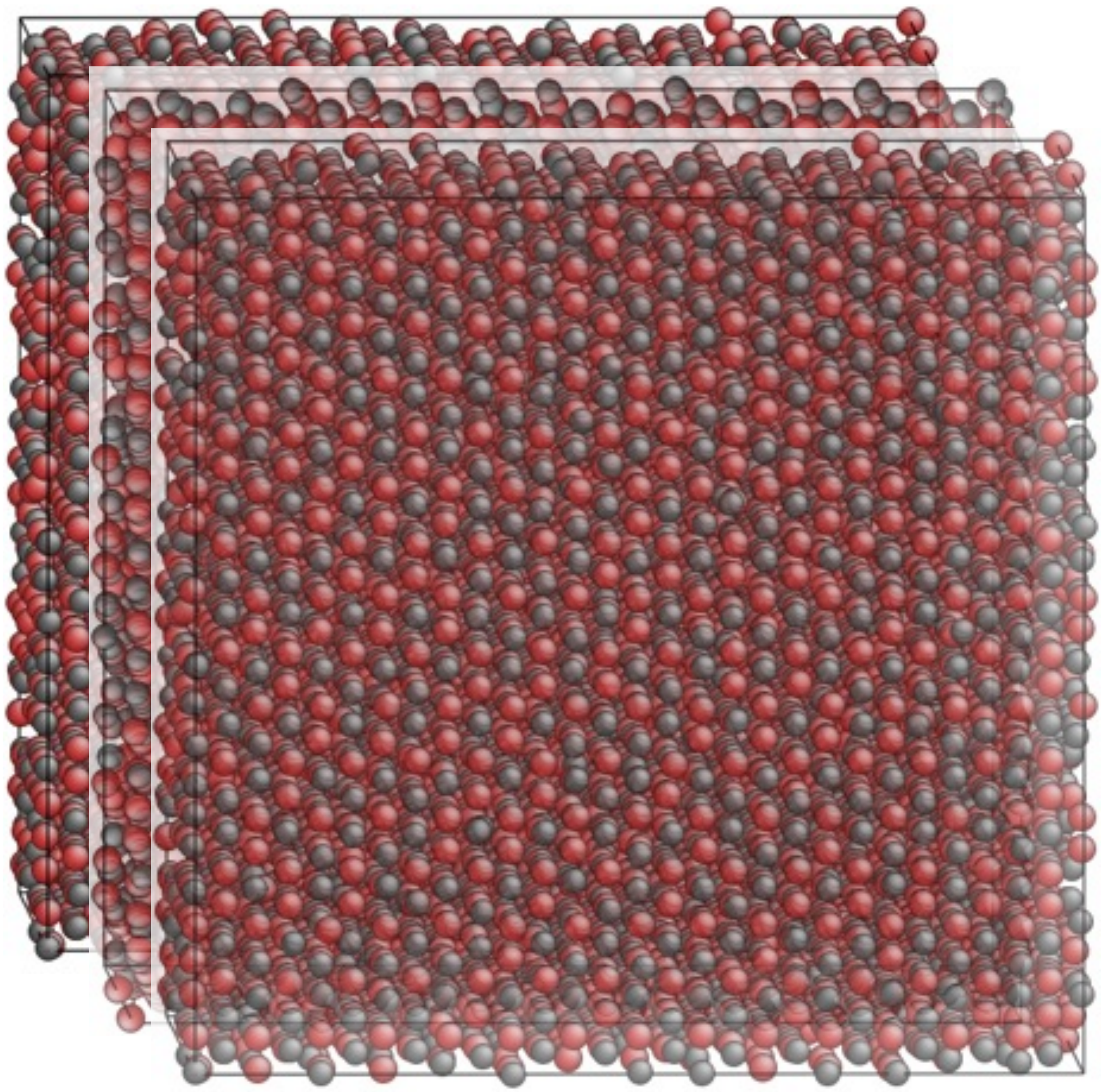
Dave Keen
ISIS

Matt Tucker
ISIS

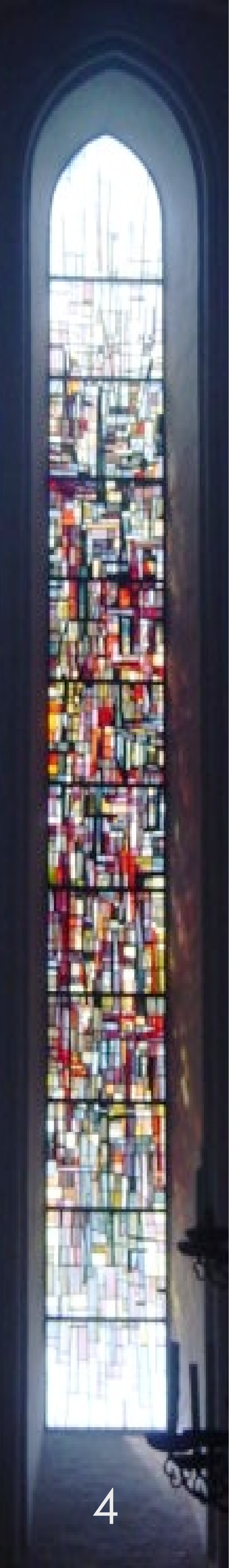
Andrew Goodwin
Oxford

Objective





We are seeking to construct large-scale atomic models of matter that best match experimental data



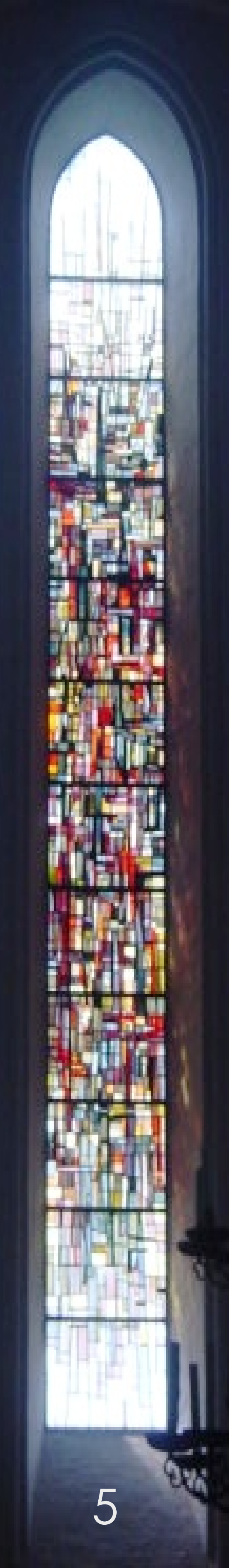
The Reverse Monte Carlo algorithm

Generate initial configuration

Move a randomly selected atom a random distance

Compute new experimental functions and compare with data

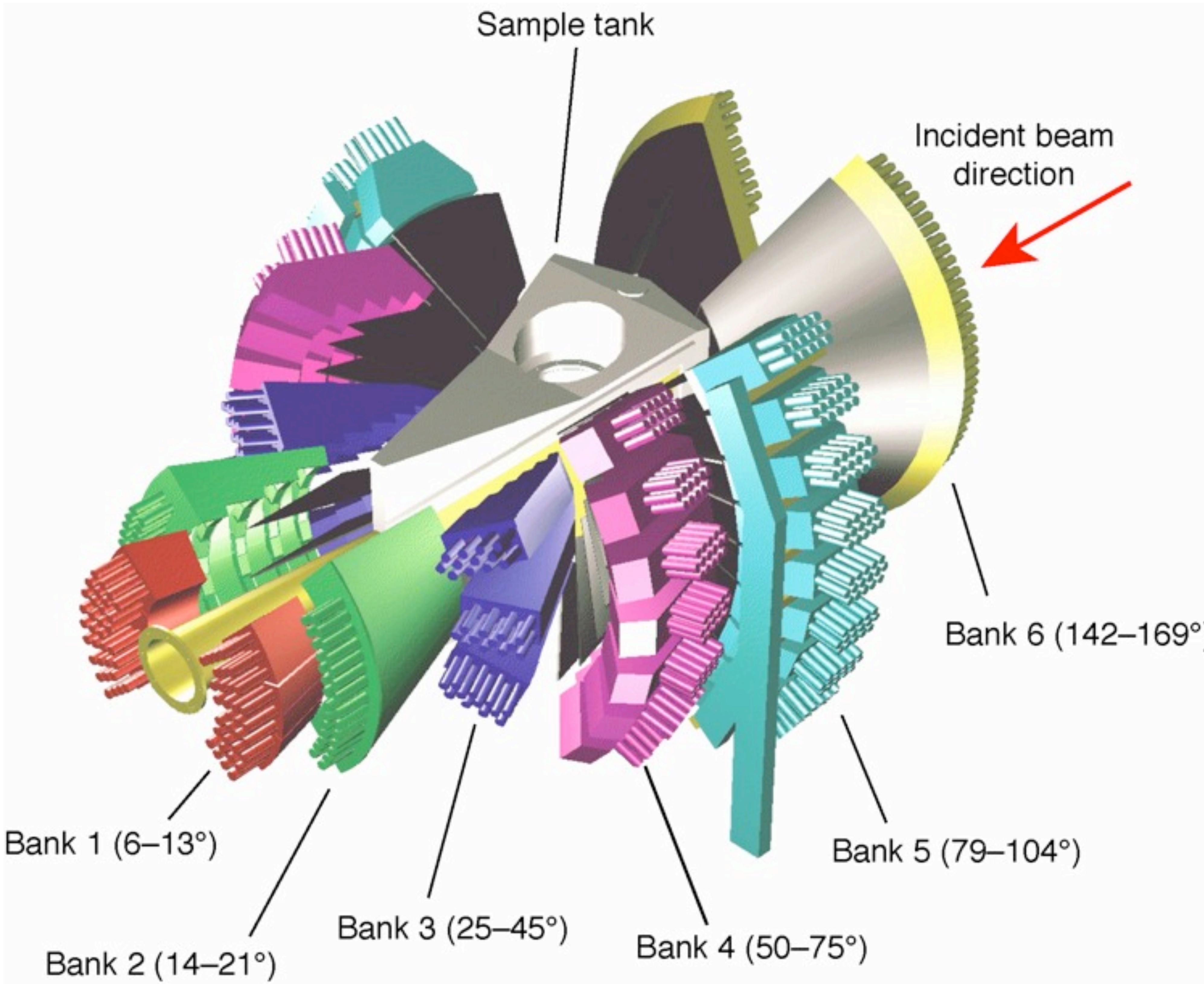
Only reject change if comparison is worse and with some probability

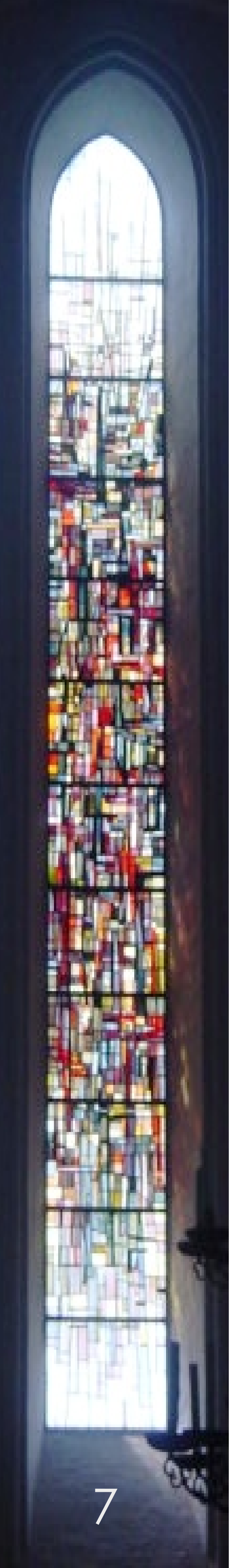


Principles of a scattering experiment

- Idea is to scatter radiation beams from matter
- The spatial Fourier transform gives information about atomic structure
- The time Fourier transform gives information about atomic dynamics
- In our work our result is an integral in the energy domain = instantaneous correlations

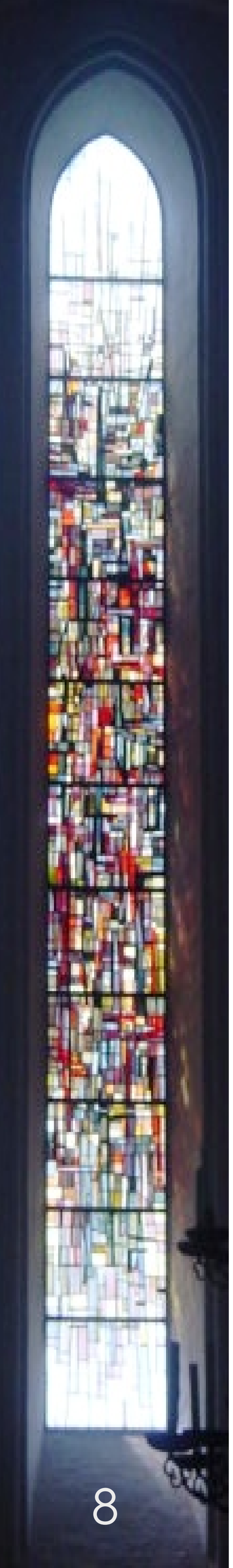
GEM @ ISIS


Sample tank
Incident beam direction
Bank 6 (142–169°)
Bank 5 (79–104°)
Bank 4 (50–75°)
Bank 3 (25–45°)
Bank 2 (14–21°)
Bank 1 (6–13°)

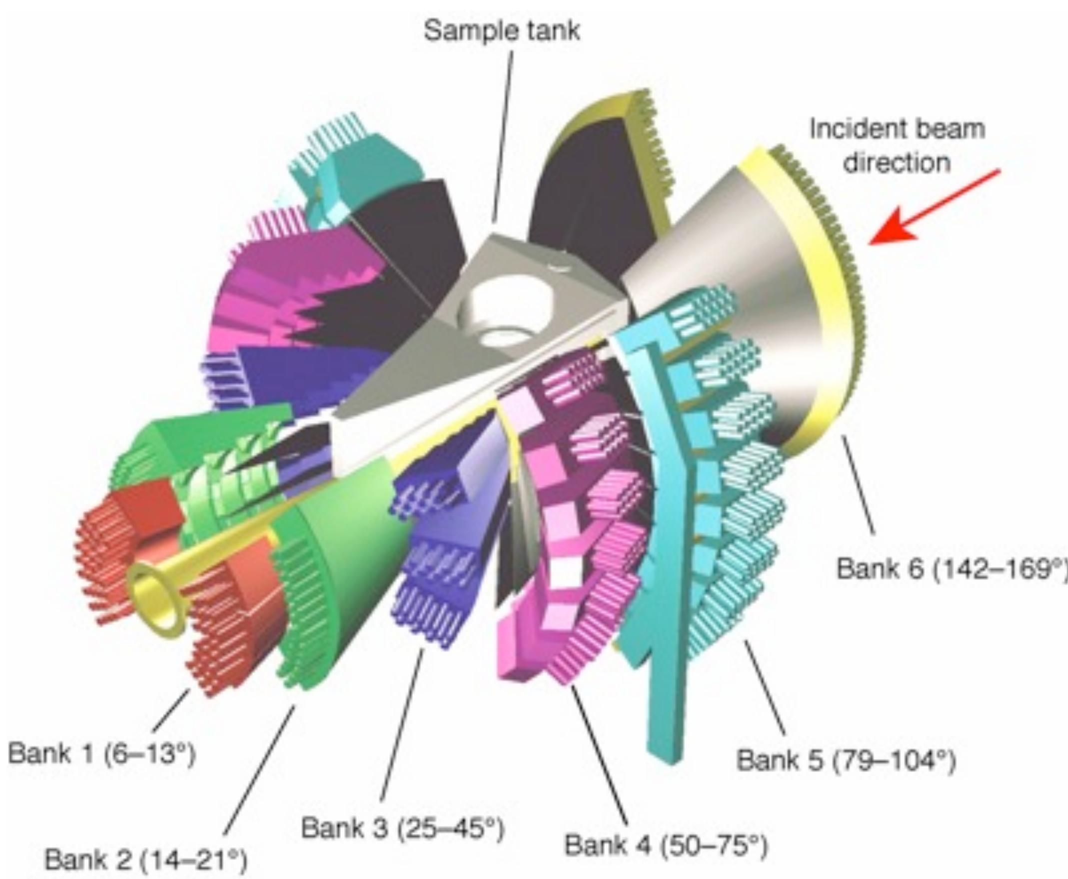


ISIS neutron source

- Produces intense beams of neutrons by firing a beam of protons at a metal target
- Neutrons are produced in tight pulses at a rate of 50 Hz
- The essential measurement is the time taken for each neutron to go from the source to the detector

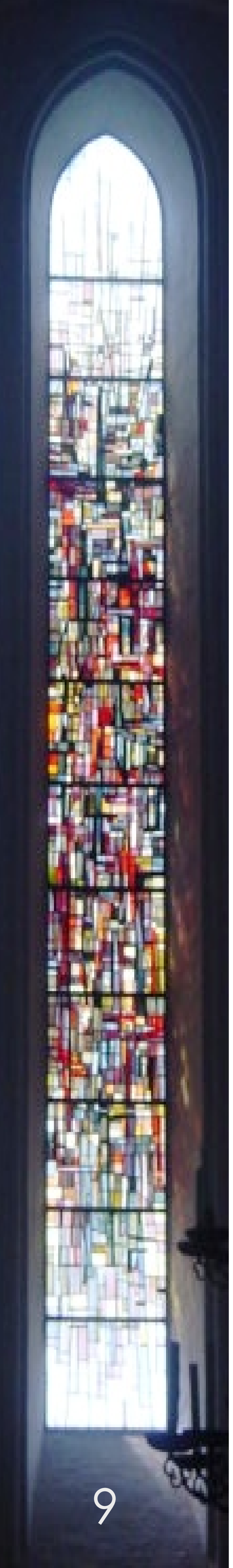


GEM histogram files



- ~4000 detectors
- Each experiment produces a histogram for each detector
- Each histogram is a binning of all neutron flight times per pulse, summing all pulses

The data reduction process has to convert these histograms into meaningful data



Converting to meaningful data 1

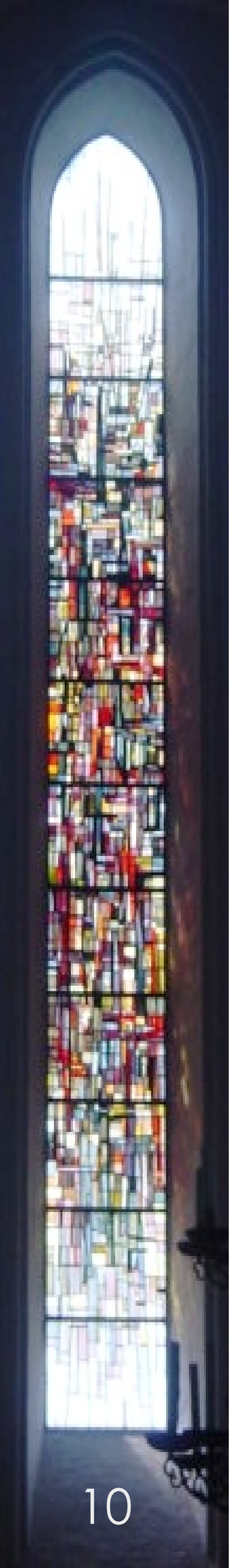
A meaningful concept is the *scattering vector*

$$Q = \frac{4\pi \sin(\phi / 2)}{\lambda}$$

The wavelength can be obtained from the flight time

$$\lambda = \frac{ht}{mL}$$

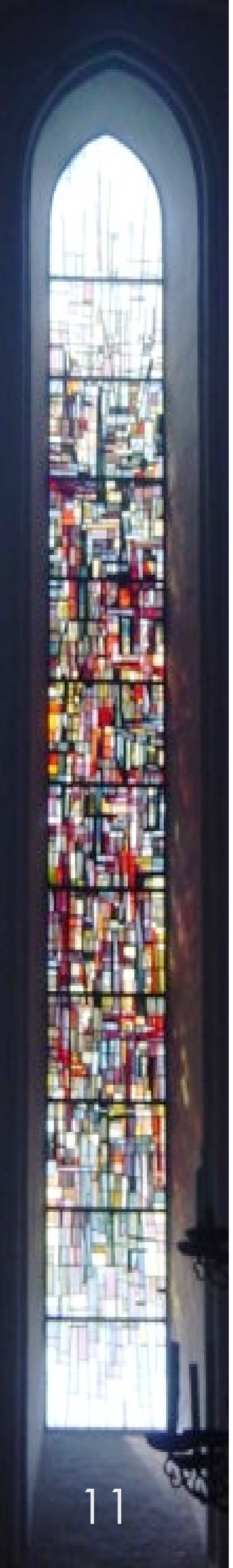
Distances and angles can be obtained by surveying and diffraction measurements



Converting to meaningful data 2

A second meaningful concept is the *intensity of the scattered beam*

We can put the intensity of the spectra for each data onto a common scale from measurements of incoherent scattering from vanadium



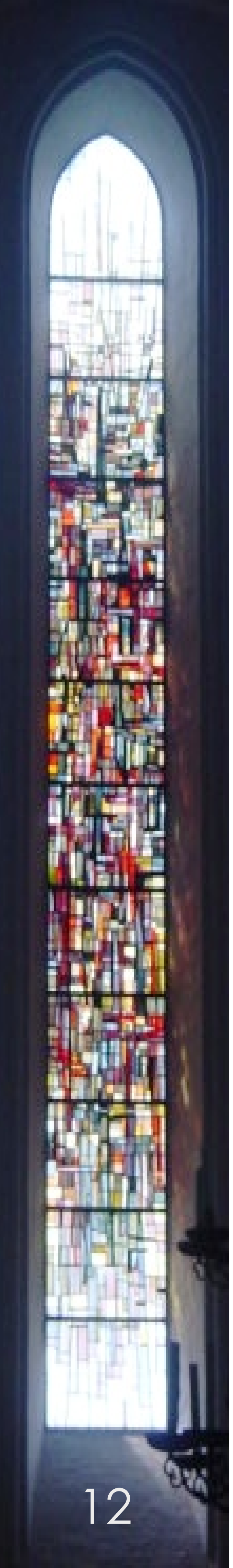
Converting to meaningful data 3

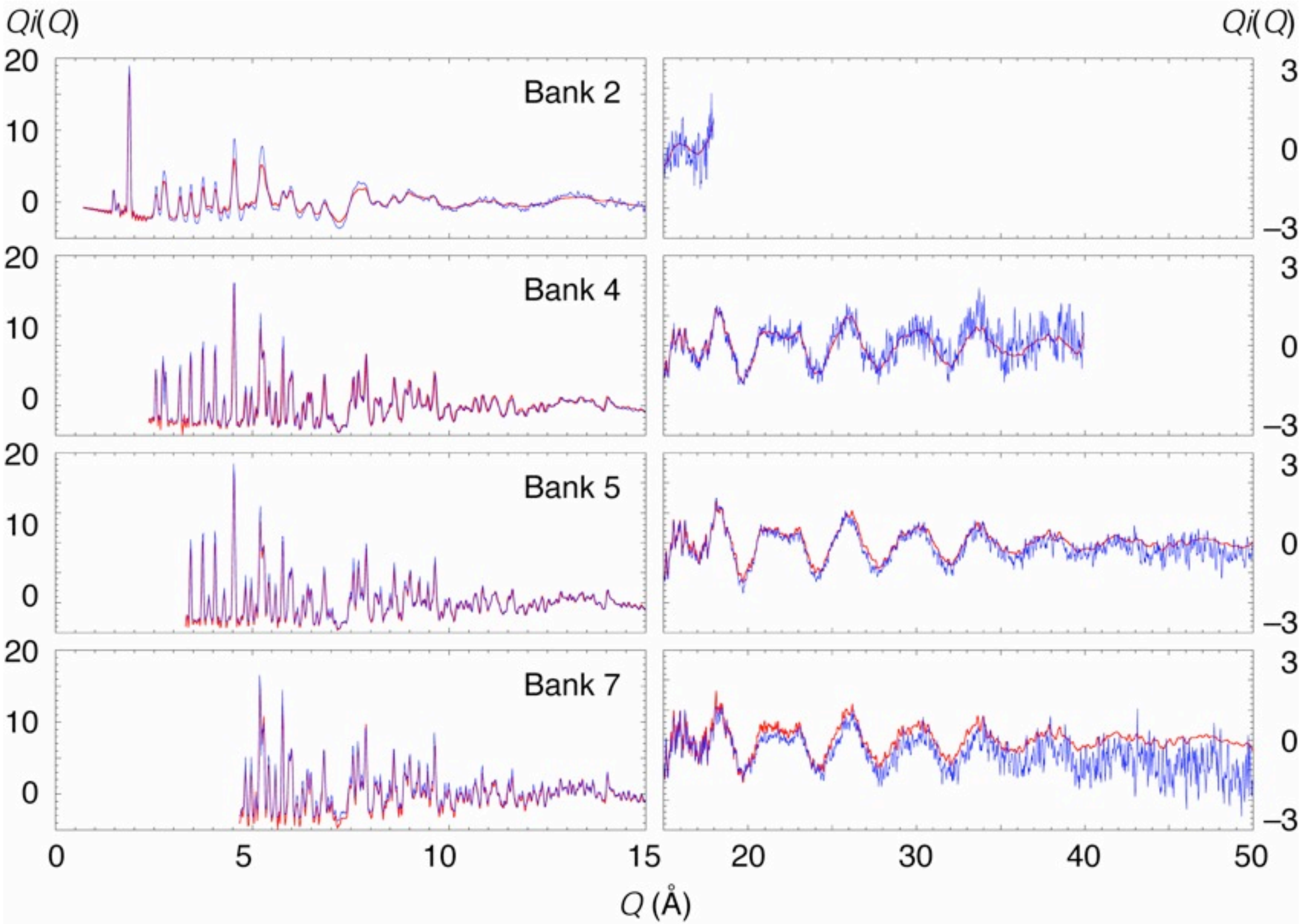
Finally, we need to subtract the scattering from the following components

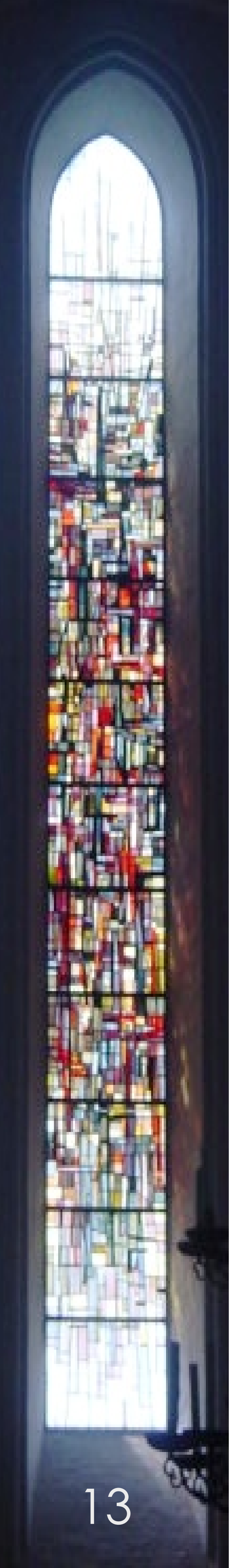
- The instrument itself
- The sample container
- The equipment used to control the sample temperature

These quantities are obtained from separate measurements (Day 1)

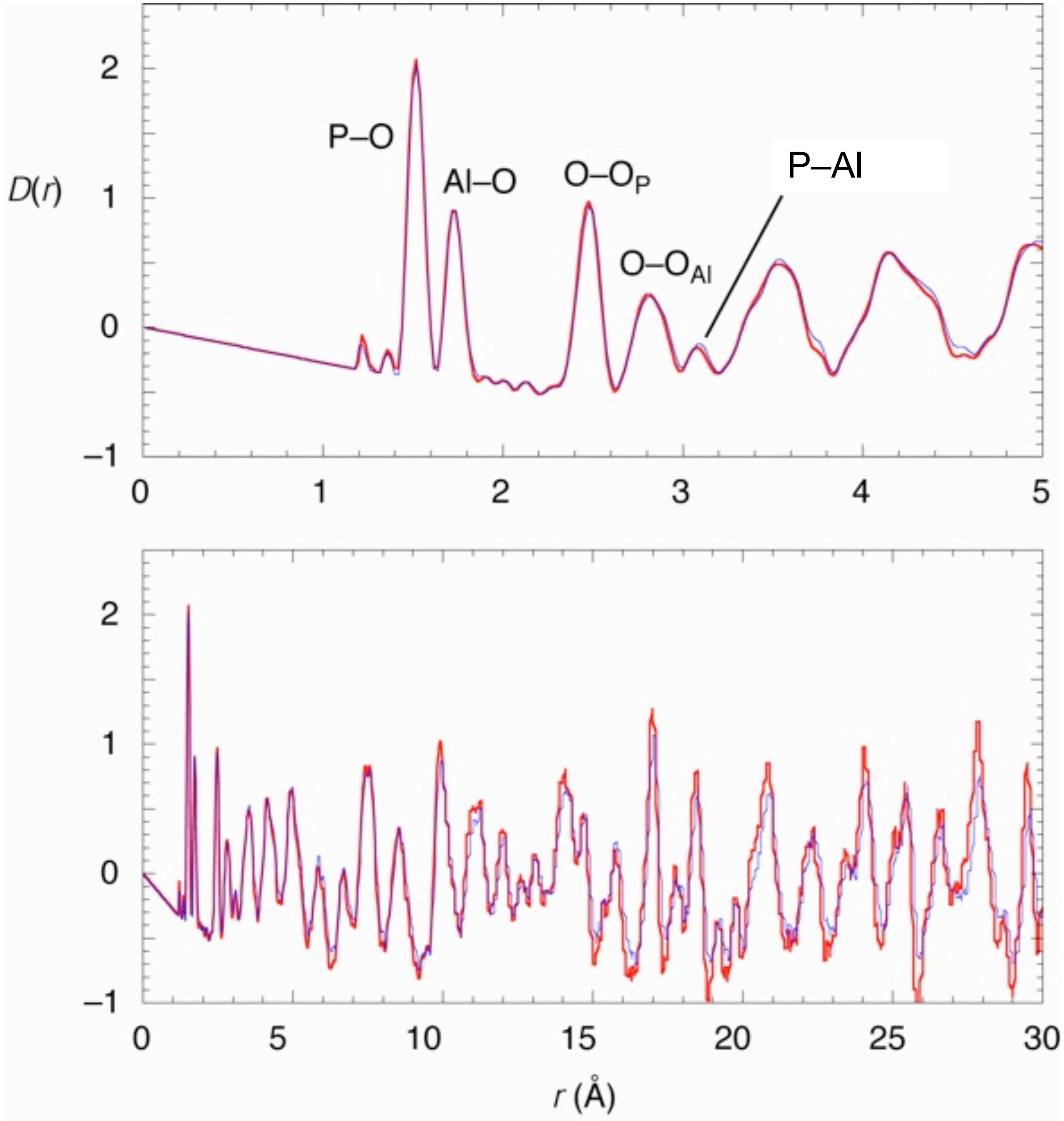
Example of $AlPO_4$



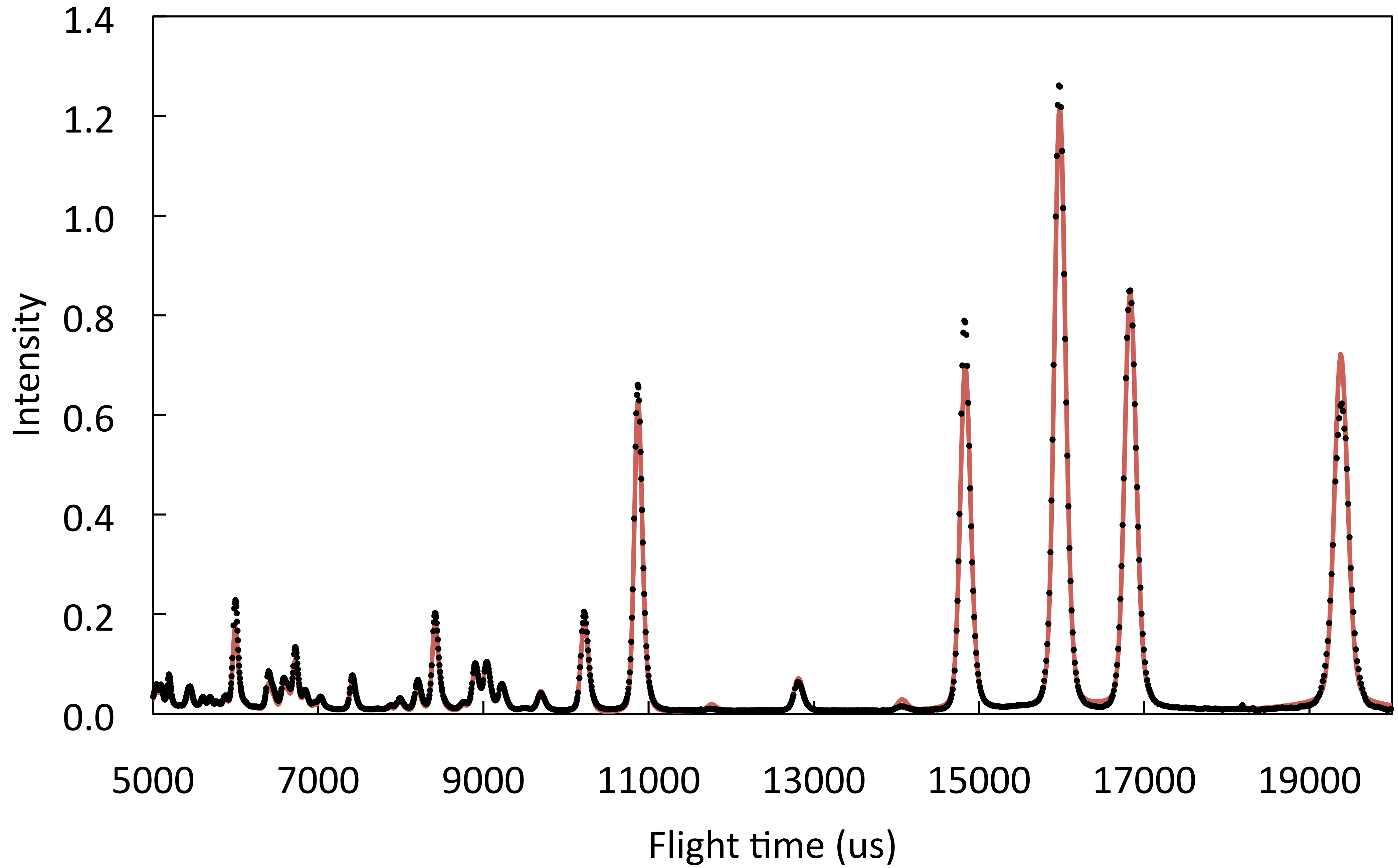


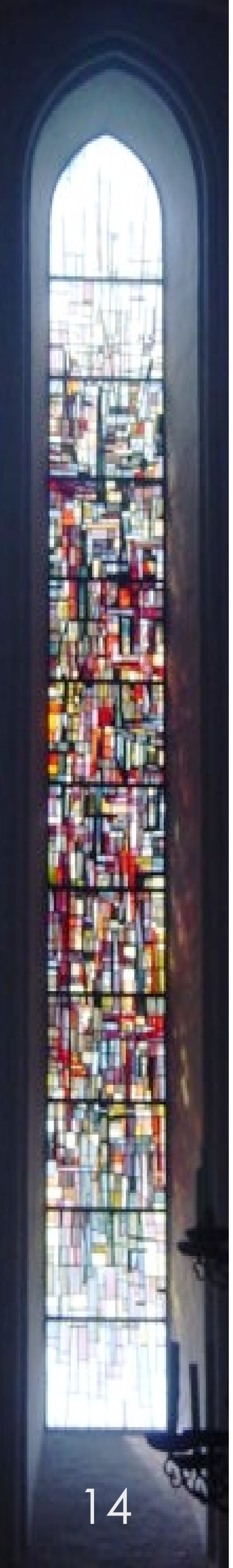


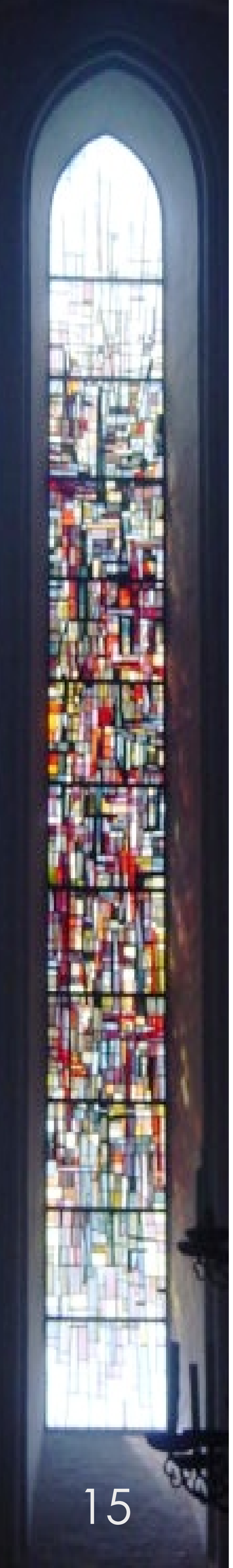
Fourier transform of the data gives the pair distribution function



Bragg diffraction (KCN)







Use of XML data representation

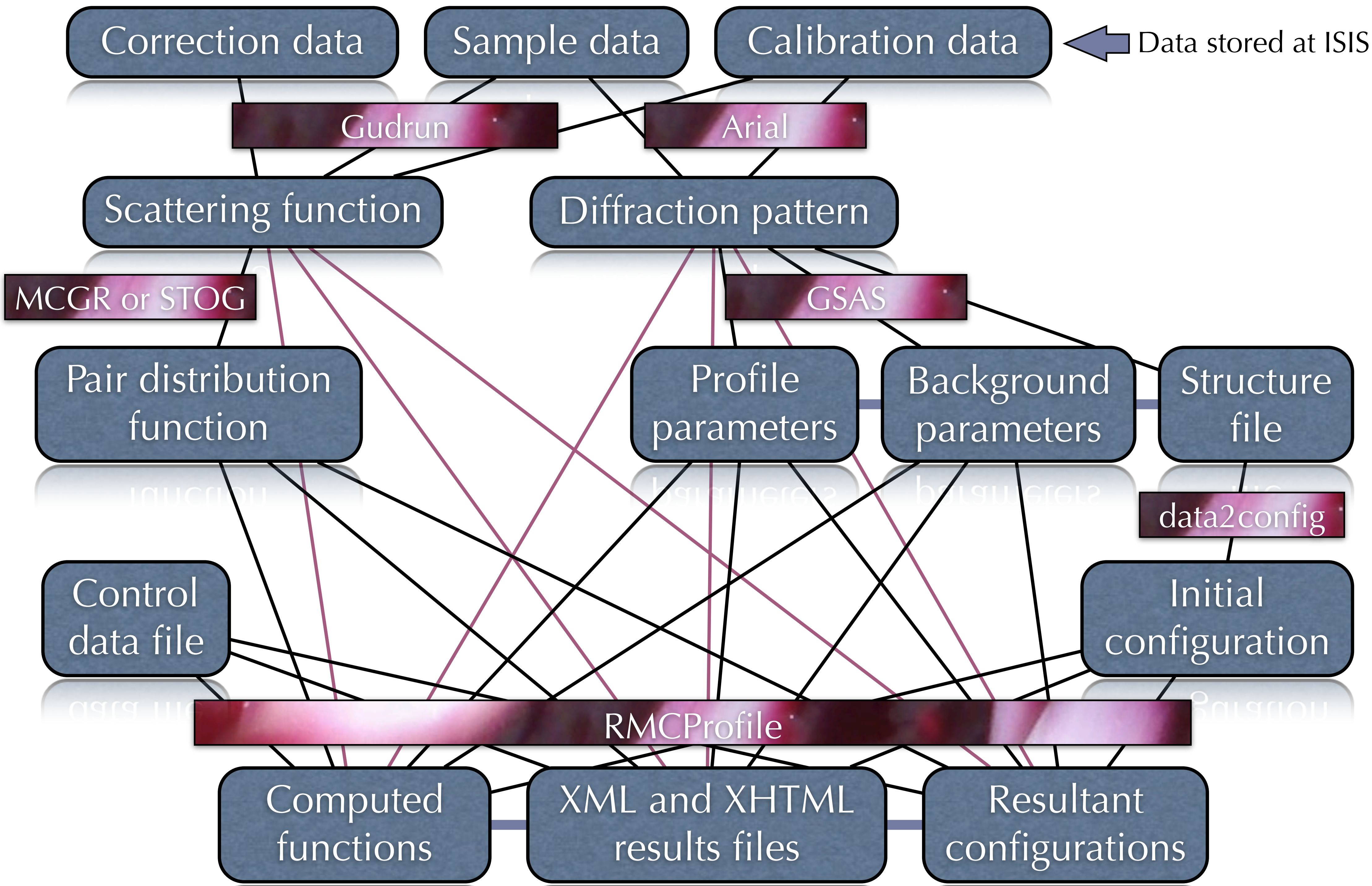
Output from RMCProfile is given in several representations, including XML

Our XML document is based on CMLcomp, which is a dialect of the *Chemical Markup Language* for computational science

Important role of metadata, parameter values, and computed properties

Motivated to support collaboration

RMC data flow



RMC data flow