APS SAC (January 2006)

Biology/Life Science Drivers for APS Upgrade –

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APS, Argonne National Laboratory, Chicago, USA

Contents

- Context of the Physical Sciences usage of APS and the APS upgrade
- Most recent overview of the biosciences at the APS was the July 2004 Workshop
- Widening the technical capabilities for the biosciences; time-resolution, high photon energies, higher flux at the sample
- Coincidental chances to upgrade the older biosciences beamlines
- Problems for sectors recently or just coming on line
- Risk analysis for the key APS parameters (those upgraded and those not)
- Overall context; LCLS/XFEL, X-ERLP, NSLS II

APS Upgrade opportunity

Thanks to the American Competitiveness Initiative

APS Strategic Planning Meeting

APS Biosciences Workshop 2004; *special focus was in the areas of*

- *Radiation Damage*
- *Biomolecules Under High Pressure*
- *Crystallography with Microfocused X-ray Beams*
- *Diffuse Scattering from Biomolecules*
- *Powder Diffraction from Proteins*
- *Dedicated protein SAXS*

Local availability of complementary facilities to develop integrated research programs, such as

- *Cryo-electron microscopy*
- *Associated biochemistry labs*
- *In-line optical spectroscopies in experiment stations*
- *Resident detector development expertise*
- *Resident physicists with long term interest in molecular dynamics theory to perform radiation damage studies, diffuse scattering and small-angle scattering modeling, etc.*

The biocrystallography future

- Professor Janet Smith (in GMCA CAT CDR Nov 2001)

"***The frontier of structural biology is in smaller, poorer crystals of larger macromolecules and complexes***."

JRH: Is the technical need to include:-

- Micron and sub-micron sized beams scanning over tiny crystals to extract ***suitable*** single crystal diffraction data?
- Ie which would benefit directly from the APS upgrade.

APS Director (JMG) quote from APS Users' Meeting May 2006

- We have the unique opportunity to bring APS to world-leading level in the next decade (proposal has been solicited by DOE-BES, due late 2006)
  - Reduce lattice emittance to ~1 nm with ID beamports unchanged
  - Most straight sections longer (8m), special undulators, utilizing unique properties of APS to tailor x-ray beams
  - "Crab" cavities for ps pulses and controlled coherence
  - Optimized and upgraded beamlines

JMG continues…

Revolutionary science from upgraded APS

- Chemical excited states give insight into photosynthesis for efficient and cheaper solar energy
- Ultrafast dynamics of magnetic and ferroelectric domains for information storage and computing
- Detecting sub zeptogram (10^{-21}g) quantities of metals in cells and soils – health and environment
- In-situ study of nucleation in liquids – leading to better controlled chemical synthesis and catalysis
- Materials under extreme magnetic fields – routes to quantum computing
- …

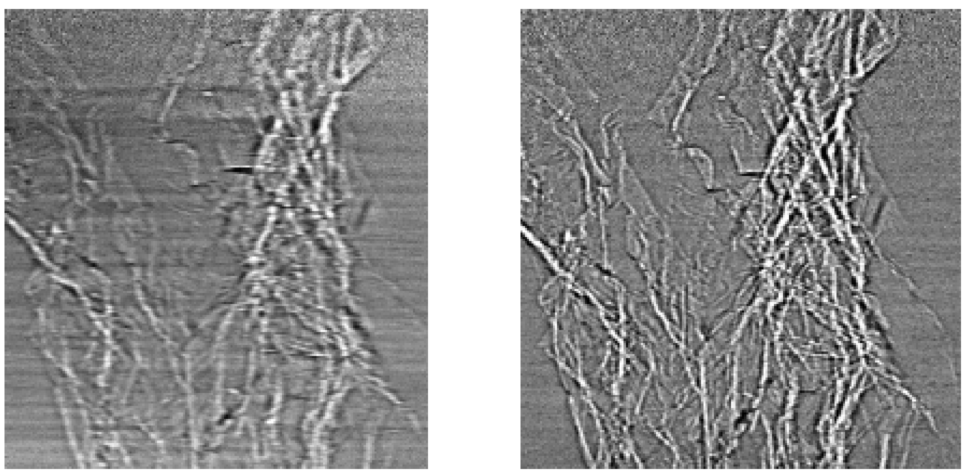
Imaging at APS Sector 32

Making a smaller x-ray source at Sector 32

APS has unique flexibility to control beta functions by sector

Normal beta $FWHM_x$ = 560 μm   Reduced beta $FWHM_x$ = 280 μm

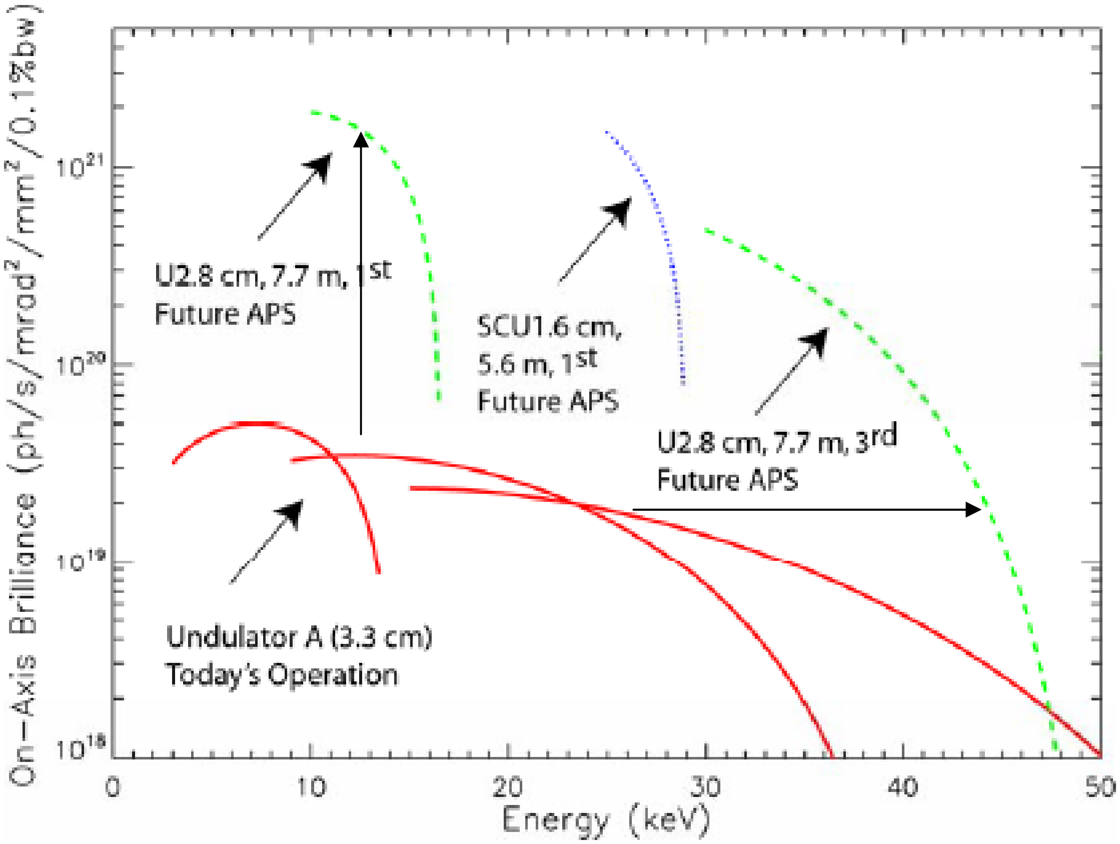
200 μm



Aluminum stress crack sample, ~3mm thick

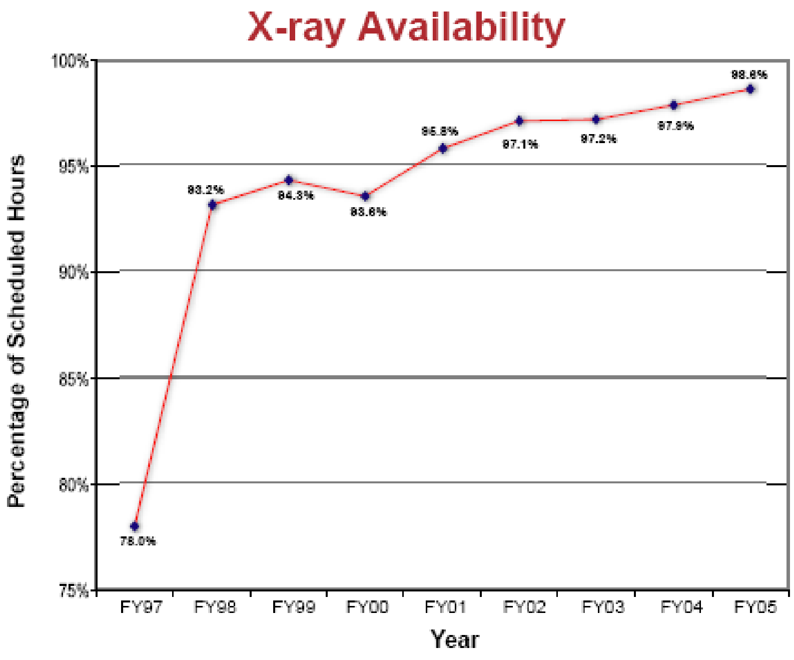
Surely strong implications for SR imaging in biology too……

APS upgrade parameters ‘catching JRH’s eye’

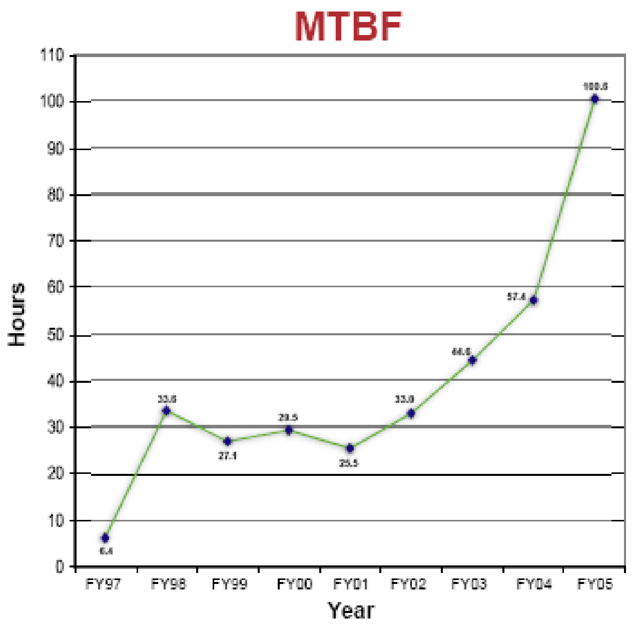


But we must note:- APS running superbly

Excellent record of improved APS reliability and availability

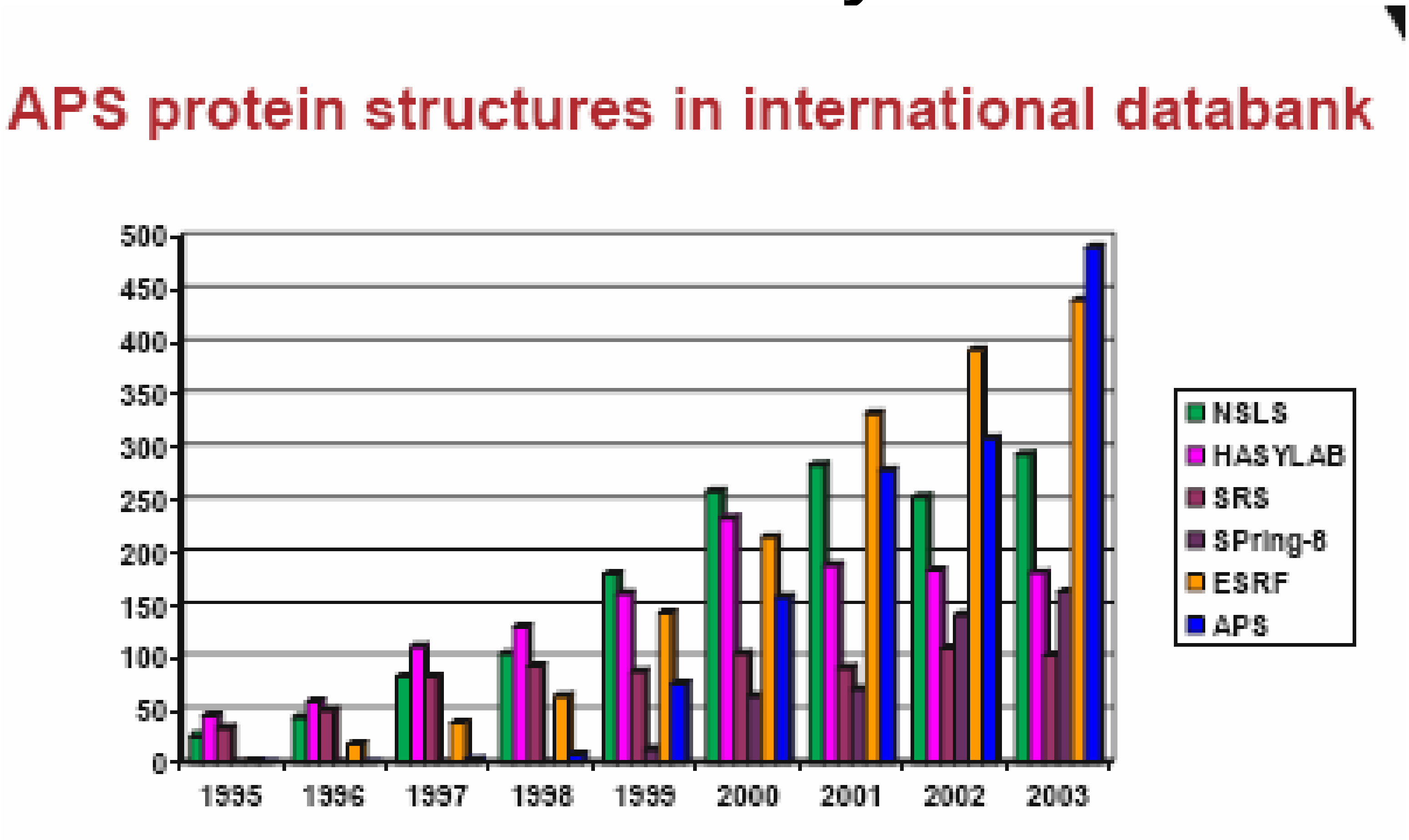


FY05 is best yearly operation for any third-generation hard x-ray source in the history of these facilities.*



*Based on data available from ESRF and SPring-8

As a measure the protein crystal structure analyses PDB depositions APS already leads the world currently



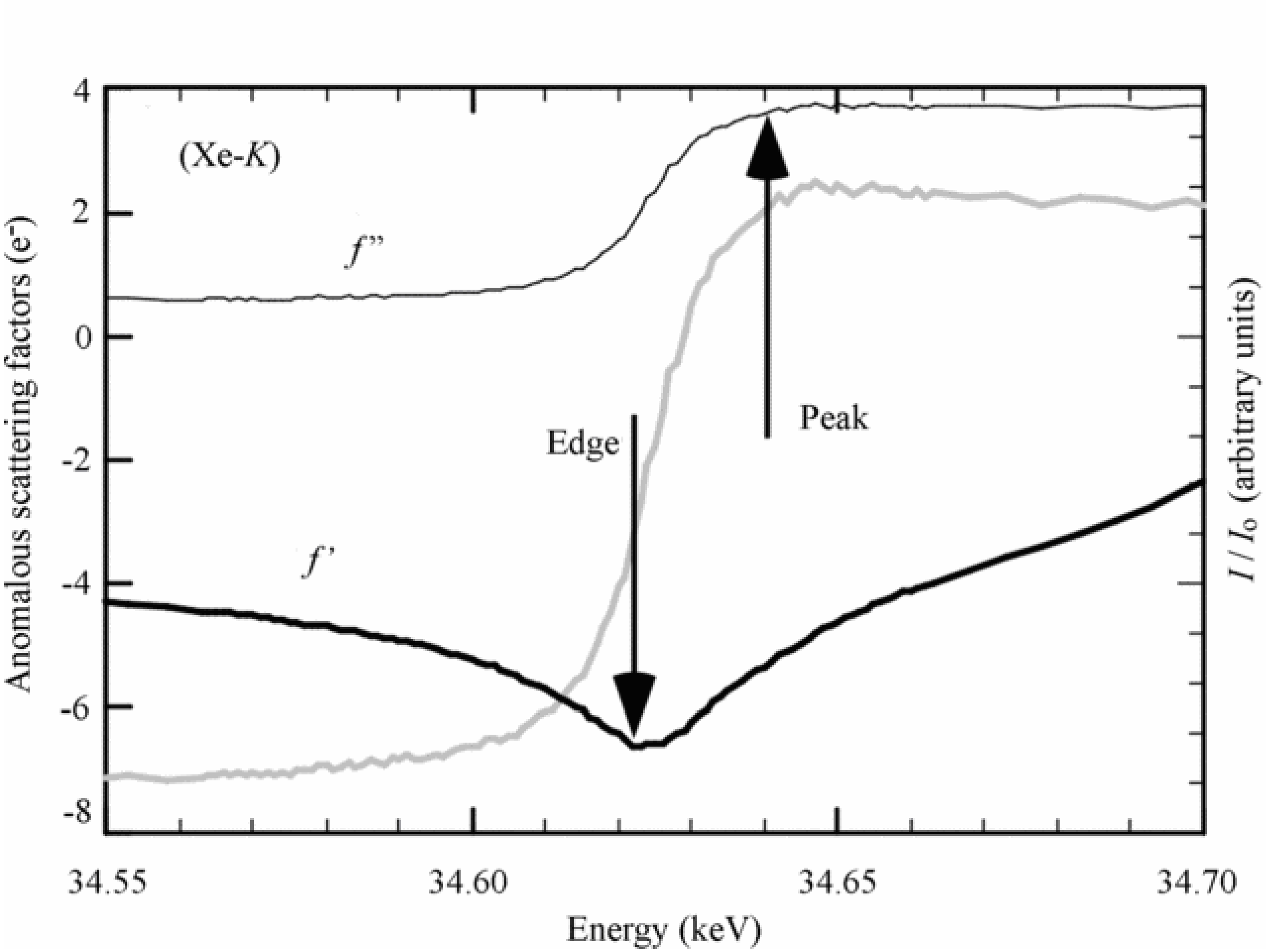
And APS has yet further PDB depositing CATS coming on line to further emphasise its global lead

- NE CAT
- GMCA CAT
- LS CAT
- The timing of the APS upgrade then has “non-ideal” aspects

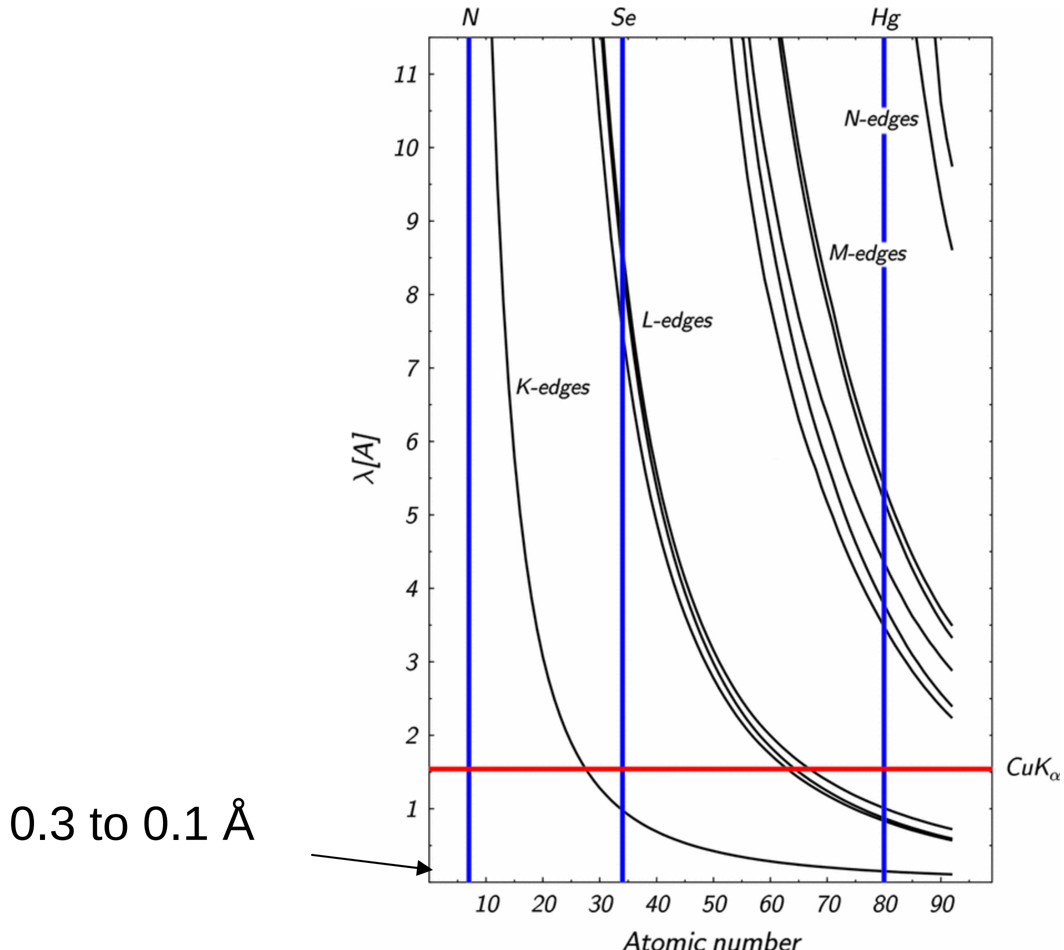
Perhaps the timing of the APS upgrade has ideal aspects

- SBC upgrade to make 19 ID-1, 19ID-2,19ID-3; SBC is the leading PDB depositing beamline in the world and the fastest accumulator of high impact Journal front covers; it needs this year to effect its own renewal/upgrade
- APS could wrestle a lead from ESRF re time-resolved research by going to a few psec time-resolution
- APS could champion high photon energy MAD R&D eg iodine/xenon Kedges, Pt, Au, Hg K edges……radiation damage behaviour of protein samples at high energy (benefits?)

K. Takeda, H. Miyatake, S.-Y. Park, M. Kawamoto, N. Kamiya and K. Miki J. Appl. Cryst. (2004). 37, 925-933:-



K, *L*, *M* and *N*-absorption edges of the first 92 elements



For reference the vertical lines at atomic numbers 7 (for nitrogen), 34 (for selenium) and 80 (mercury) are also given, as is the Cu *K* wavelength of 1.5418 Å as a horizontal line.

Case study: Anomalous Diffraction at Ultra High Energy for Protein Crystallography

- **Jean Jakoncic,[ab] Marco Di Michiel,[c] Zhong Zhong,[a] Veijo Honkimaki,[c] Yves Jouanneau,[d] and Vivian Stojanoffa***

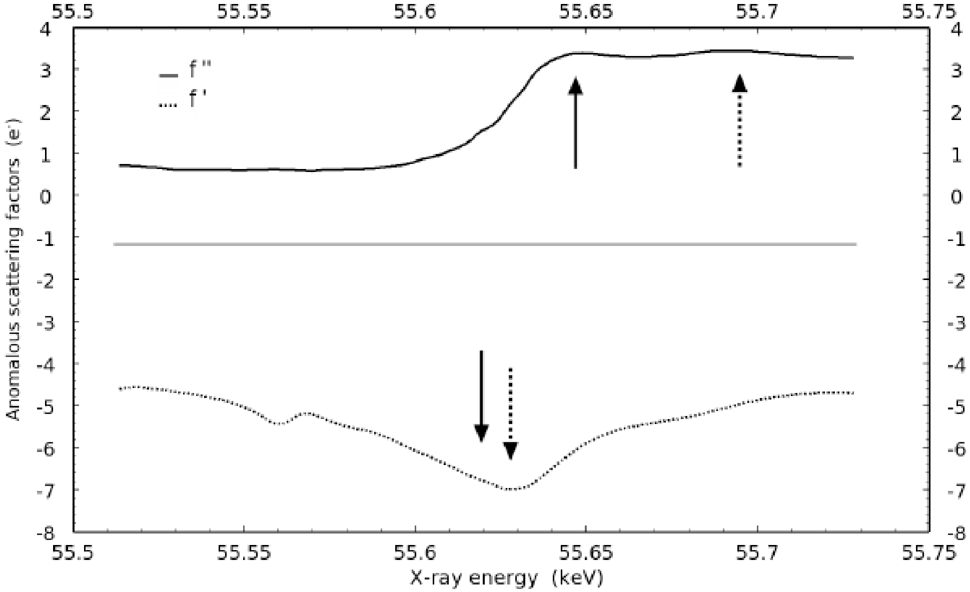
- *[a]Brookhaven National Laboratory, National Synchrotron Light Source, Upton, NY, USA, [b]Universite Joseph Fourrier, Grenoble, France, [c]European Synchrotron Radiation Facility, Grenoble, France and [d]CNRS CEA, Grenoble, France.*

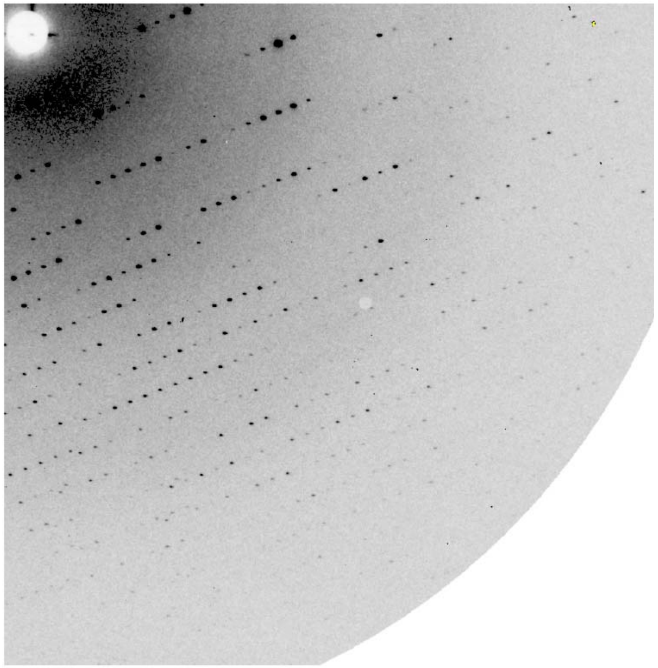
- *Submitted to Acta Cryst D*

Singlewavelength Anomalous Diffraction (SAD), Multiwavelength Anomalous Diffraction (MAD) and Single Isomorphous Replacement with Anomalous Scattering (SIRAS) phasing at ultra high X-ray energy, 55 keV, using Holmium at the K-edge for lysozyme sufficient to obtain a remarkable electron density and build the first lanthanide structure for HEWL in its entirety.

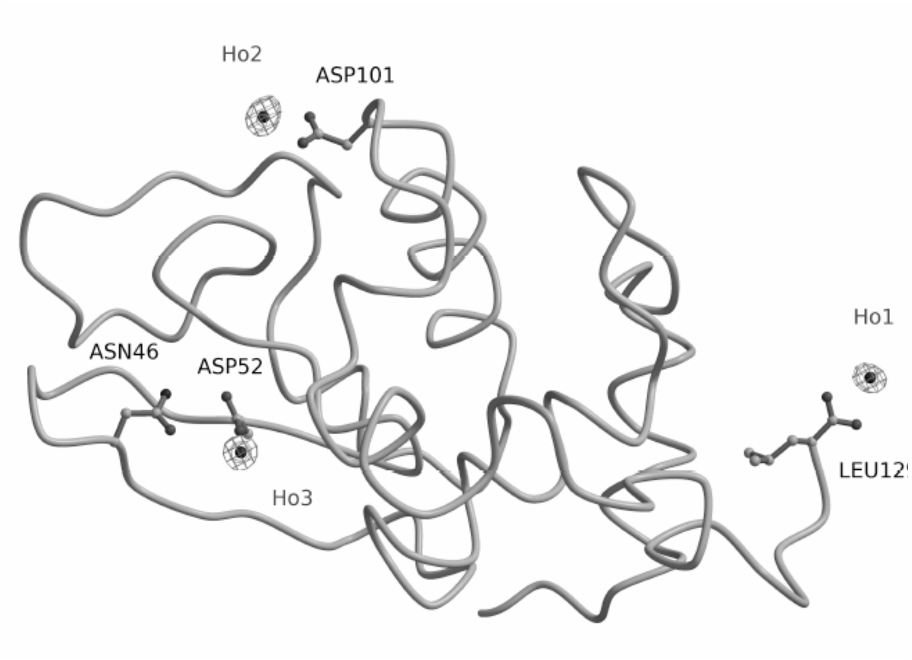
ID15B, at the European Synchrotron Radiation Facility in Grenoble, France (ESRF) and X17B1 at the National Synchrotron Light Source, Upton, NY, USA. Both beamlines deliver either monochromatic beam or white beam in the high energy range, typically higher than 50 keV.

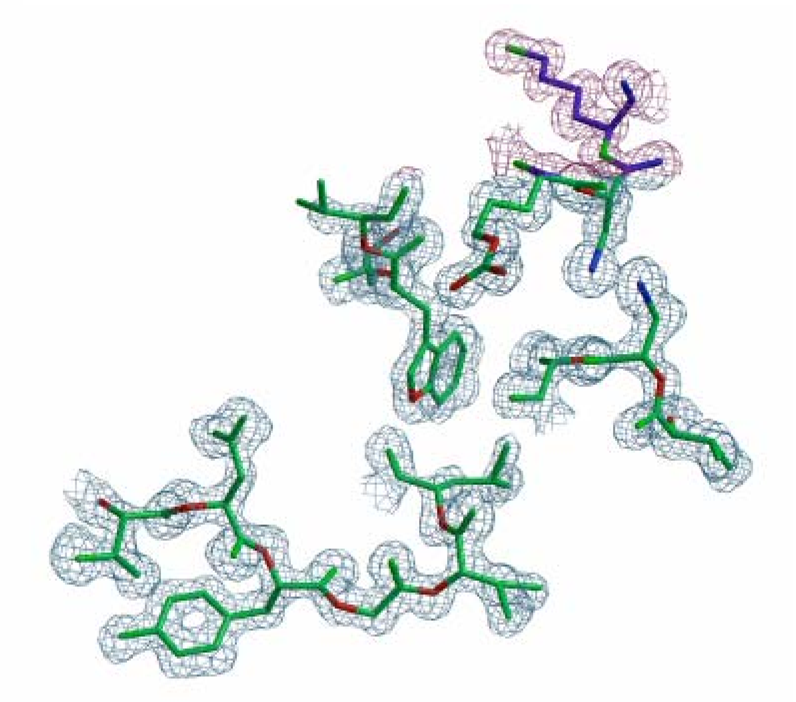
Actual energies used for data collection are indicated by the plain arrows; 55.62 (0.2229 Å), 55.68 (0.2227 Å) and not shown the remote energy, 56.34 (0.22 Å) keV.





Holmium sites anomalous difference density and resulting MAD protein map





Re-reading my 1992 book final chapter Future developments

- The preceding slides included much on microcrystallography, high photon energies, radiation damage. However…
- I mentioned in 1992 that (much of) the R&D work to harness nuclear anomalous dispersion effects, with huge f “ eg ~500e-, had been done. Could this come to reality after upgrade.
- Also biological uses of magnetic scattering eg with iron proteins; a low scattering efficiency effect that again would benefit from big increases in intensity at the sample…..?

Perhaps the timing of the APS upgrade has ideal aspects contd

- Microfocus to nanofocus beams…ESRF upgrade is coming…coherence imaging opportunities….10x10x10 or 100x100x100 unit cells…….competition with X-ERLP(?)....precursor to atomic resolution single particle structural analyses at LCLS/XFEL

APS Upgrade Risk Analysis; key risks

- Beam stability affected?
- Delays to coming back on line?
- Delay in recouping PDB depositions world lead?
- Loss of key staff from eg APS PX sectors?
- Loss of key users to APS competing SR Facilities (and their publications from work done there)?

APS and CAT Risk Management strategies; some ideas

- Risk 1; defocus the beam at the sample position
- Risk 2; delays; unthinkable!
- Risk 3; The PDB lead will be lost for a period; that is inevitable BUT in JRH experience a shutdown offers chance to write up work that is maybe not the ‘definite Nature front cover’ but in that category and ‘worth a shot’. Thus publication in the shutdown period should be a focussed effort by all CATS to keep APS in the researcher and public eye.
- Risk 4; staff sabbaticals at cognate SR sources and beamlines (eg ESRF, SPRing 8)
- Risk 5; Manage the access of key users at ‘competing SR facilities’

Overall remarks; Upgrades are often controversial

- eg SRS high brightness lattice 1985 (a mere 4 years after I brought SRS 7.2 online and a mere 1 year after bringing SRS 9.6 online); but we were major beneficiaries of that upgrade
- Eg planning ESRF in 1985 or so onwards a mere 4 years after bringing on line the SRS the world’s first dedicated SR X-ray source. The ESRF has been an astounding success for European science. As UK SR researchers we are proud to have taken part.
- At APS controversy is from the APS PX sectors who are very happy with APS current performance and reliability!

Overall, the circumstances here at APS for the upgrade have the major beneficiaries of the APS upgrade being:-

- time-resolved inc biosciences (eg psec studies, Ultra-fastSAX);
- microfocus
- high photon energies (MAD);
- Imaging;
- radiation damage amelioration?
- Detecting sub-zeptogram quantities of metals in cells and soils-important for health and environment studies.

Thankyou!