PAUL SCHERRER INSTITUT

PSI

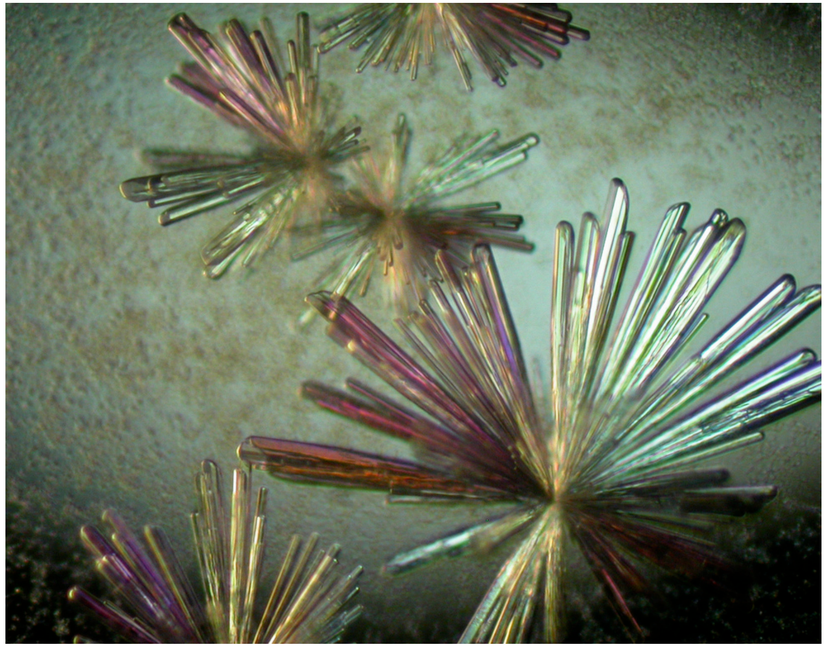
Rasmus Ischebeck

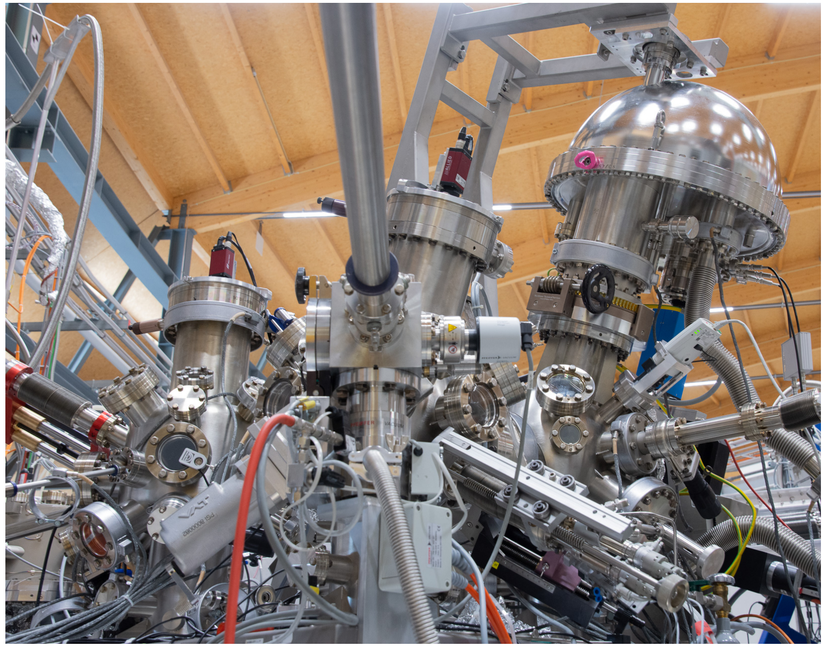
Uses of Synchrotron Radiation

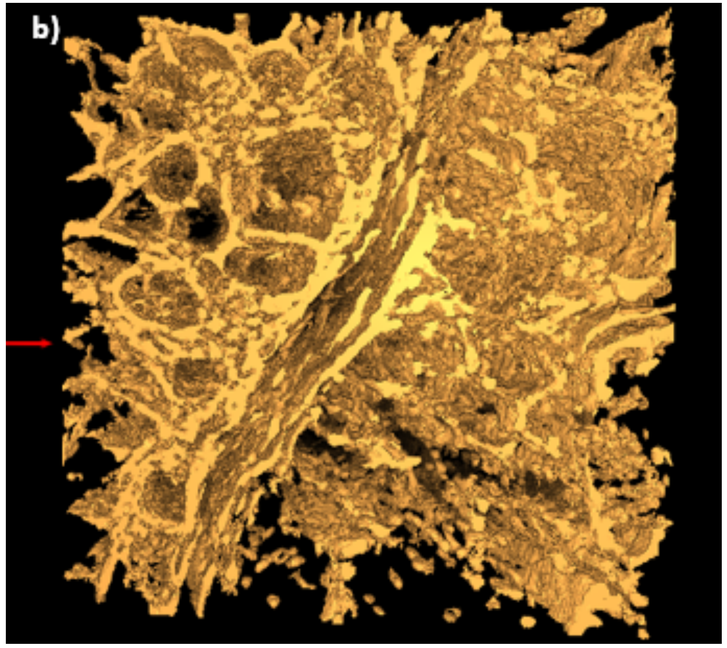
Joint Universities Accelerator School

Uses of Synchrotron Radiation

- Diffraction and crystallography
- Spectroscopy
- Imaging



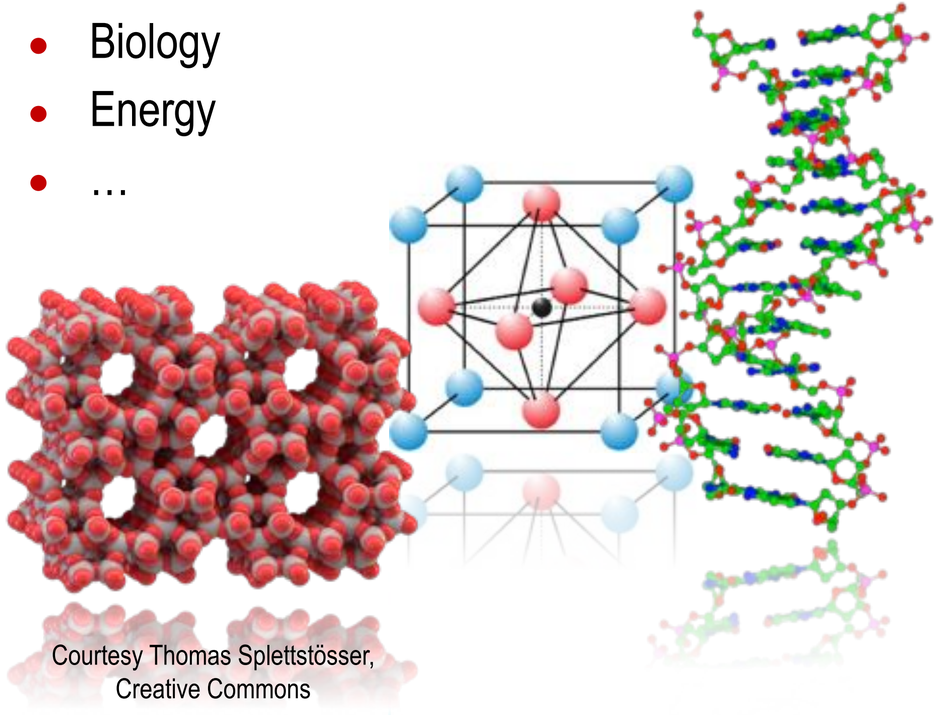




flickr/orinoco14 (left), Federica Marone (right)

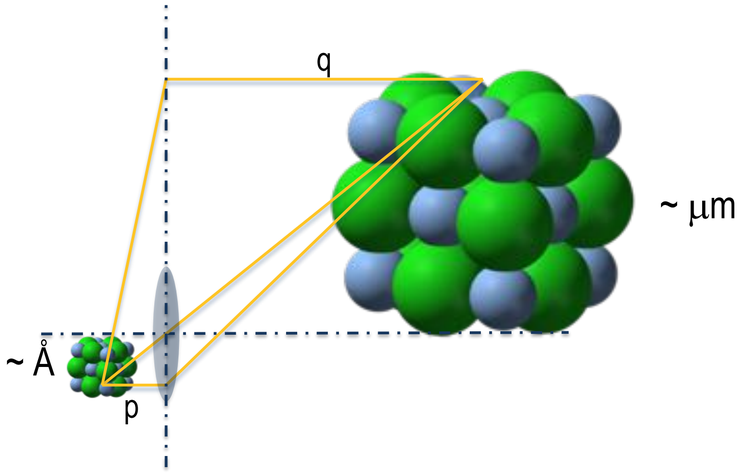
Diffraction and Crystallography

- Atomic structure
  - Functionality
    - Electronics
    - Biology
    - Energy
    - …



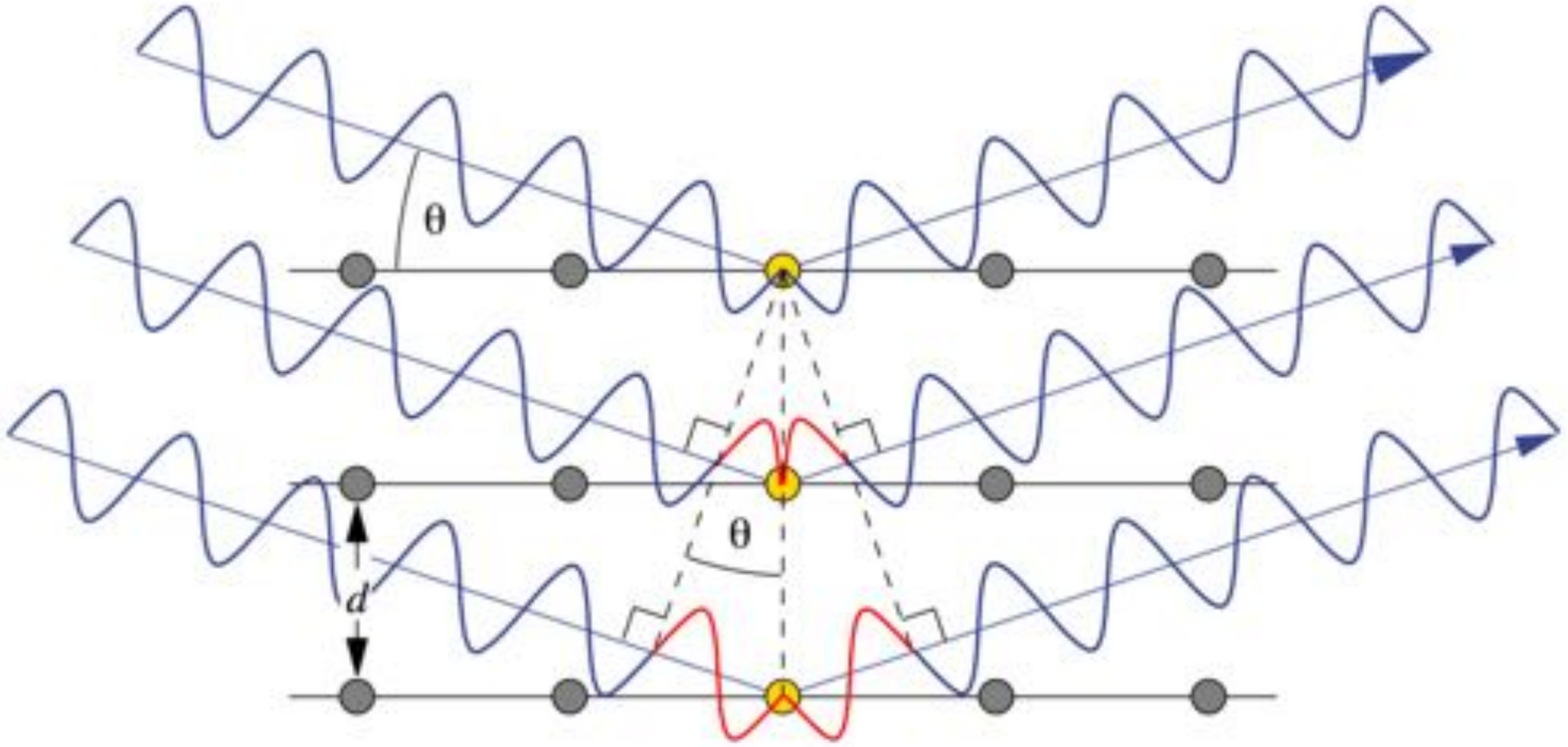
Courtesy Thomas Splettstösser, Creative Commons

- X-ray lens?
  - Required magnification q/p ~ 10^4



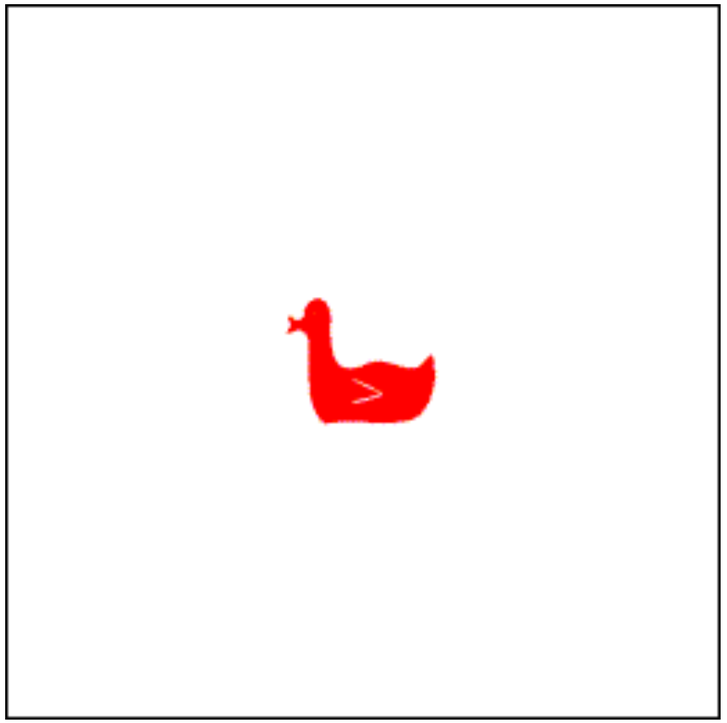
  - No x-ray lens can provide this

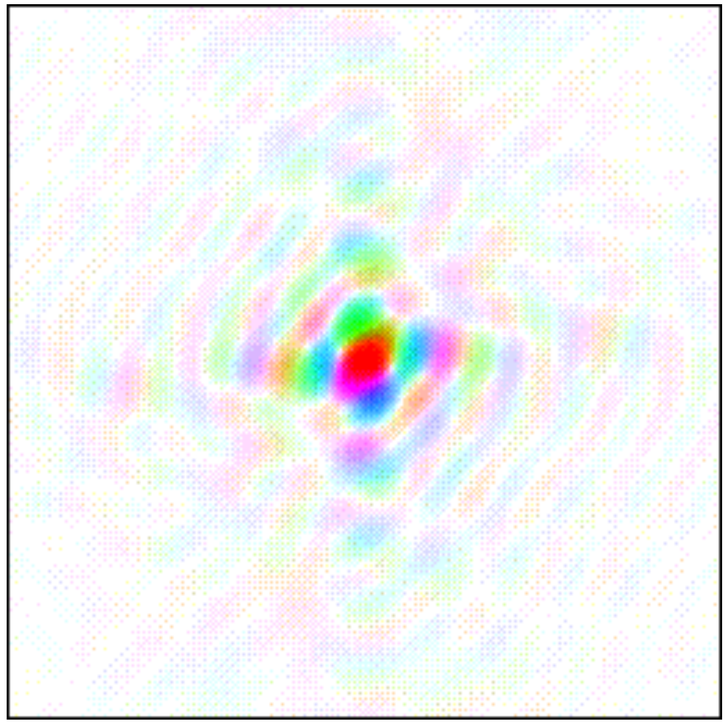
Diffraction



The Phase Problem

- A (two-dimensional) duck



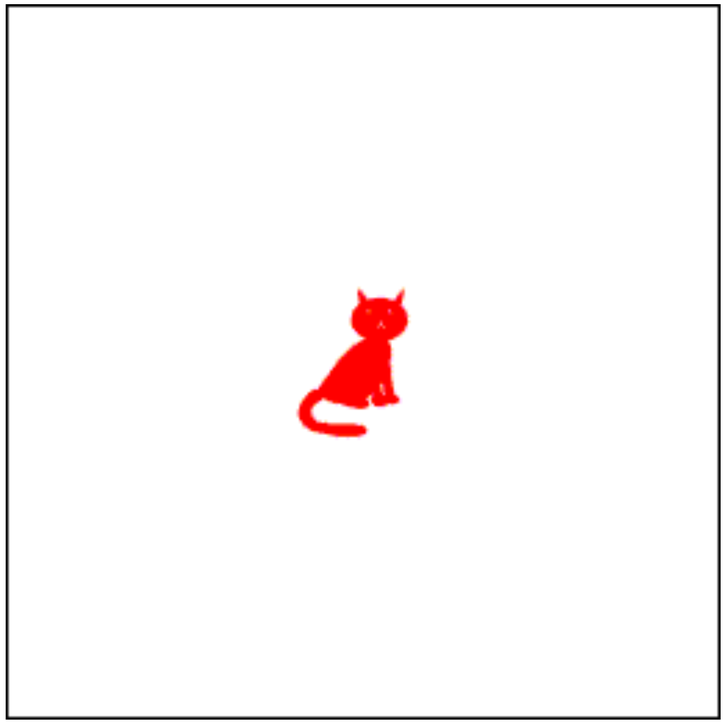


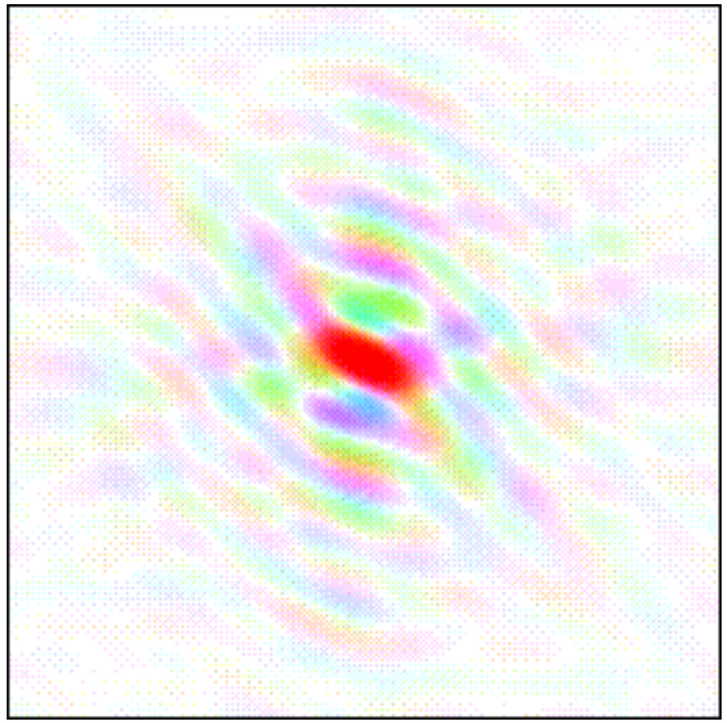
Images by Kevin Cowtan, Structural Biology Laboratory, University of York

The Phase Problem

- A Cat

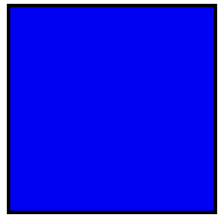
... and its Diffraction Pattern



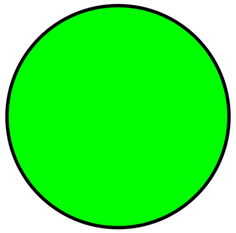


Images by Kevin Cowtan, Structural Biology Laboratory, University of York

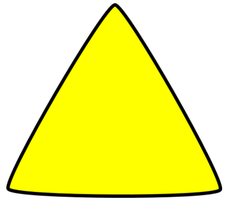
Combine the Amplitude of the Diffraction Pattern of the Cat With the Phase of the Diffraction Pattern of the Duck…



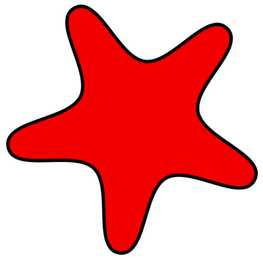
You reconstruct a cat



You reconstruct a duck



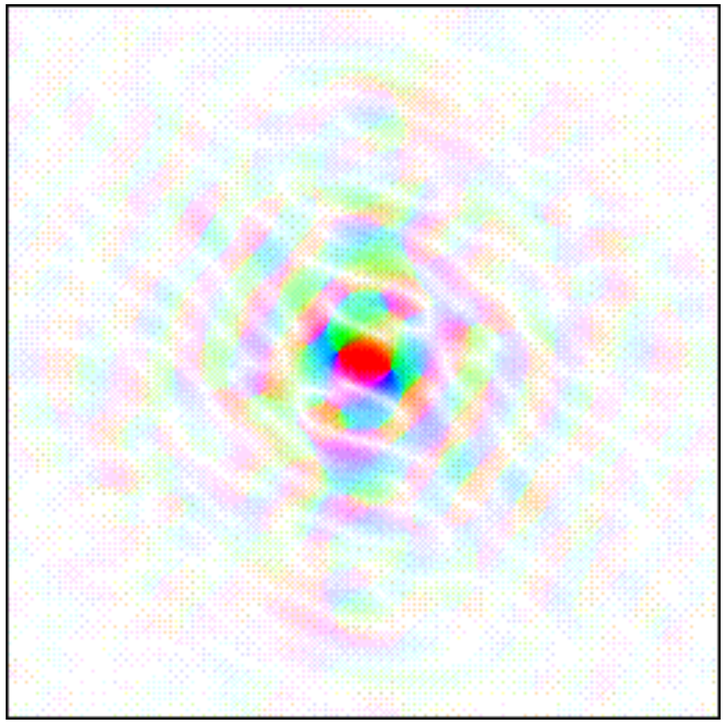
You reconstruct random noise

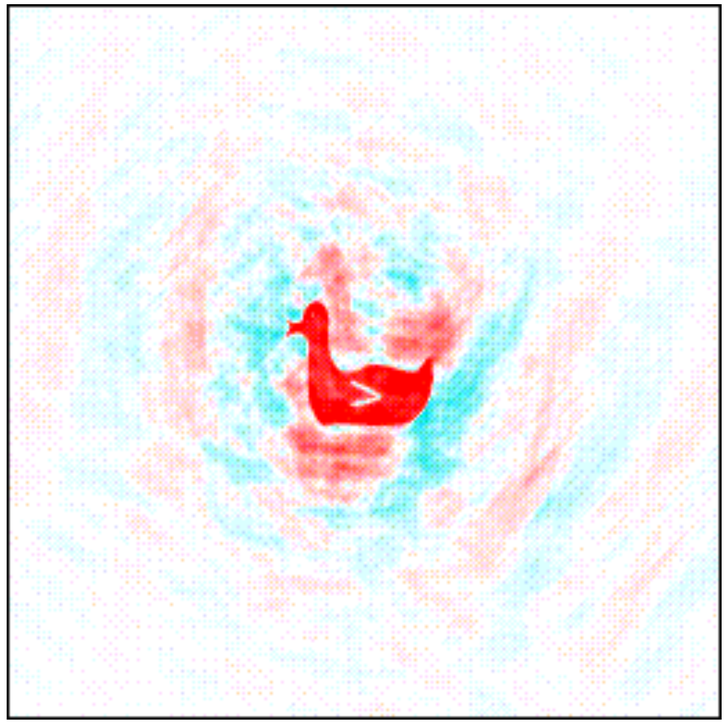


You reconstruct a cat with a duck hat

Reconstruction

- Combine the amplitude of the diffraction pattern of the cat
- and the phase of the diffraction pattern of the duck



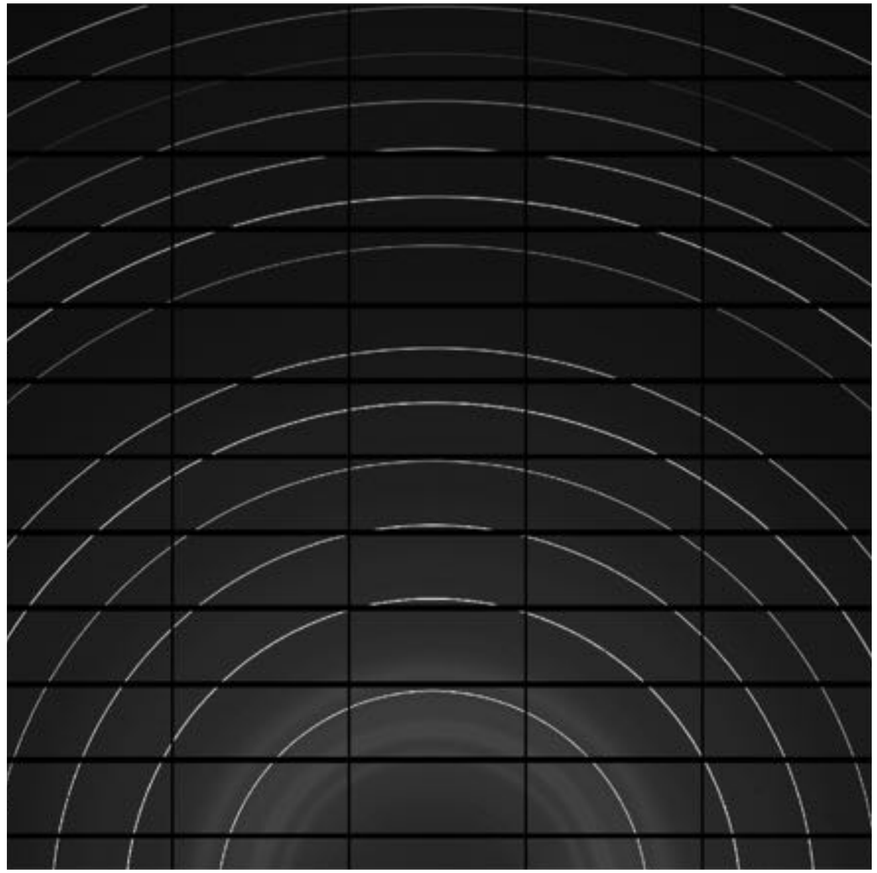


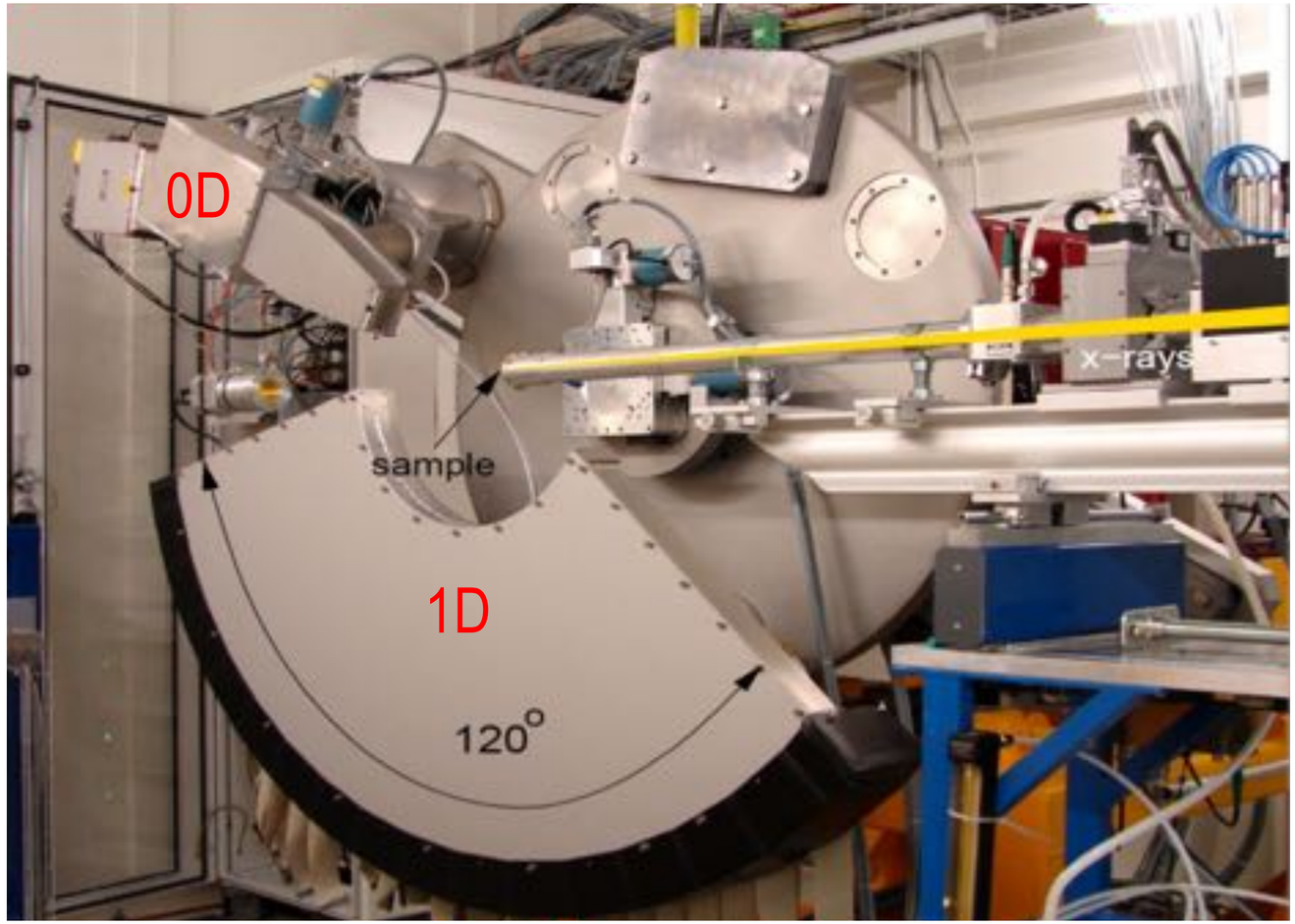
The result: a duck!

Images by Kevin Cowtan, Structural Biology Laboratory, University of York

Powder Diffraction

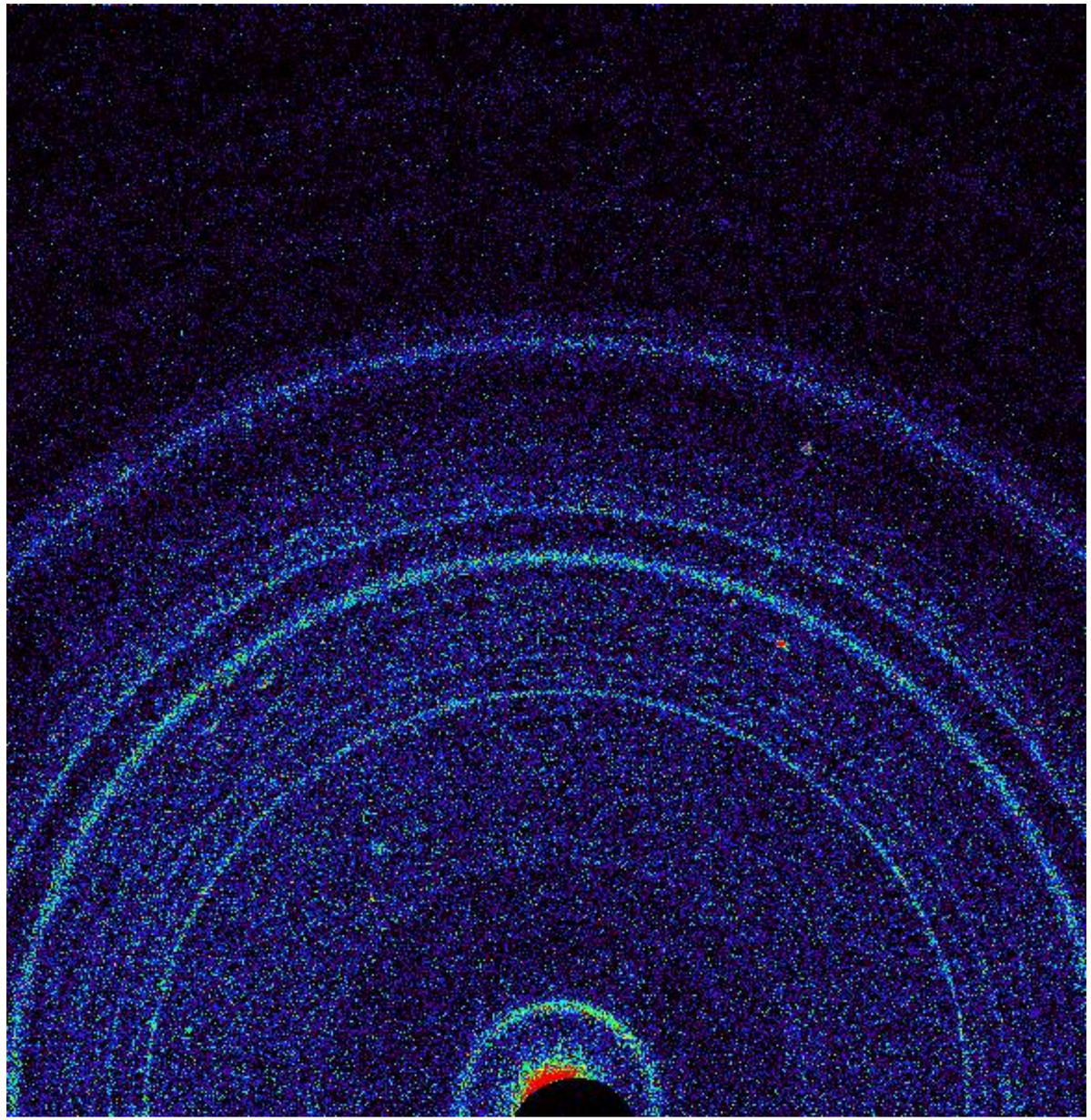
- Diffraction pattern of LaB_6





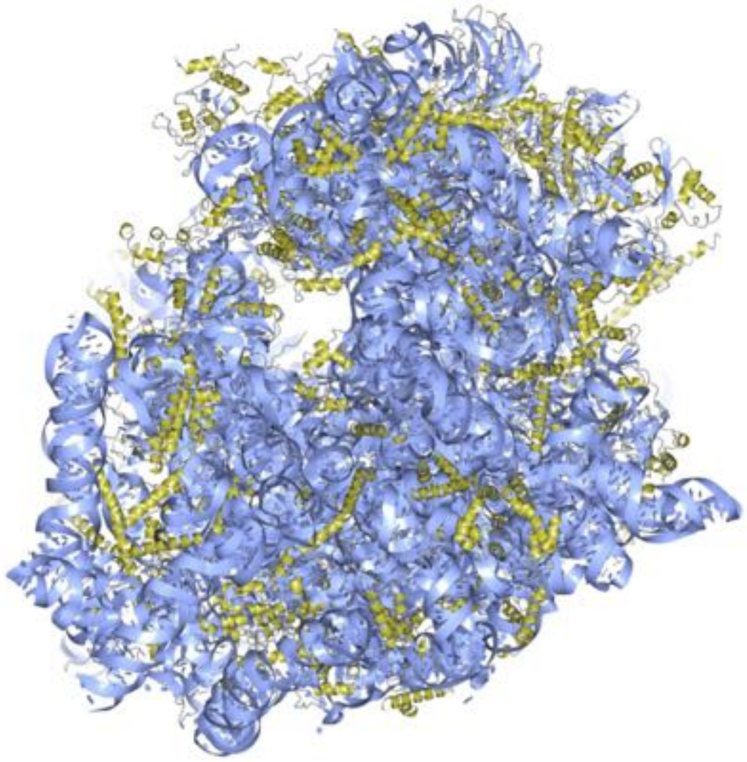
Powder diffraction station at the SLS

Powder Diffraction on Mars

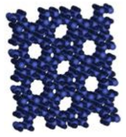


NASA

Large Molecules



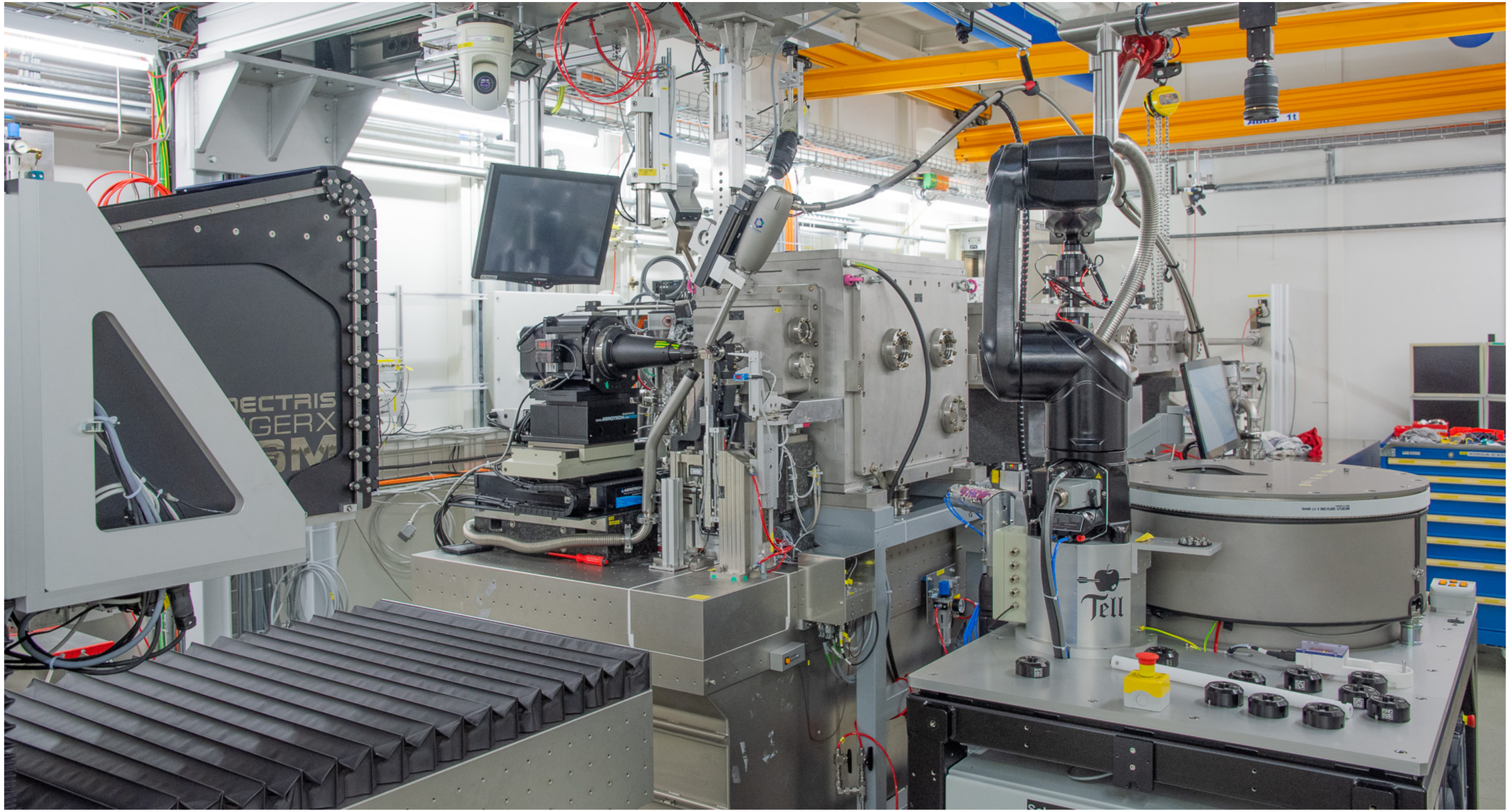
80S ribosome subunit, 1.8 MDa



ZSM-5 zeolite,
5.7 kDa

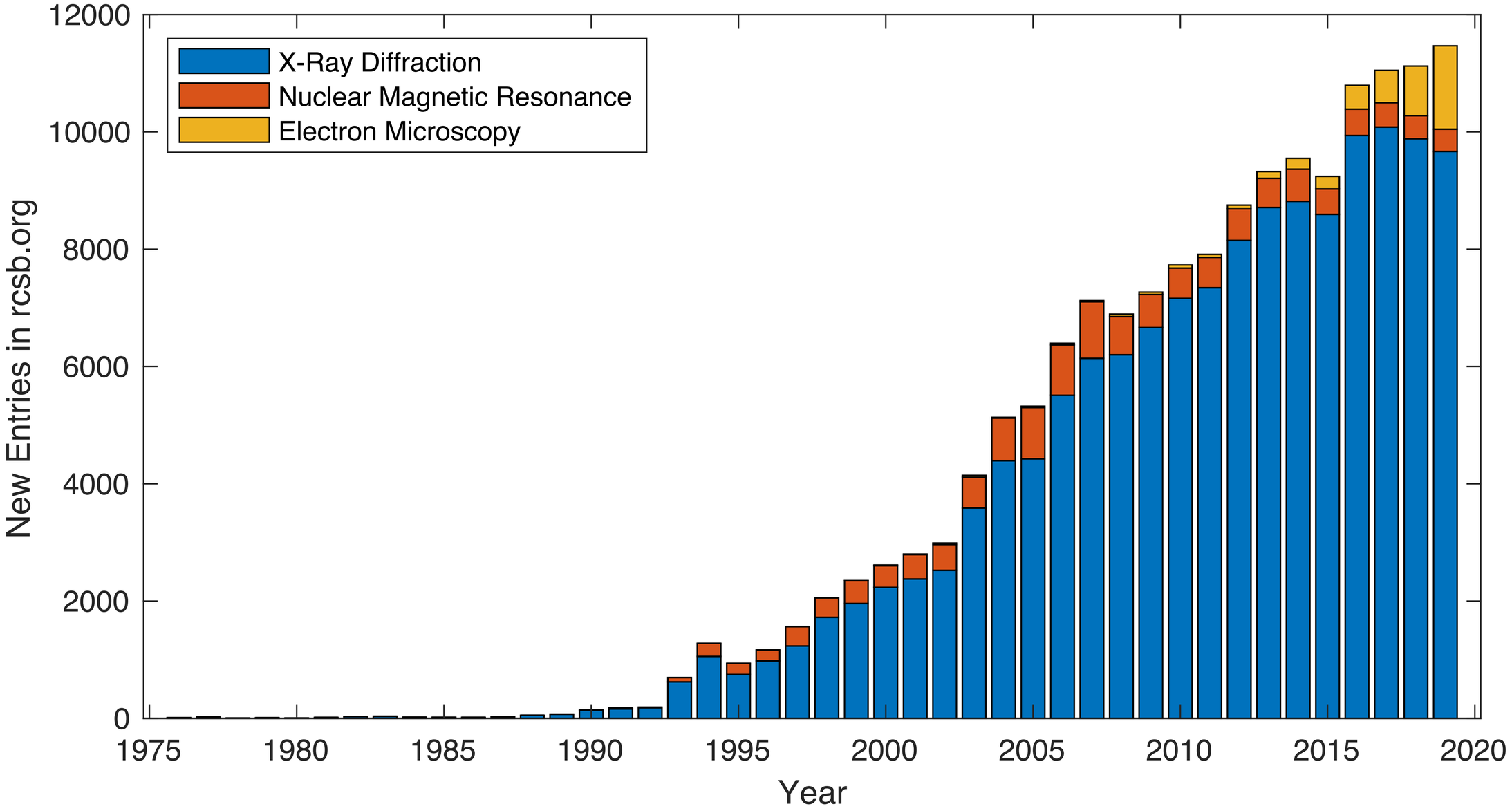
- # atoms/unit cell
  - Phase problem (see later in course)
- # unit cells/unit volume N
  - Diffraction signal $\propto N^2$
- Density of Bragg spots in reciprocal space
  - Mosaicity
  - Beam divergence
- Sample preparation
- Radiation damage

Protein Crystallography Beamline at the SLS



Frozen Samples

RCSB Protein Database



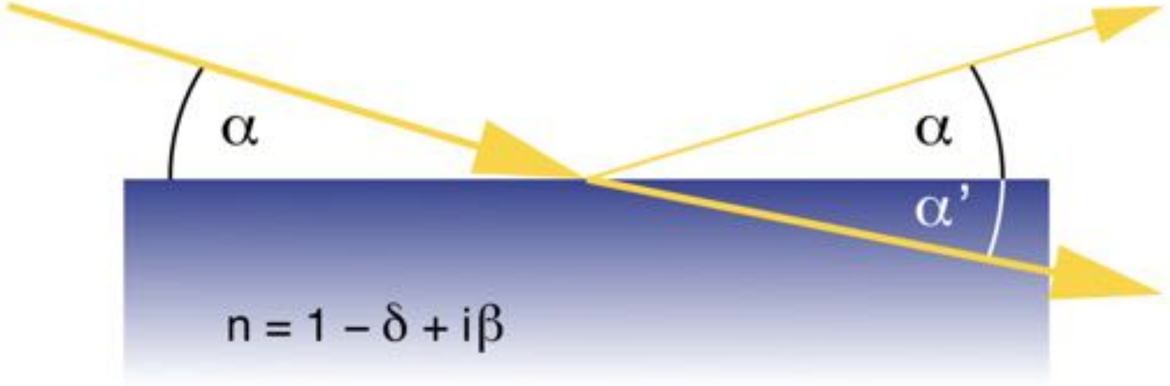
As of December 31, 2019. rcsb.org

SAXS — Small Angle X-Ray Scattering

- Measure reflectivity at grazing incidence
- Input angle = output angle

- Provides information on
  - Electron density profiles
  - Surface / interface roughness
  - Film thickness
  - Film density
  - Multilayer structures
  - Film-growth kinetics
  - …

$$r = \frac{a_r}{a_i} = \frac{\alpha - \alpha'}{\alpha + \alpha'}$$



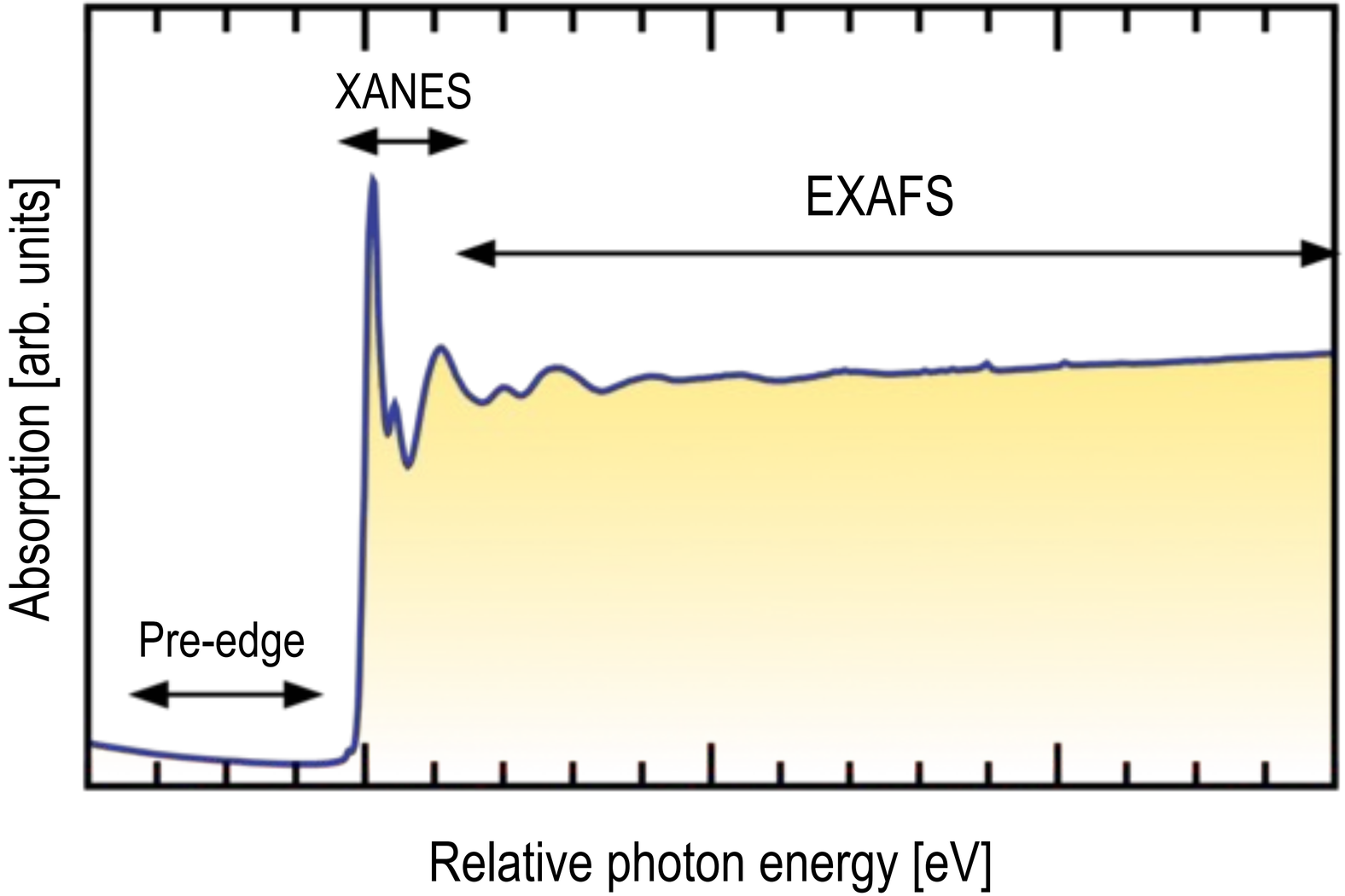
Spectroscopy

- Absorption Spectroscopy
  - XANES — X-ray absorption near edge structure
  - EXAFS — Extended X-ray absorption fine structure

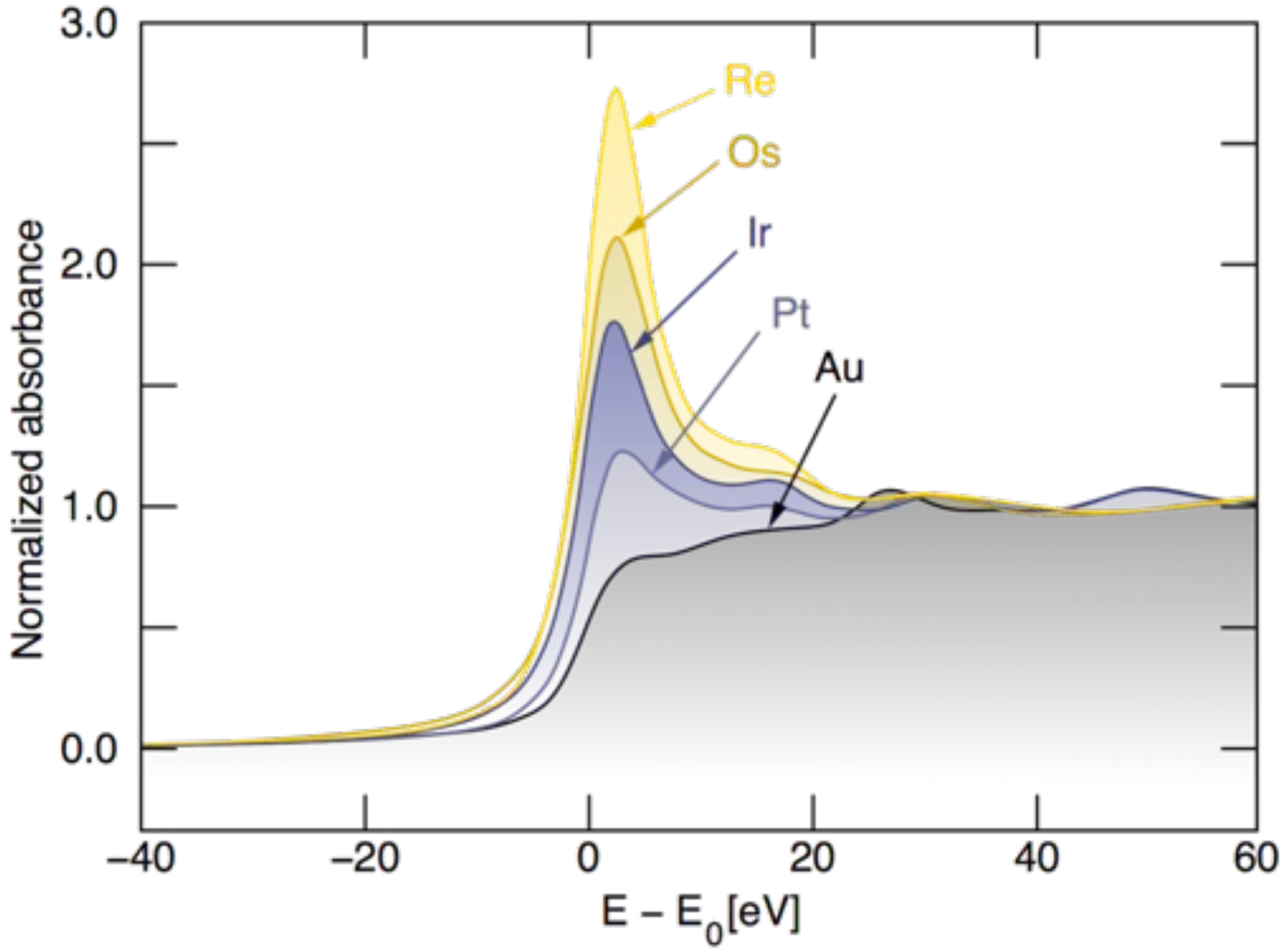
- XRF — X-Ray Fluorescence
  - Fixed $\hbar\omega_{in}$
  - RIXS — Resonant inelastic X-ray scattering: $\hbar\omega_{out}$ vs $\hbar\omega_{in}$

- Photoemission Spectroscopy
  - XPS — X-ray photoelectron spectroscopy
  - XPD — X-ray photoelectron diffraction
  - ARPES — Angle-resolved photoemission spectroscopy
  - HAXPES — Hard X-ray photoelectron spectroscopy

Absorption Spectroscopy

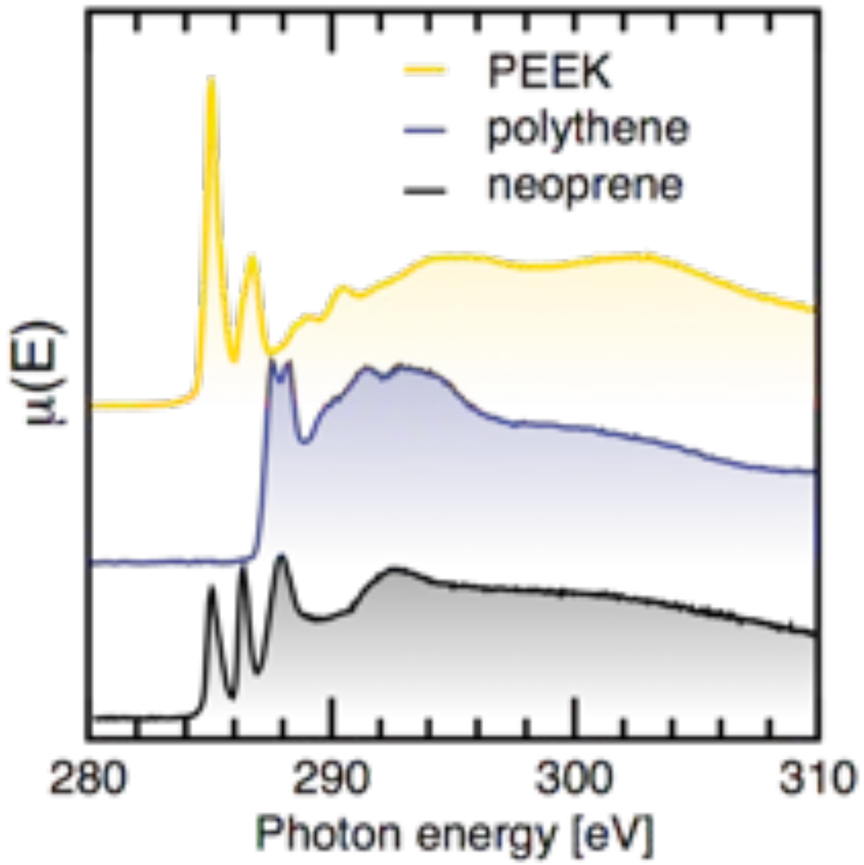


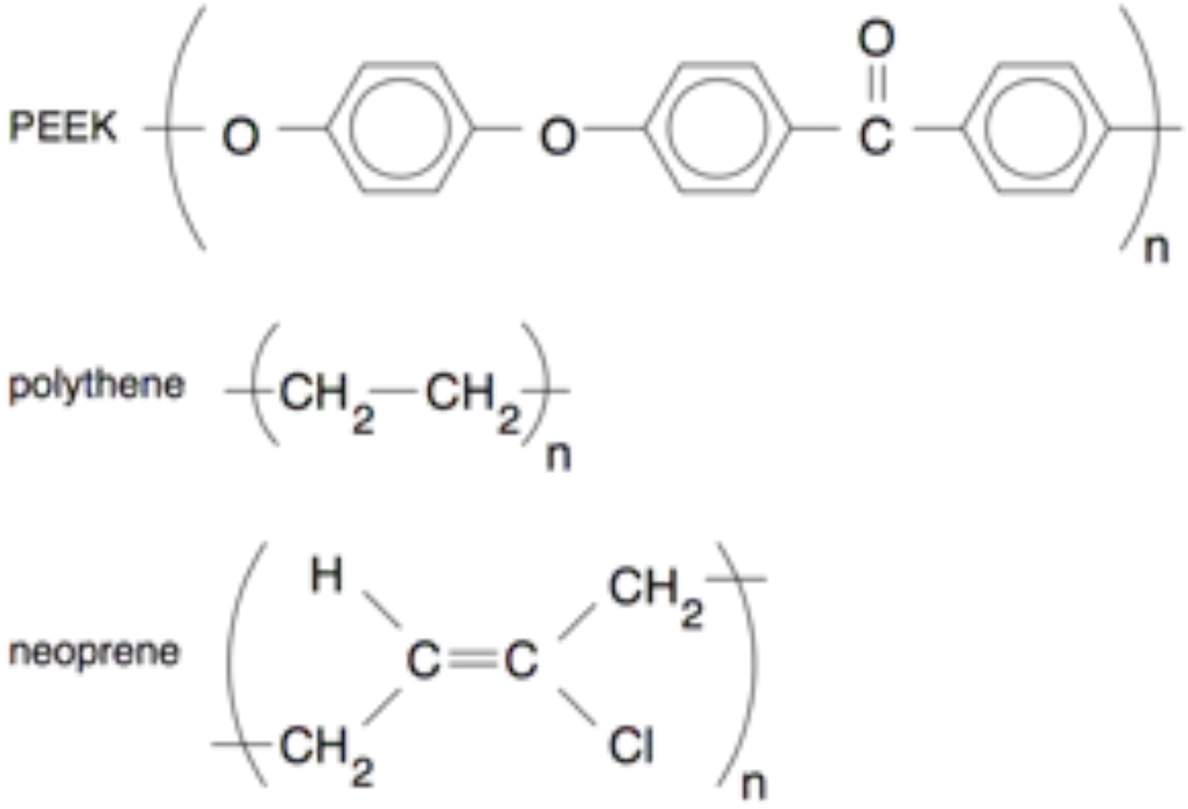
XANES — Illustrative Example



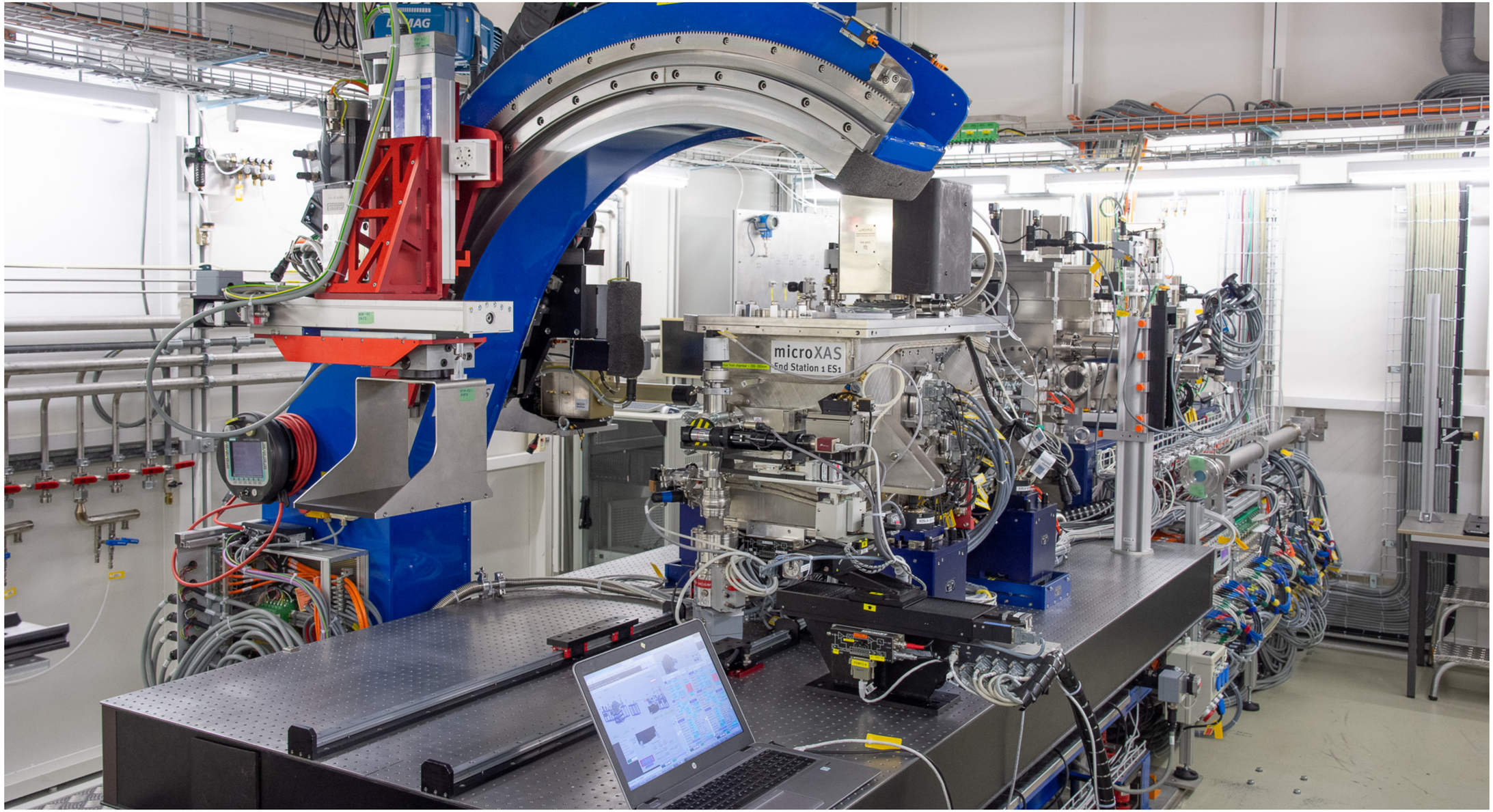
G. Meitzner et al., J. Phys. Chem. 96 4960 (1992)

Polymer Research

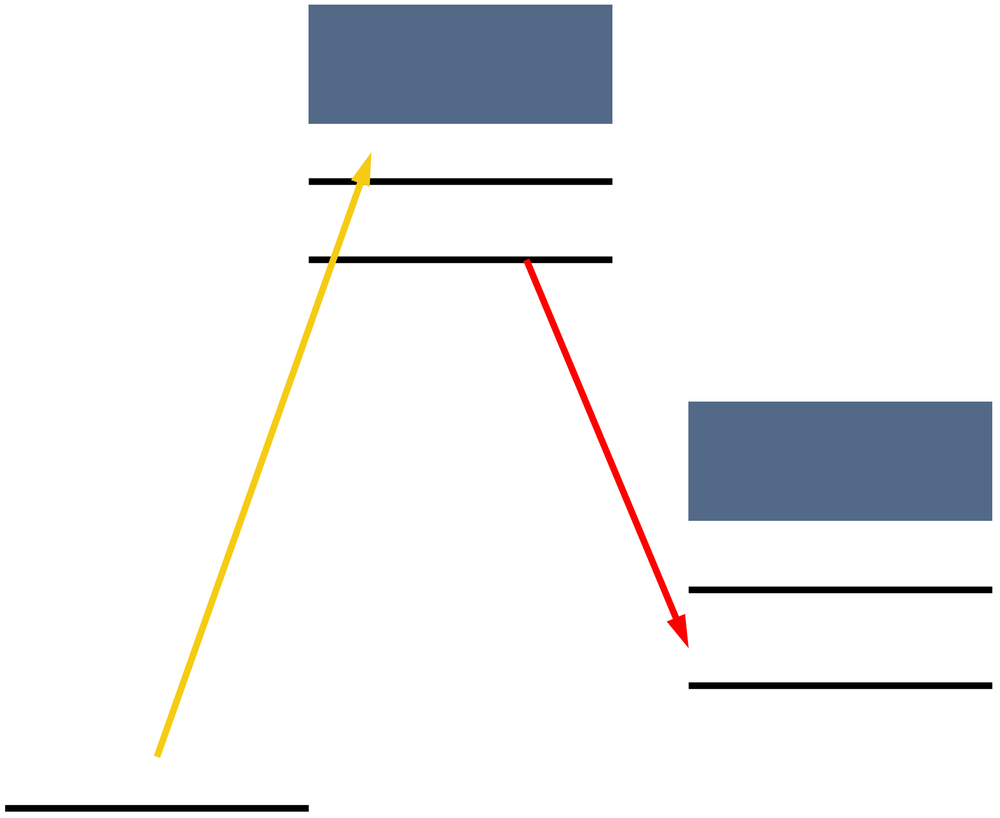


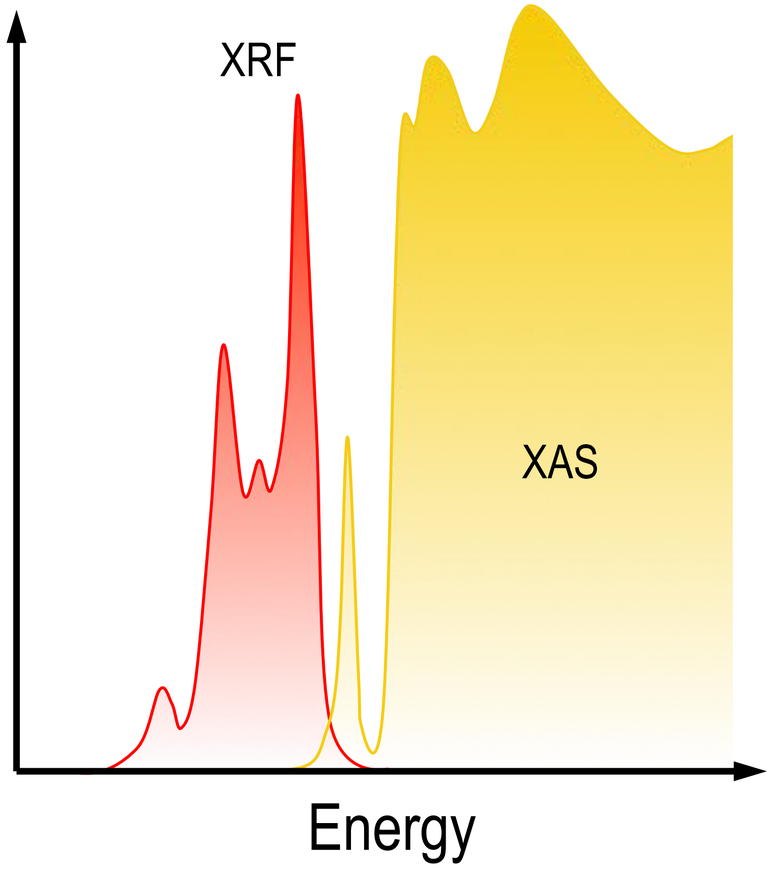


Micro-X-Ray Absorption Spectroscopy at the SLS

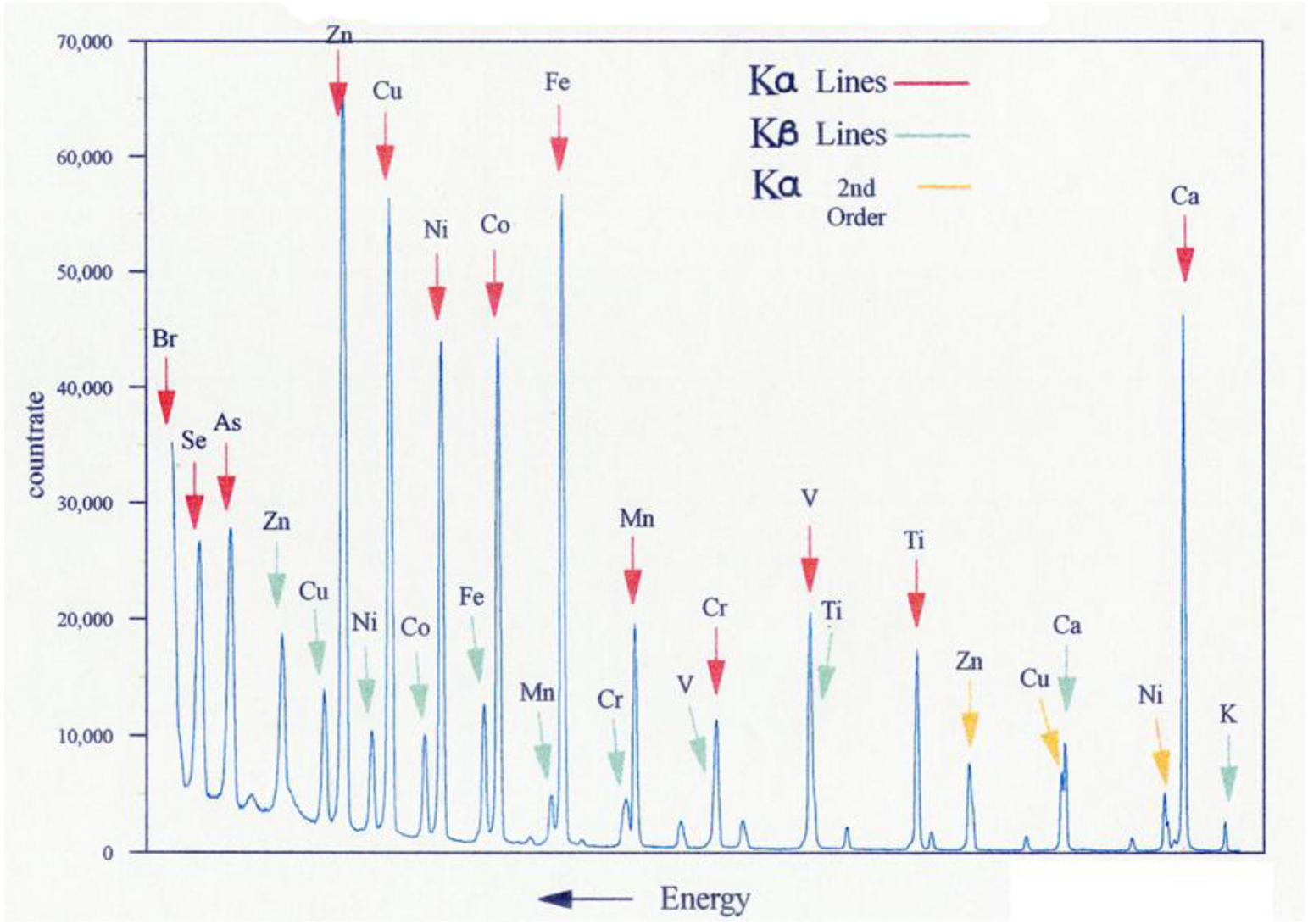


X-Ray Fluorescence



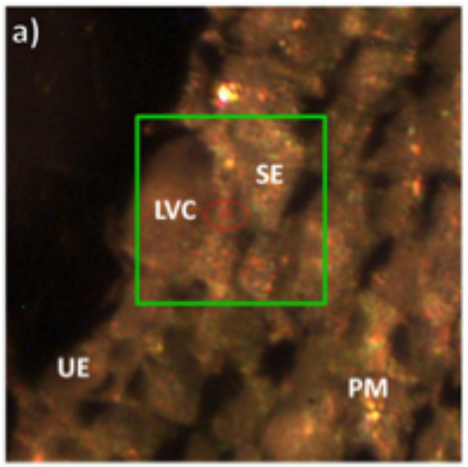


X-Ray Fluorescence Spectroscopy

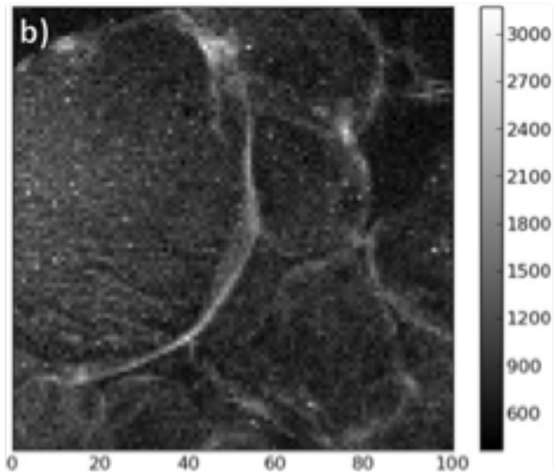


Wikimedia Commons

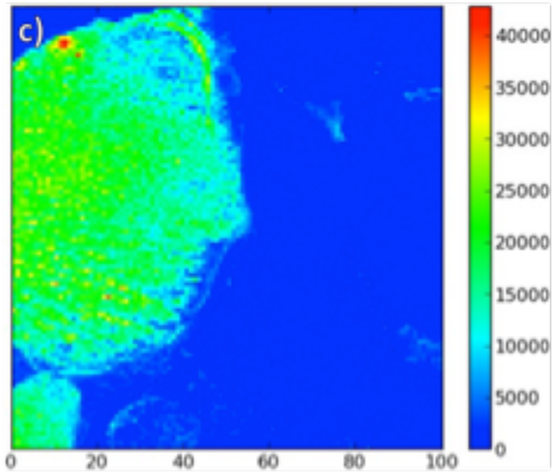
X-Ray Fluorescence of Thlaspi Praecox



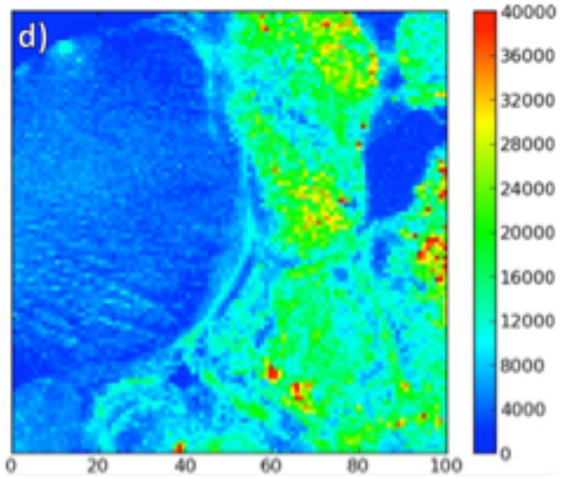
Visible Light



X-Ray Absorption



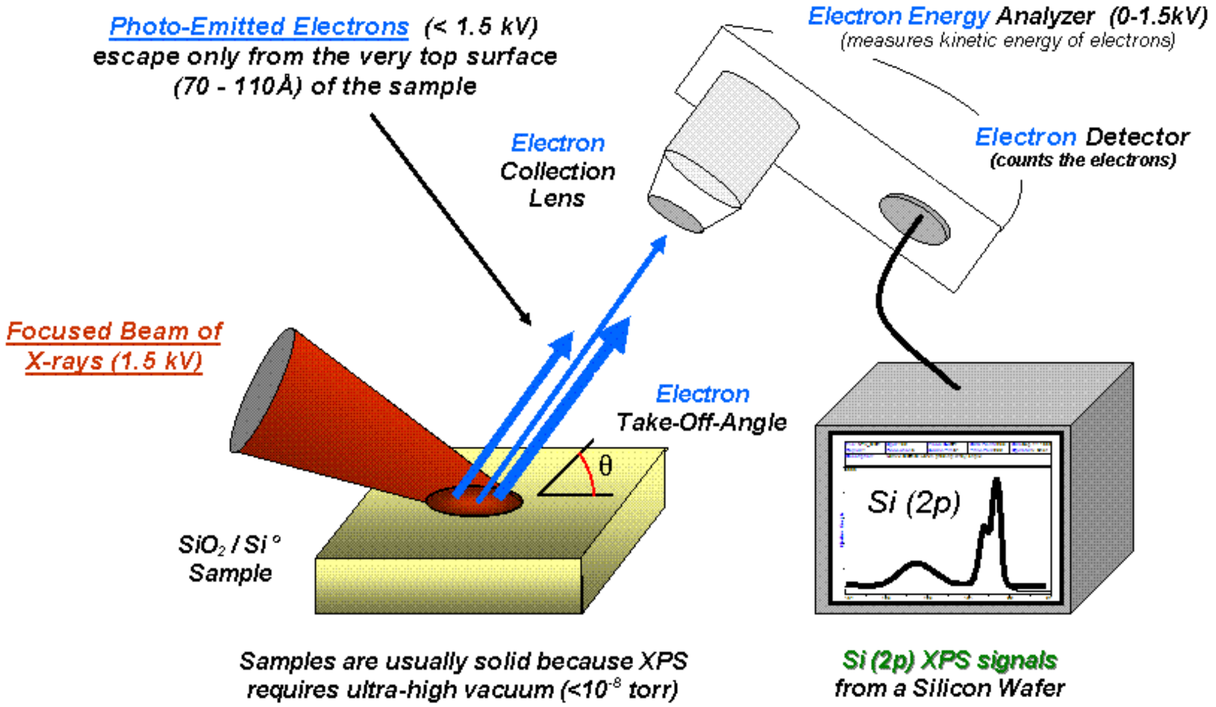
Cadmium

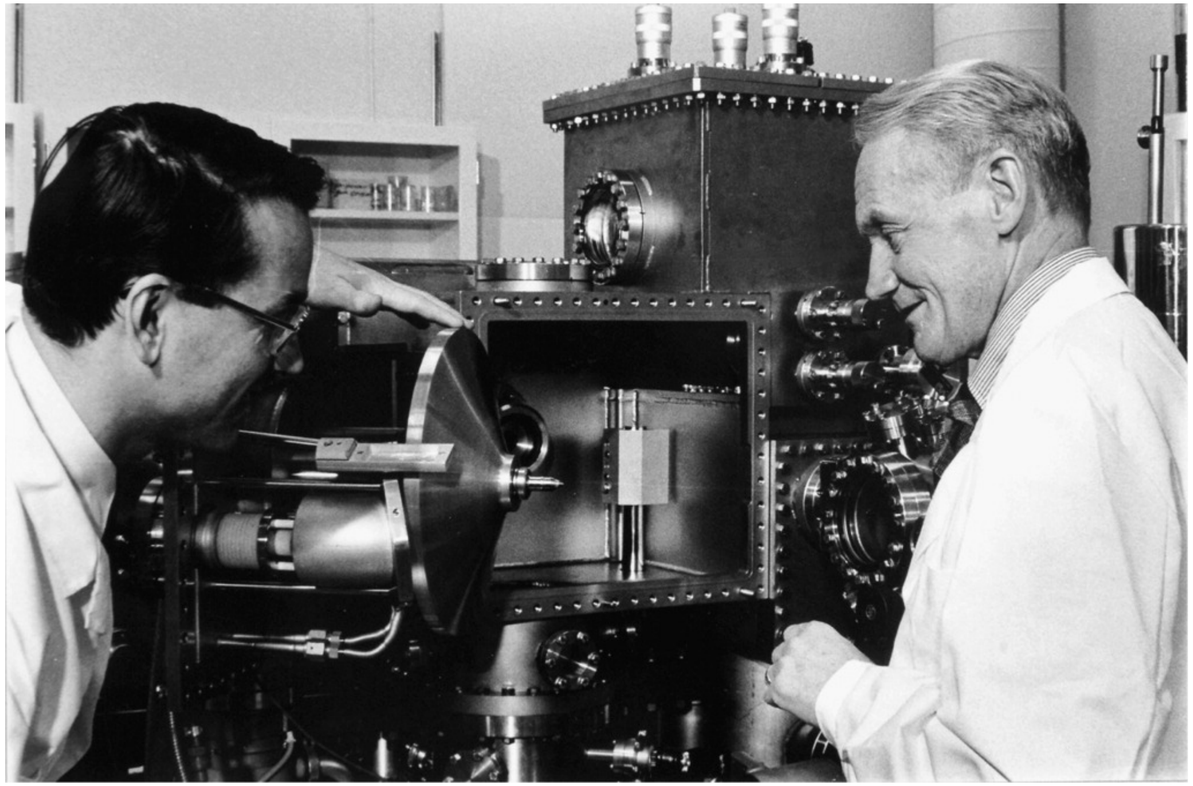


Sulphur

Wikimedia Commons (top), Koren et al., Plant and Soil 370, 1–2, 125 (2013) (bottom)

Photo-Emission of Electrons

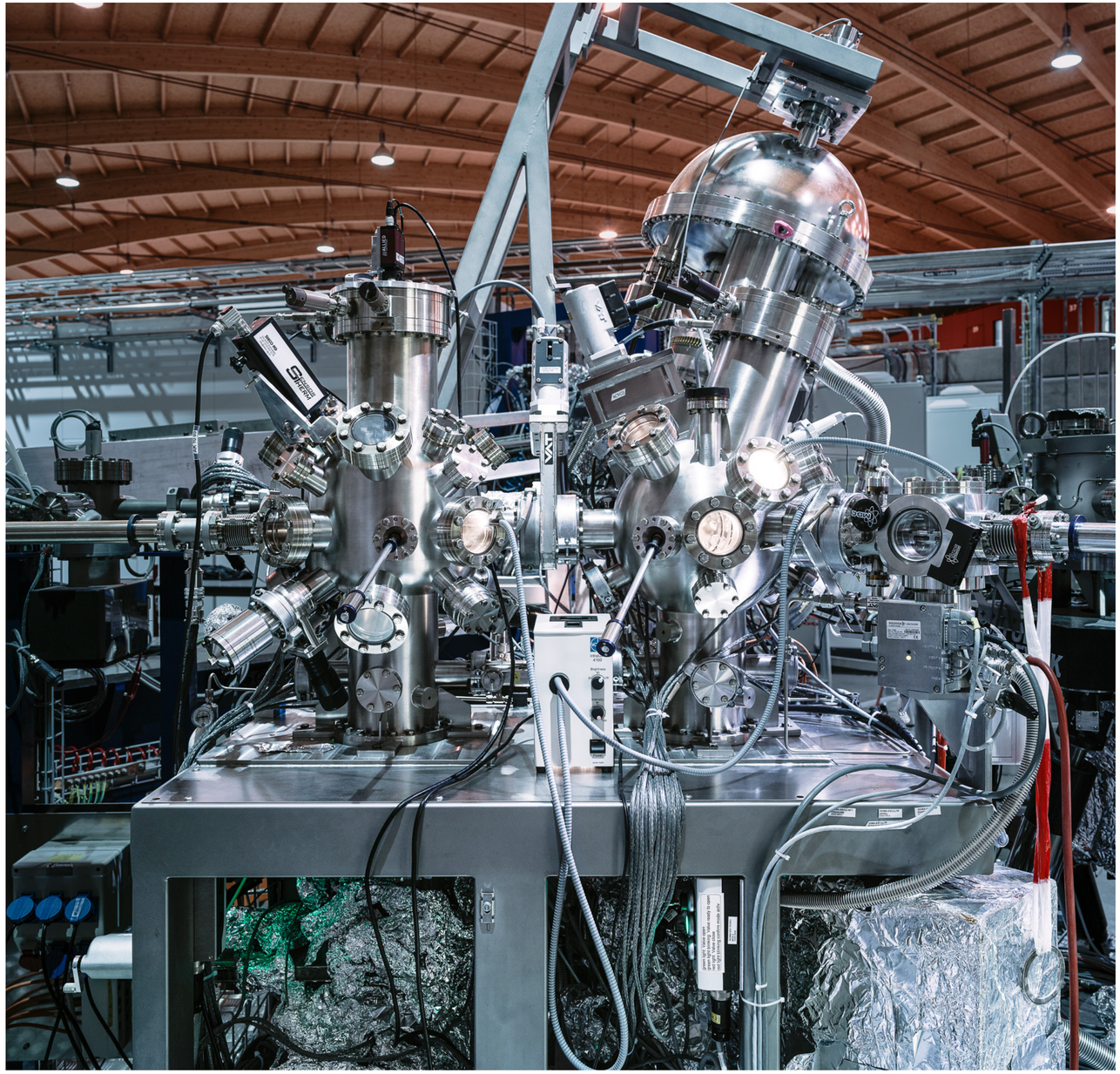




Wikimedia Commons (left), Karlsson & Siegbahn: NIM-A 601,1-2 (2009) (right)

Photoemission Spectroscopy at the SLS

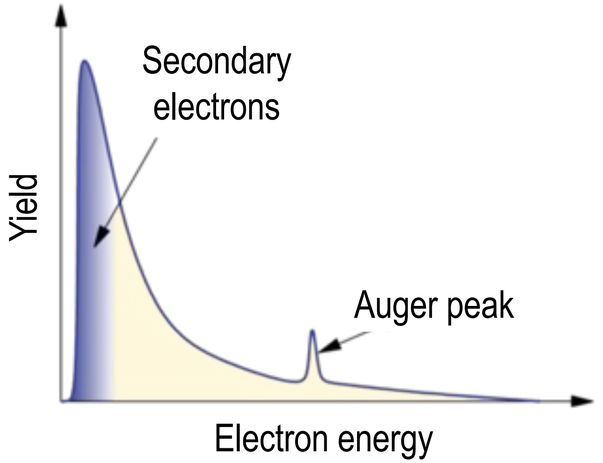
- Soft X-Ray beamline requires no hutch



PSi Bildarchiv

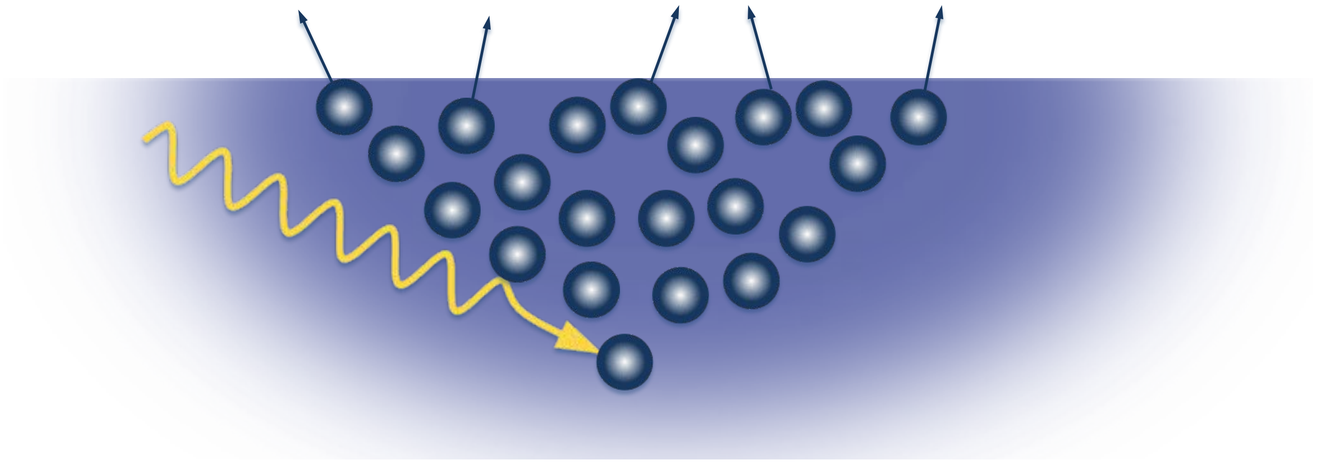
PEEM
Photoemission Electron Microscopy

- X-ray absorption
  - Products
    - Direct “photoelectrons”
    - “Secondary electrons”
  - Secondary electron yield proportional to absorption
  - Electrons are easily focussed!! (unlike x-rays)
  - Use secondary electrons to image a sample via electron microscopy



Secondary electrons

Cascade effect, many of these low energy



Questions?

Nick Veasey