diamond

A Century of X-rays
and still
a Brilliant Future

accelerator requirements for the next 50 years

Gerd Materlik
Diamond Light Source Ltd.

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Thanks for some ppt's to

- Janos Kirz
- Joe Stoehr
- Richard Walker
- Ian Robinson

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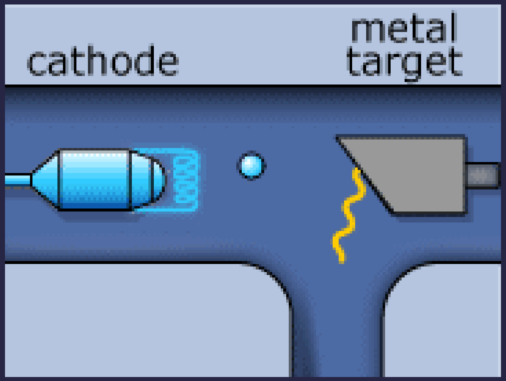
C. W. Röntgen

November 8, 1895, Röntgen discovered X-rays

– The birth of X-ray Science



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Scientific American, January 25, 1896

Vol. LXXIV, No. 4, p.51.

particular line in which they had studied; and, secondly, that the electrical graduate is paid from 20 to 23 per cent less than the mechanical or the civil graduate.

Professor Routgen's Wonderful Discovery.

There have been received from Europe by cable very insufficient accounts of a discovery attributed to Professor Routgen, of Wurzburg University. By the use of a radiant state of matter tube, a Crookes tube, it is stated that he has succeeded in obtaining photographic effects through opaque objects. It has long been known that ether waves of long period would pass through matter opaque to short waves, and that such a screen as is afforded by a plate of blackened rock salt will sift out short waves, while long waves pass through it. In some unexplained way Professor Routgen, it is claimed, has succeeded in affecting the sensitive plate with waves which had passed through an opaque body. Metals cutting off all rays alike would produce a shadow, so that a metallic object in a box or embedded in the human system could be made to give some kind of an image. The operations are said to have been conducted without a lens, entirely by shadow.

This is about the substance of the reports. It is yet too soon to indulge in the wild possibilities that have been suggested for the process. When the details reach us, the process will probably prove to be of scientific rather tha f practical interest.

A New Horseless Carriage Race in France.

The Automobile Club, of Paris, have arranged a race which is to take place in June, the course being from Paris to Marseilles and return. One of the conditions laid down for the race is that the contestants are to proceed only in the daytime. The carriages are to be

supply ten millio
the ocean at a poi
almost directly
would run some
pumping station
settling tank, fro
to a near-by reser
pumping would t
thence by gravity
a storage reserve
level, and water
have sufficient pr
high buildings. B
as Plymouth, Yar
enhead, and othe
flushing, and the
of sea water, clai
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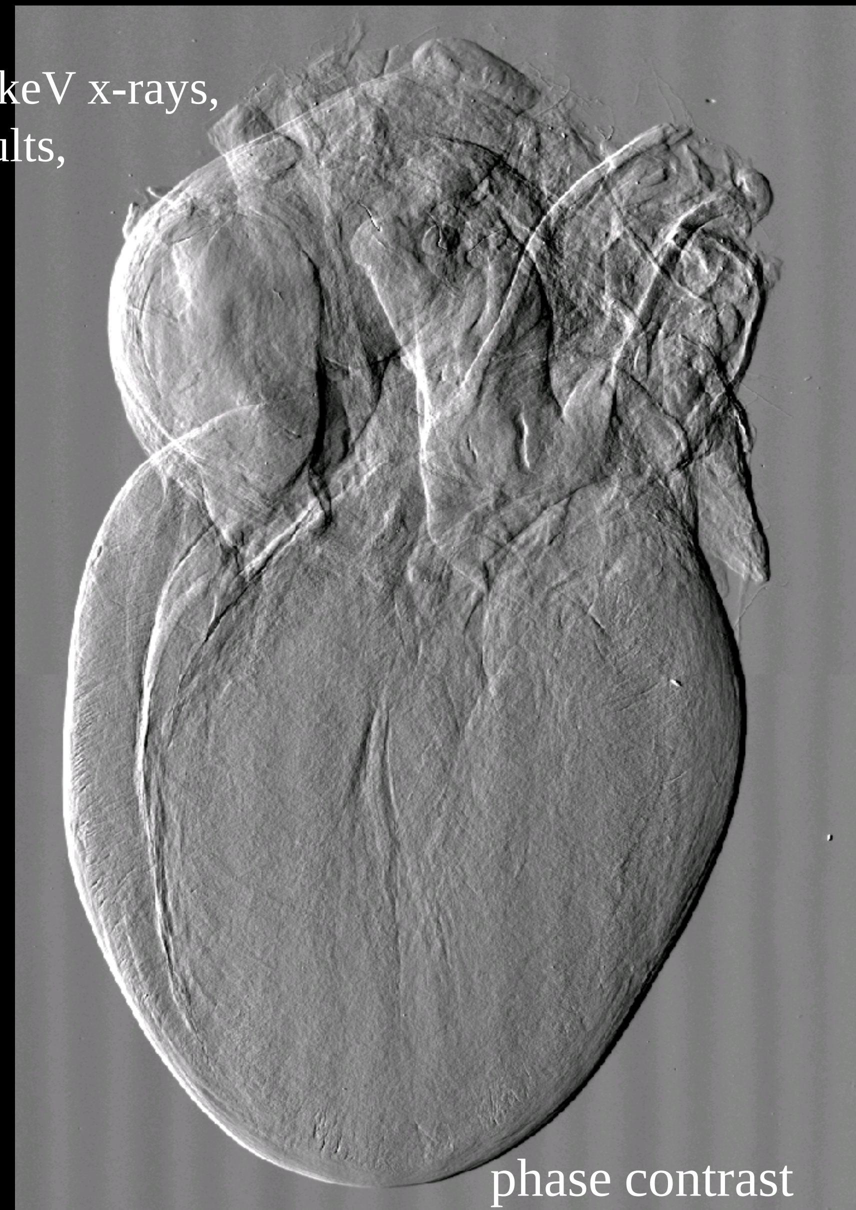
urged by some of
Health, in partic
detrimental to t
and promote the
However, are not
bathing lakes an
a sea water bath
tem would affor
of. For such use
the new compa
find ample use.
day is not much
five millions of

Today with Sy. Light we even get phase contrast images

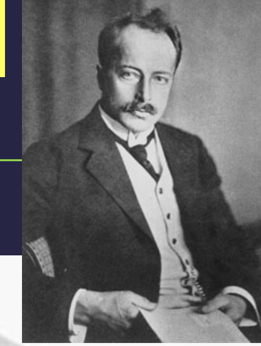
F. Pfeifer et al. ,
July 2005, 17.5 keV x-rays,
synchrotron results,
ID 19/ ESRF

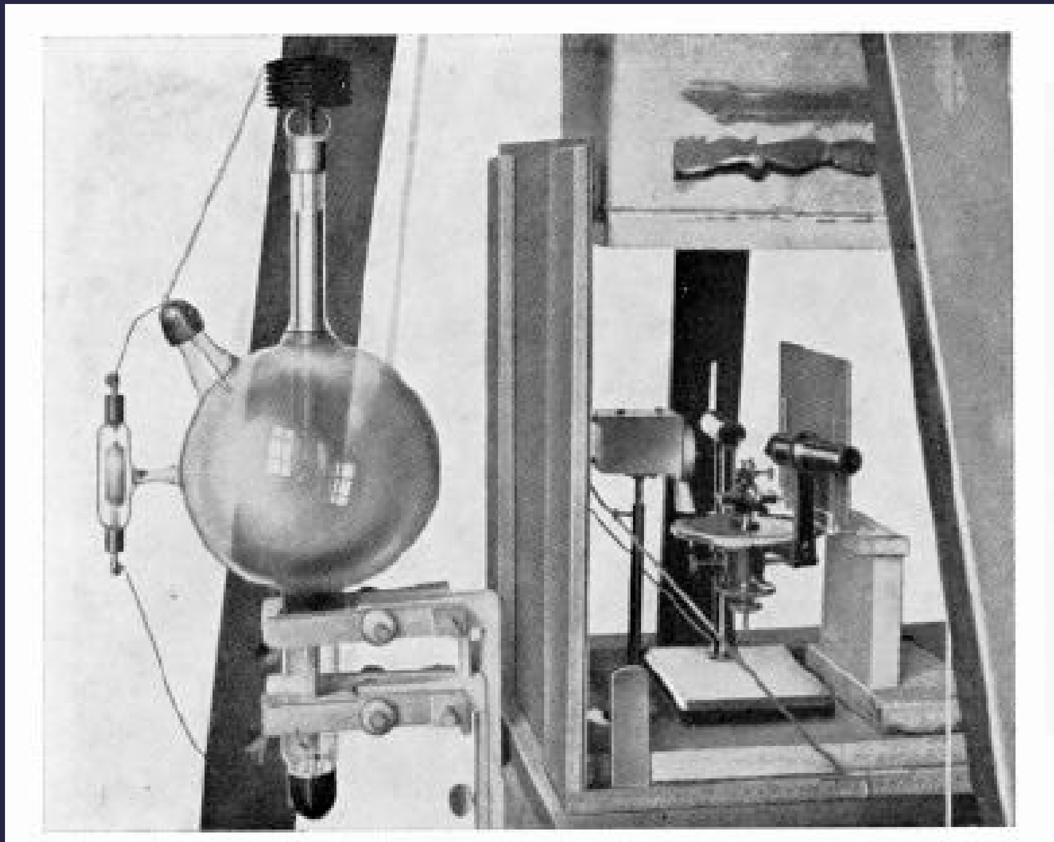


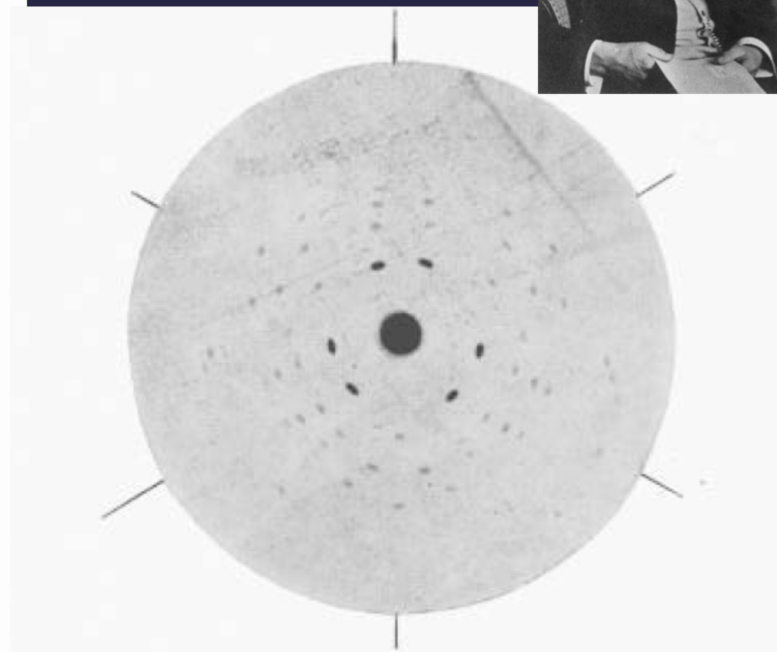
Centennial of X-ray diffraction

in 1912 – Friedrich, Knipping, Laue

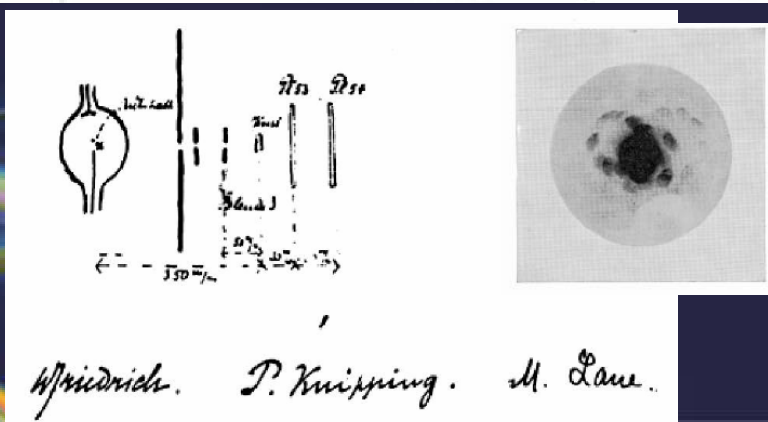
Max von Laue

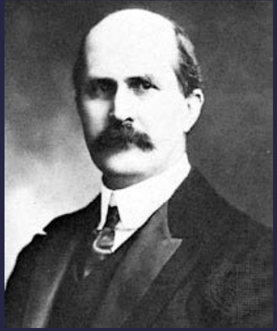






ZnS – diffraction pattern

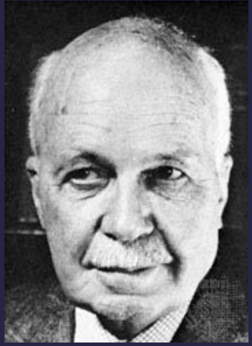




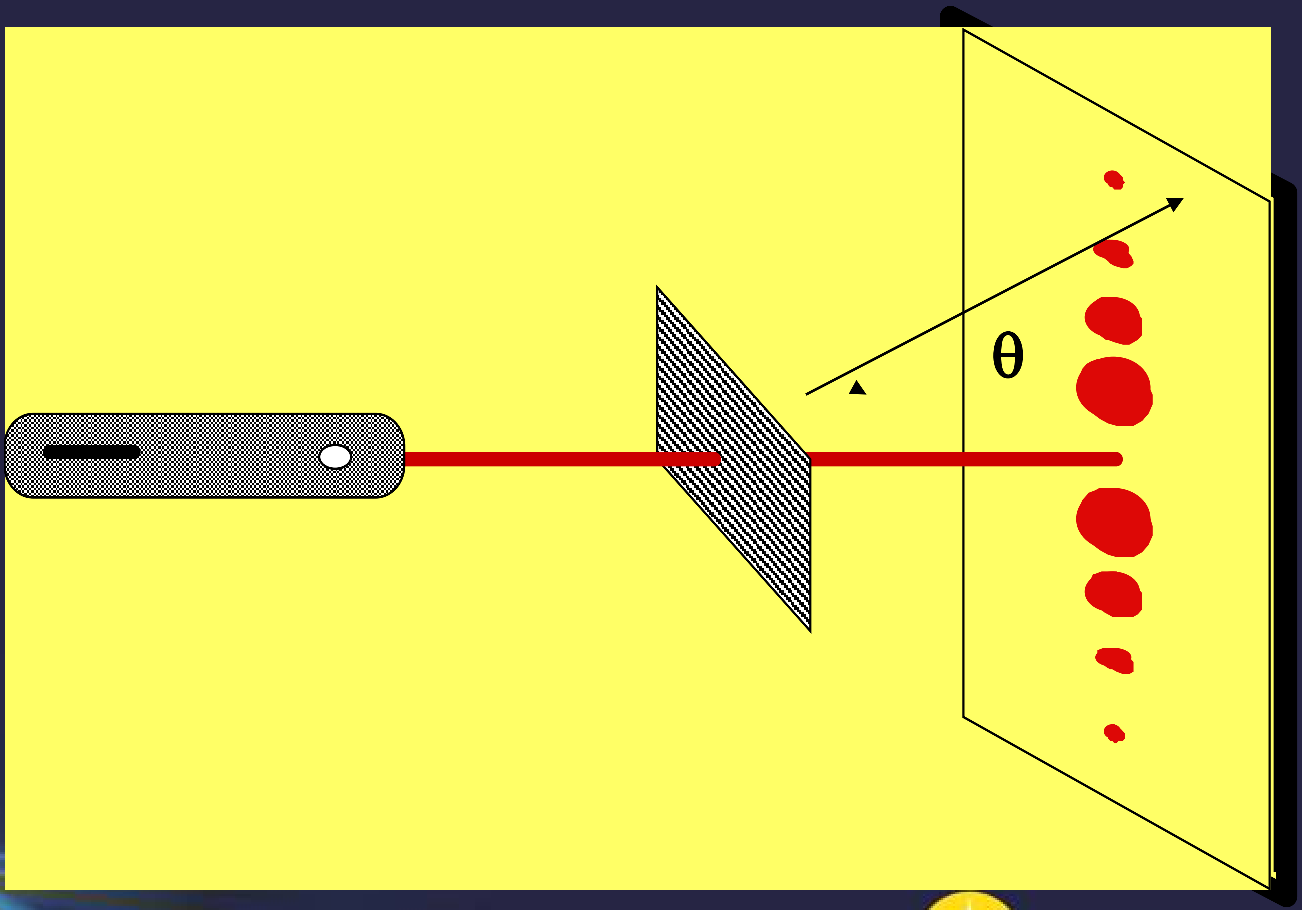
Sir William Bragg

Diffraction & Spectroscopy

Sir Lawrence Bragg



- X-rays
- Neutrons
- Visible light



- Braggs Law
  λ = 2dsinθ

1912/13

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1960's

- The era:
  - Cold War
  - Vietnam War
  - Cultural Revolution in China
  - Student revolution and flower power
  - First electronic calculators
  - Pope Paul VI declares opposition to the pill
  - First tabletop microwave ovens on market
  - Beatlemania starts
  - First Apollo Moon landing 1969

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Still to come…

- First large storage ring SPEAR and DORIS
- Personal computer ~1978
- WWW ~ 1990
- FELs ~2000

Accelerators in the 60's

- Synchrotrons NINA, DESY, BONN, Cornell…

  -Tomboulian and Hartmann (1956); first spectroscopy;

  -Parratt (1959) realized that such machines with larger electron energies " would be a boom in many aspects of X-ray physics"

First SR tests on the DESY Synchrotron 1965

  -spectroscopy on atoms and gases starts

  -photoemission spectroscopy starts – bandstructure made visible

- First storage rings came into operation in the 70's
  - 1976 I saw my first EXAFS spectrum taken at SSRL – a storage ring!!!

Conclusion: this is the source of the future!!!

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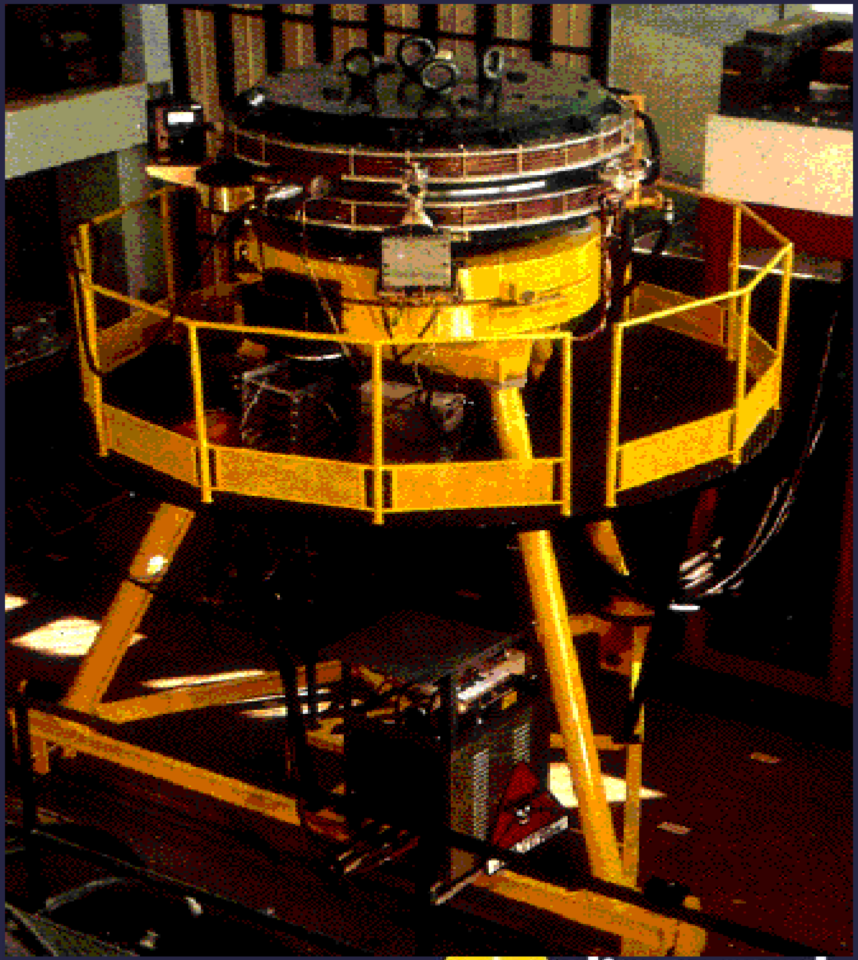
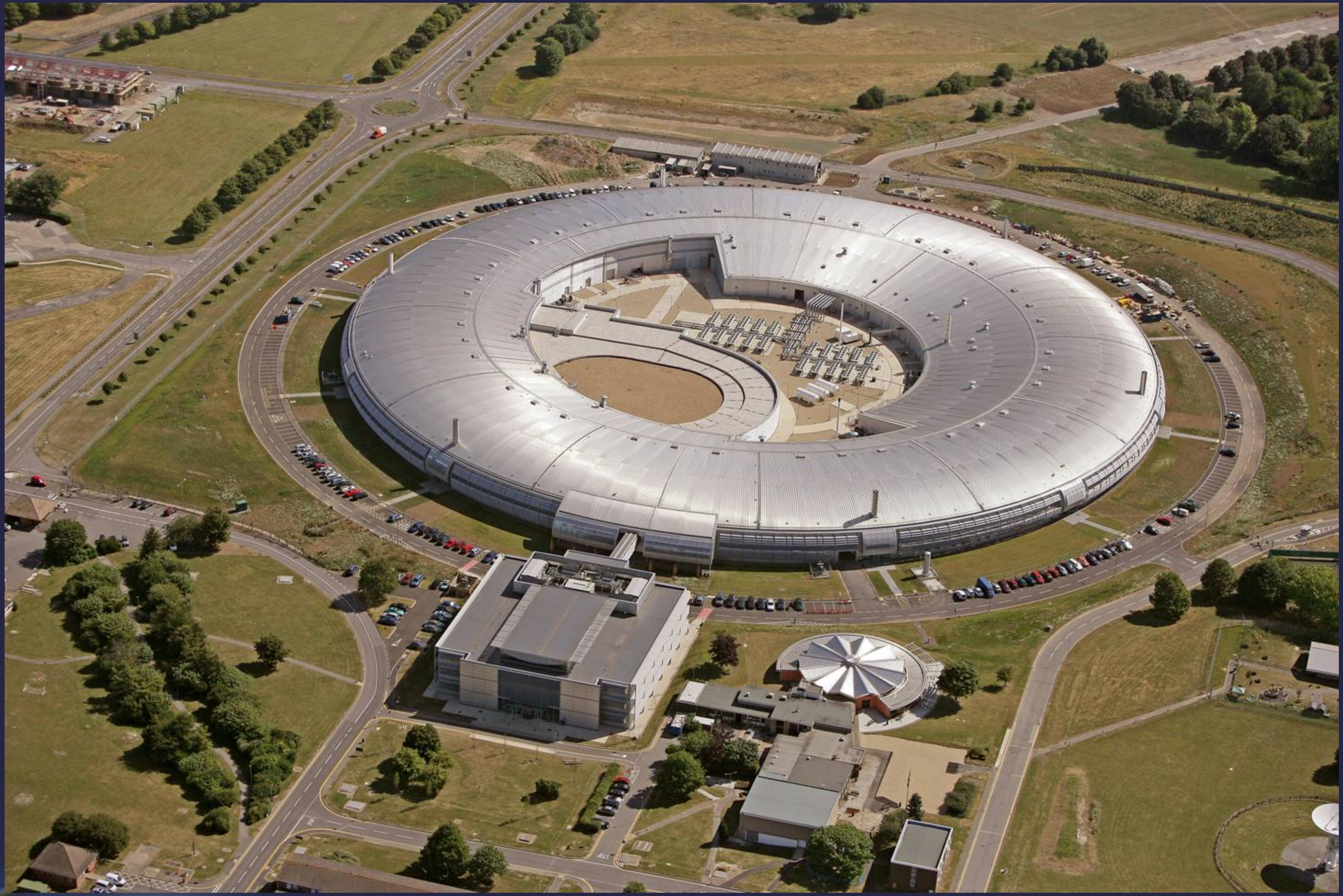
Colliders Global Origins

– AdA
– Bruno Touschek
  Frascati

e+ - e- 250MeV

~1960





Diamond Light Source

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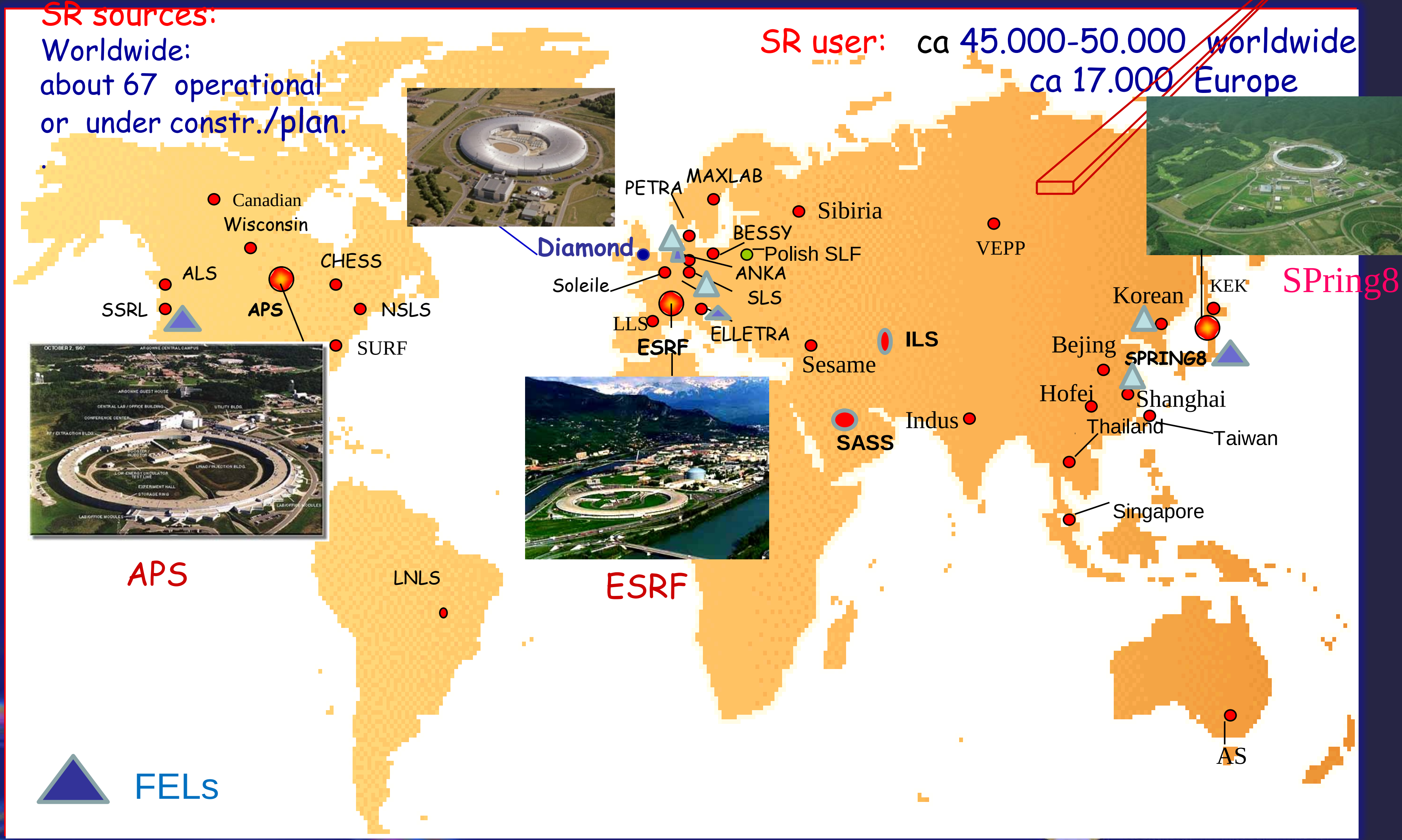
Synchrotron Radiation Research worldwide

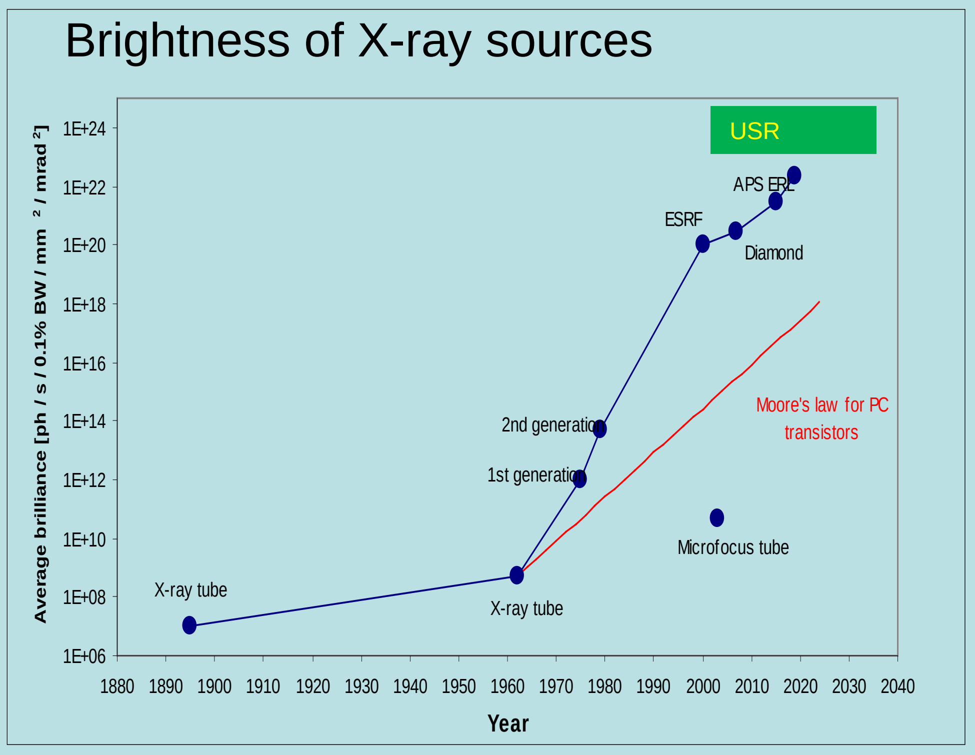


Diamond is a 3rd -Generation SL Source

Challenge is to make it a Next Generation SL USER Facility

- **1st generation:**
  machines originally built for other purposes e.g. high energy physics
- **2nd generation:**
  purpose-built machines for synchrotron radiation (e.g. SRS)
- **3rd generation:**
  higher brightness machines using special "insertion devices" (e.g. ESRF)

- **Next Generation Facility:**
  remote automatic control, robots for sample handling, grid access



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Needs stable accelerators and beamlines…

sub-micrometer,
sub-microradian,
constant electron current,
few pico-second bunch length

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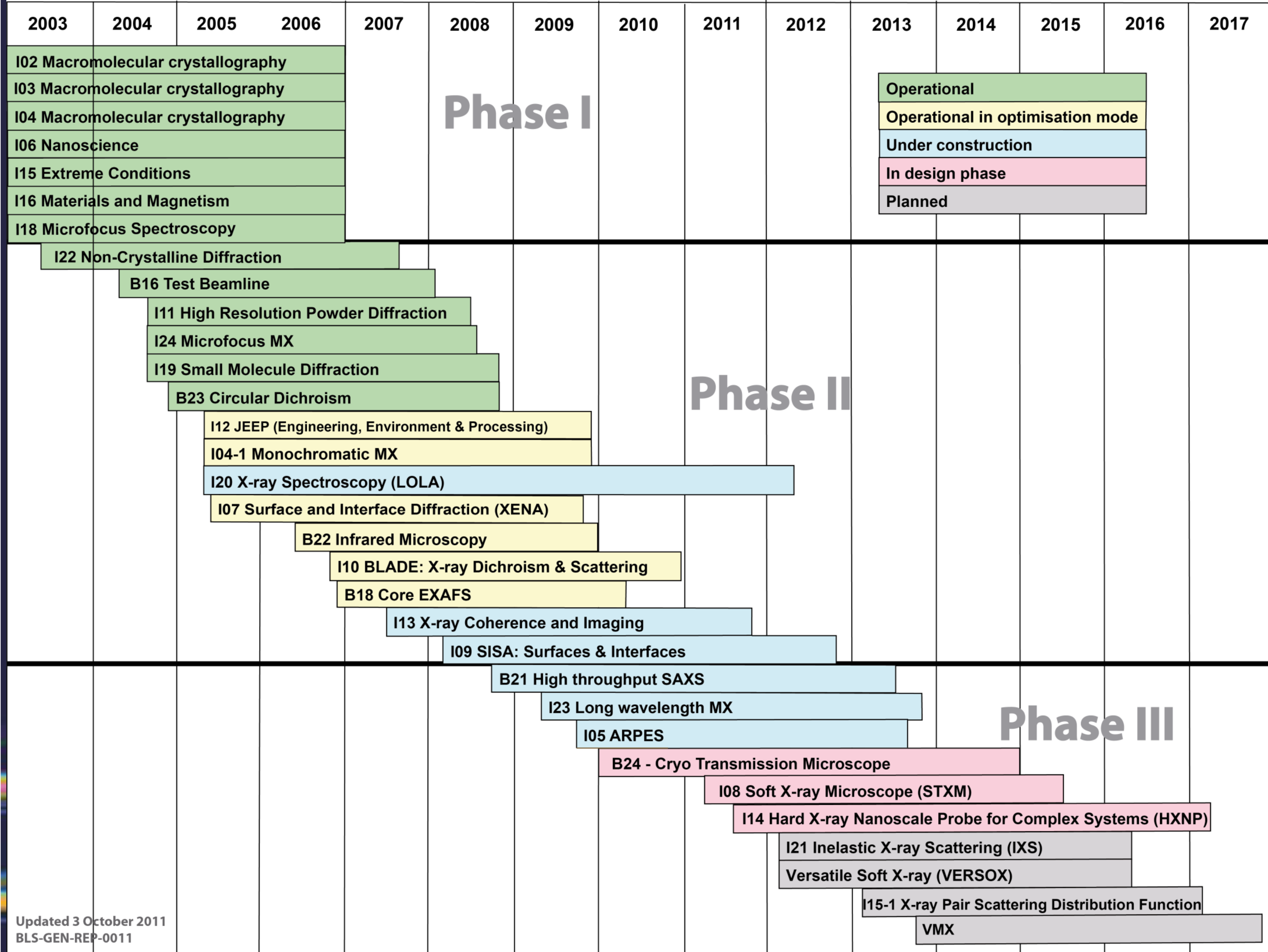
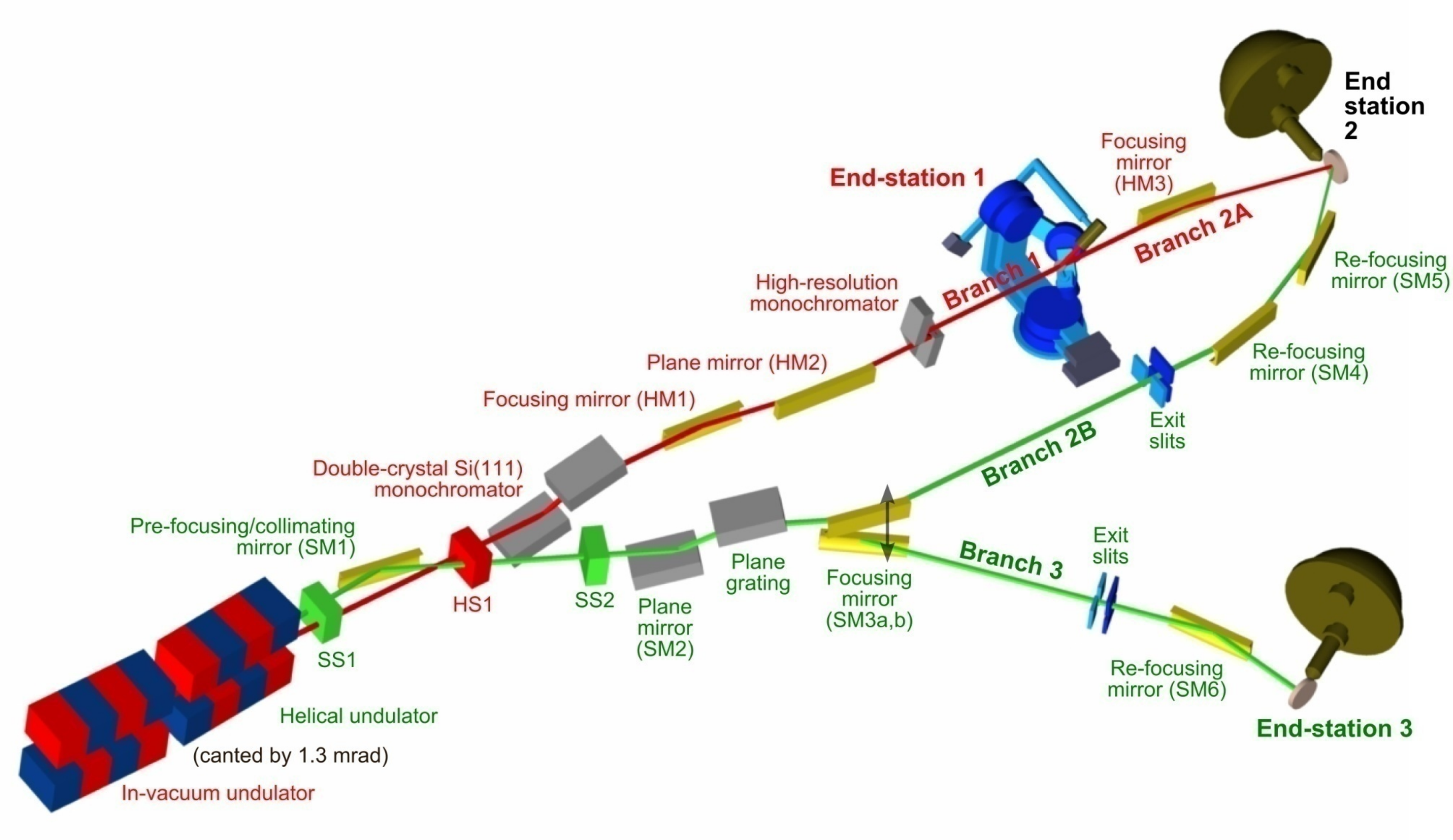
How do we do experiments ?


2003
2004
2005
2006
2007
2008
2009
2010
2011
2012
2013
2014
2015
2016
2017
Phase I
Phase II
Phase III
Operational
Operational in optimisation mode
Under construction
In design phase
Planned
I02 Macromolecular crystallography
I03 Macromolecular crystallography
I04 Macromolecular crystallography
I06 Nanoscience
I15 Extreme Conditions
I16 Materials and Magnetism
I18 Microfocus Spectroscopy
I22 Non-Crystalline Diffraction
B16 Test Beamline
I11 High Resolution Powder Diffraction
I24 Microfocus MX
I19 Small Molecule Diffraction
B23 Circular Dichroism
I12 JEEP (Engineering, Environment & Processing)
I04-1 Monochromatic MX
I20 X-ray Spectroscopy (LOLA)
I07 Surface and Interface Diffraction (XENA)
B22 Infrared Microscopy
I10 BLADE: X-ray Dichroism & Scattering
B18 Core EXAFS
I13 X-ray Coherence and Imaging
I09 SISA: Surfaces & Interfaces
B21 High throughput SAXS
I23 Long wavelength MX
I05 ARPES
B24 - Cryo Transmission Microscope
I08 Soft X-ray Microscope (STXM)
I14 Hard X-ray Nanoscale Probe for Complex Systems (HXNP)
I21 Inelastic X-ray Scattering (IXS)
Versatile Soft X-ray (VERSOX)
I15-1 X-ray Pair Scattering Distribution Function
VMX
Updated 3 October 2011
BLS-GEN-REP-0011

Surface and Interface Structural Analysis Beamline SISA at Diamond (Tien-Lin Lee et al)



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Expect huge advances in beamline instrumentation:

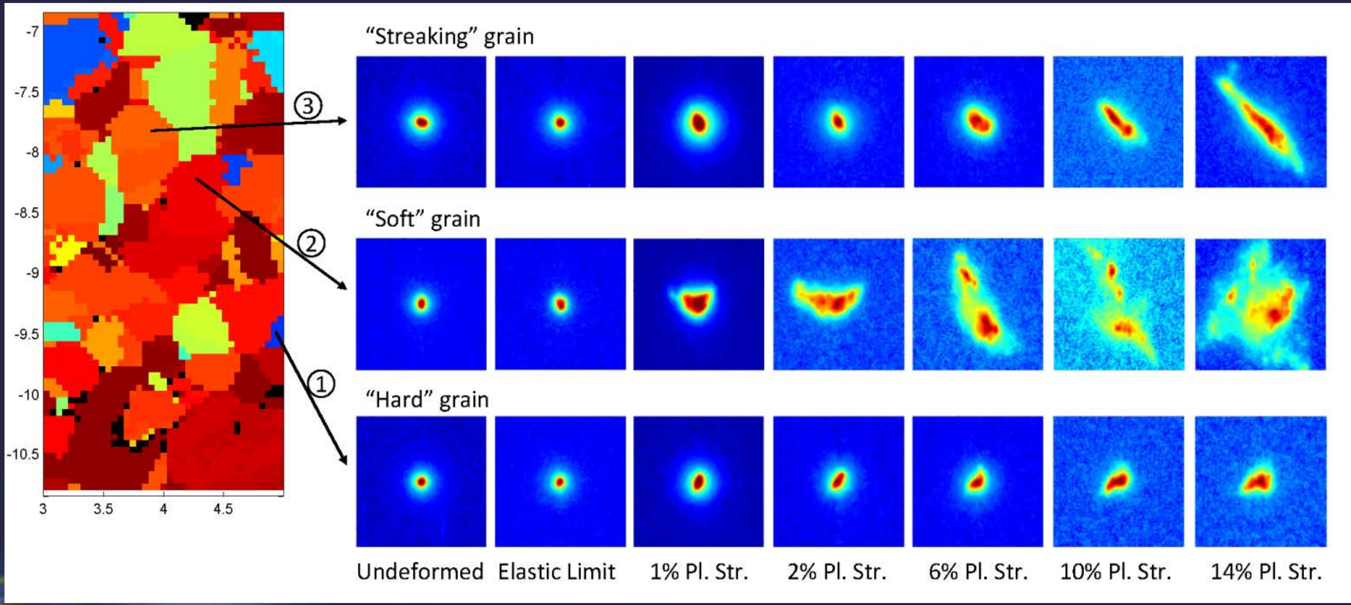
detectors, computing, mirrors, lenses…

What about material science and engineering?

Probing Intragranular Deformation by Micro-beam Laue Diffraction (A Korsunsky, et al, Oxford Univ., I Dolbnya)

B16

- Developed a novel microbeam Laue diffraction setup on B16
- for determination of dislocation density distribution and micro-level strains



Plot of Laue Spot evolution with loading in a “Streaking” grain, a “Soft” grain and a “Hard” grain.

Tomography of crack formation

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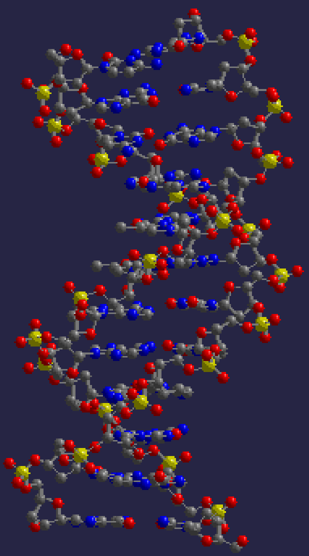
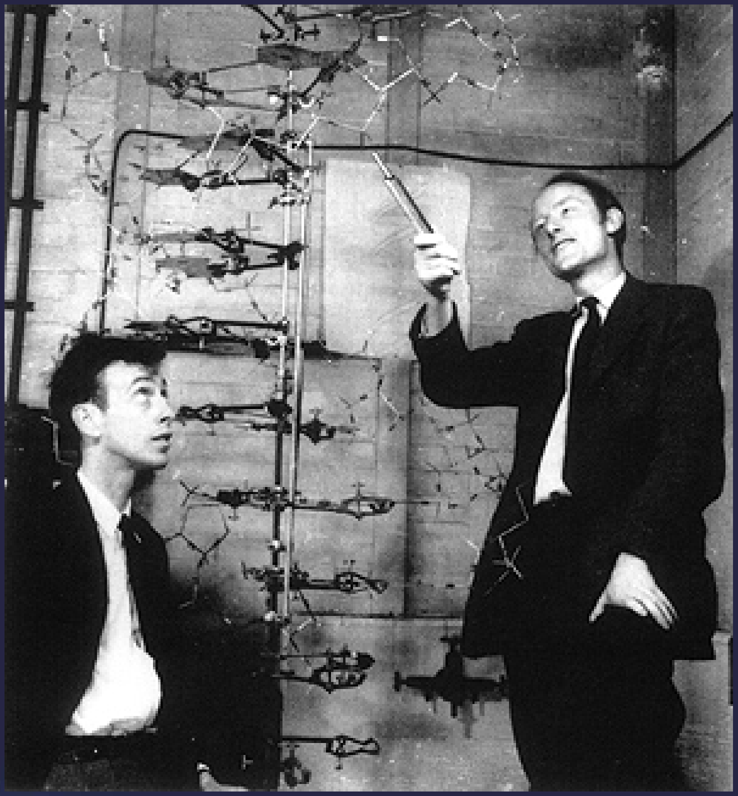
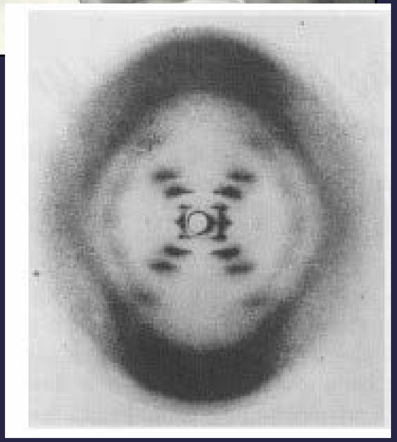
Let’s diffract from a crystal…

1953 Crick & Watson solve the structure of DNA - the famous Double Helix



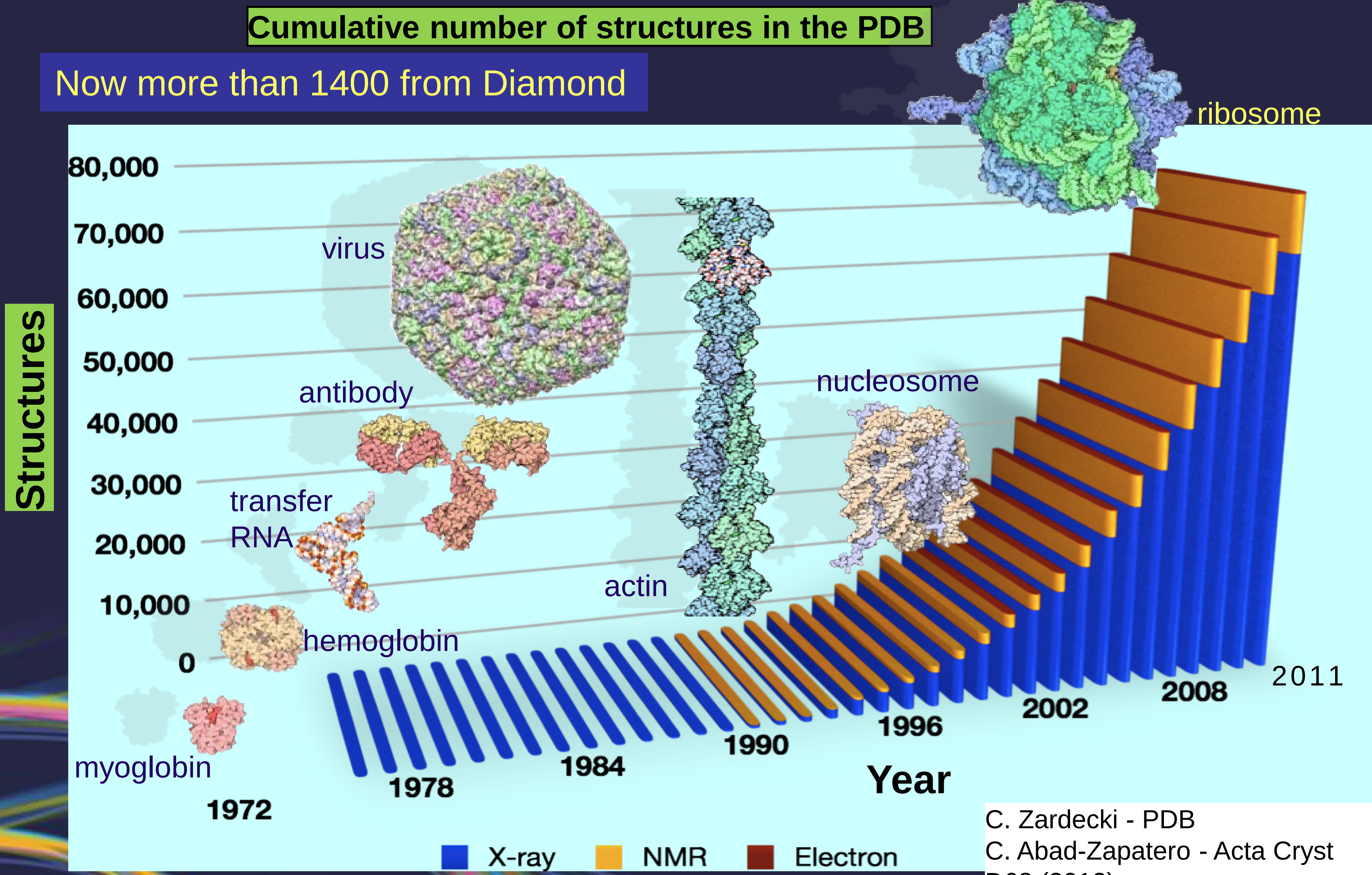




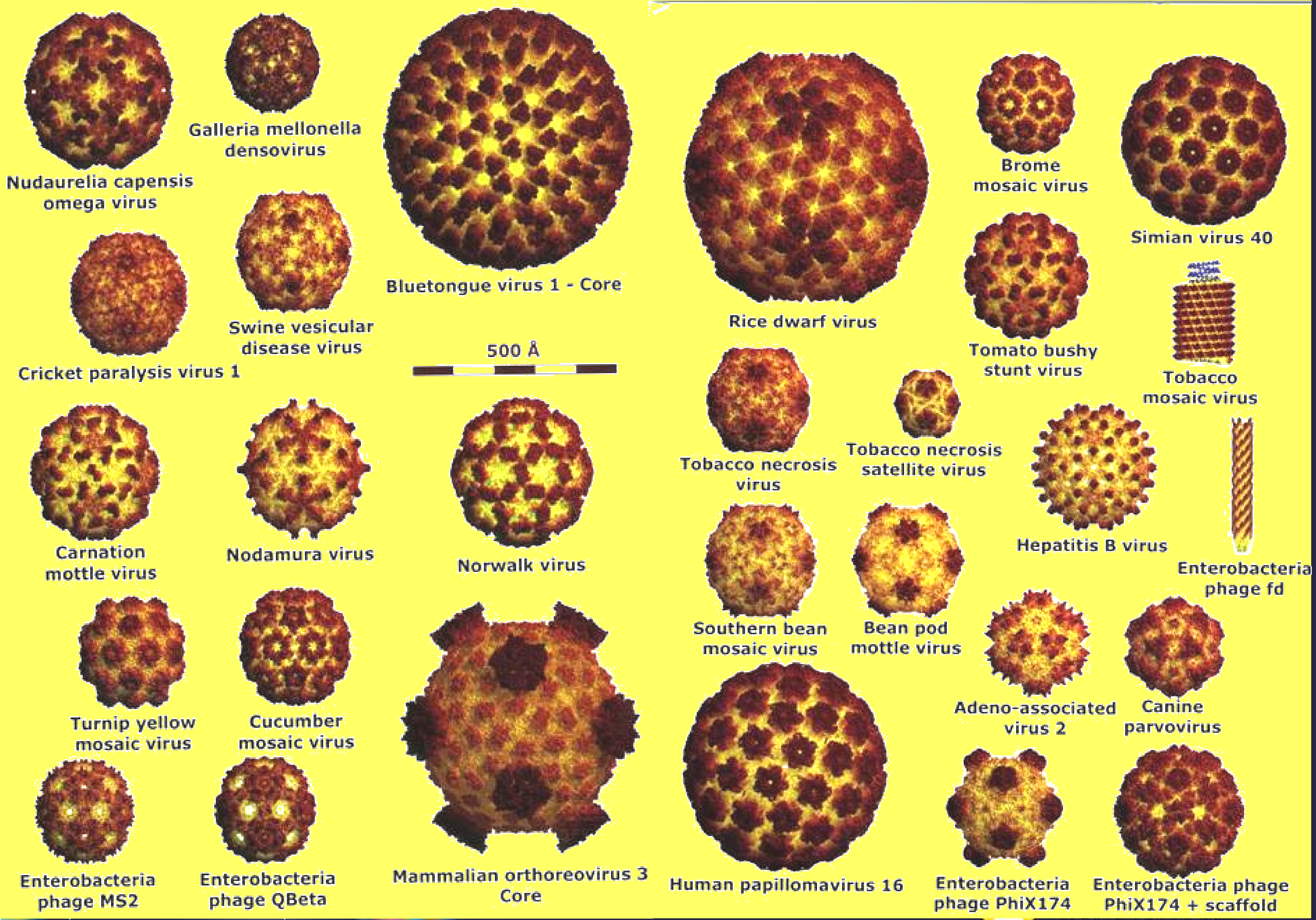
Rosalind Franklin - Measured the first high-quality X-ray diffraction pattern from DNA and deduced the basic helical structure of DNA.

Biological Structure: X-Rays are the key tool

(courtesy H. Chapman, J Stoehr)



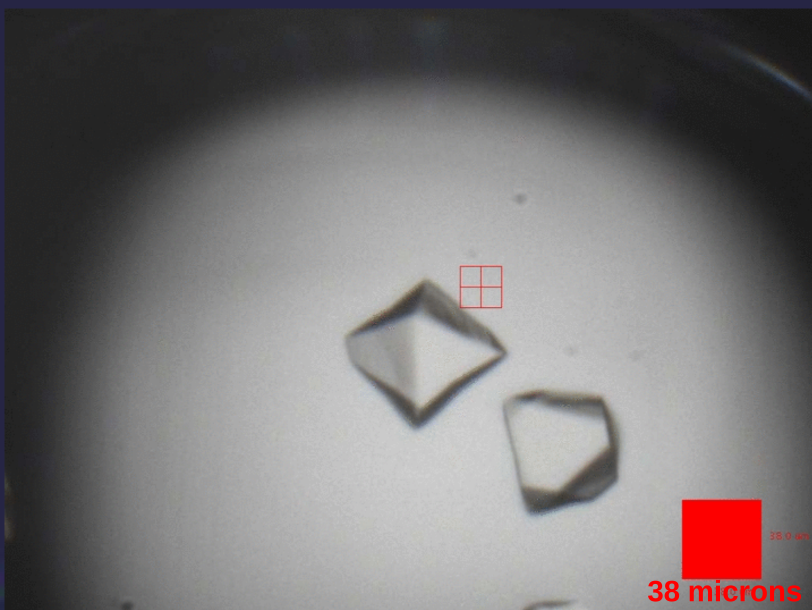
C. Zardecki - PDB
C. Abad-Zapatero - Acta Cryst D68 (2012)



BUT ~100 structures of viruses, suggest a new approach…

The difference I24 made...

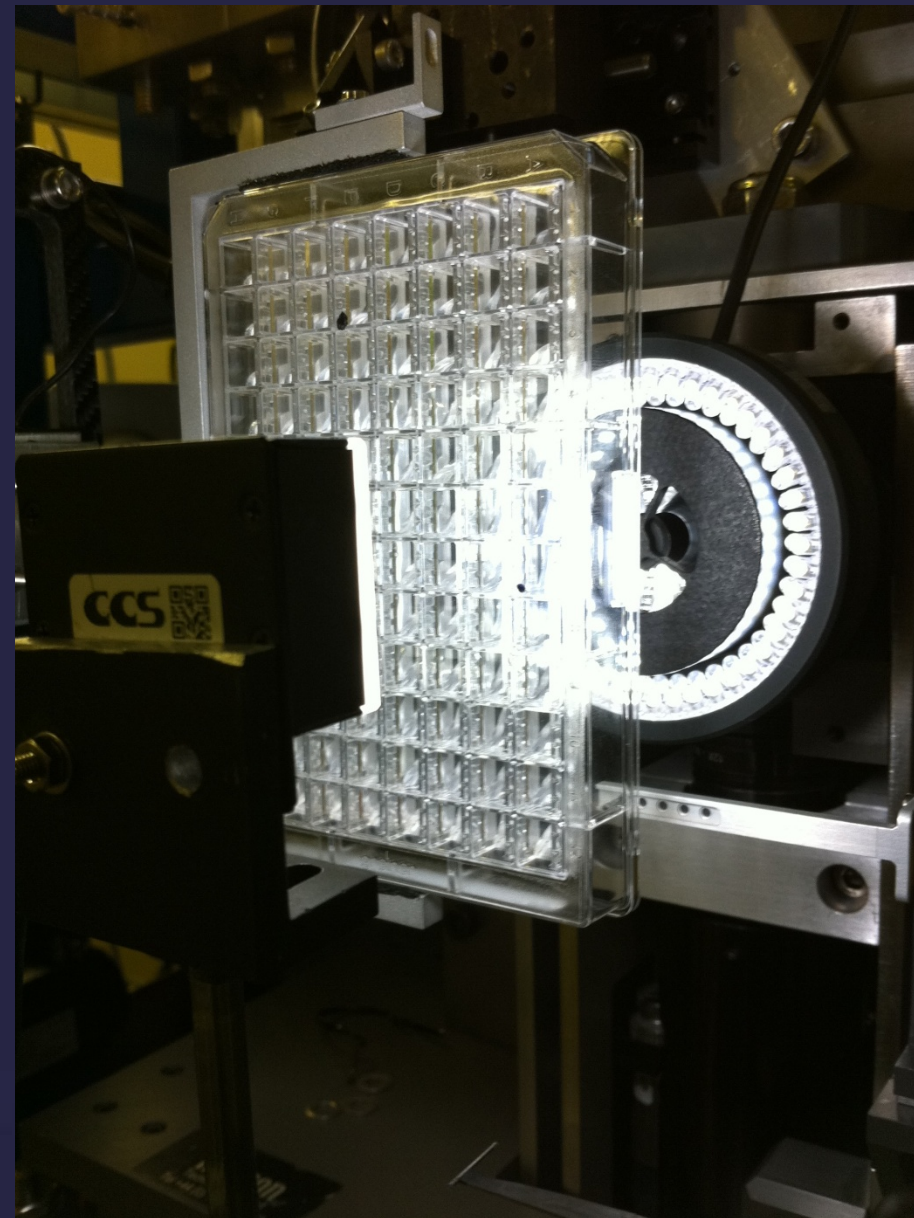
In situ room temp diffraction
(this means using smallish crystals in the nano-drops in which they have been grown, after being set-up robotically) ...



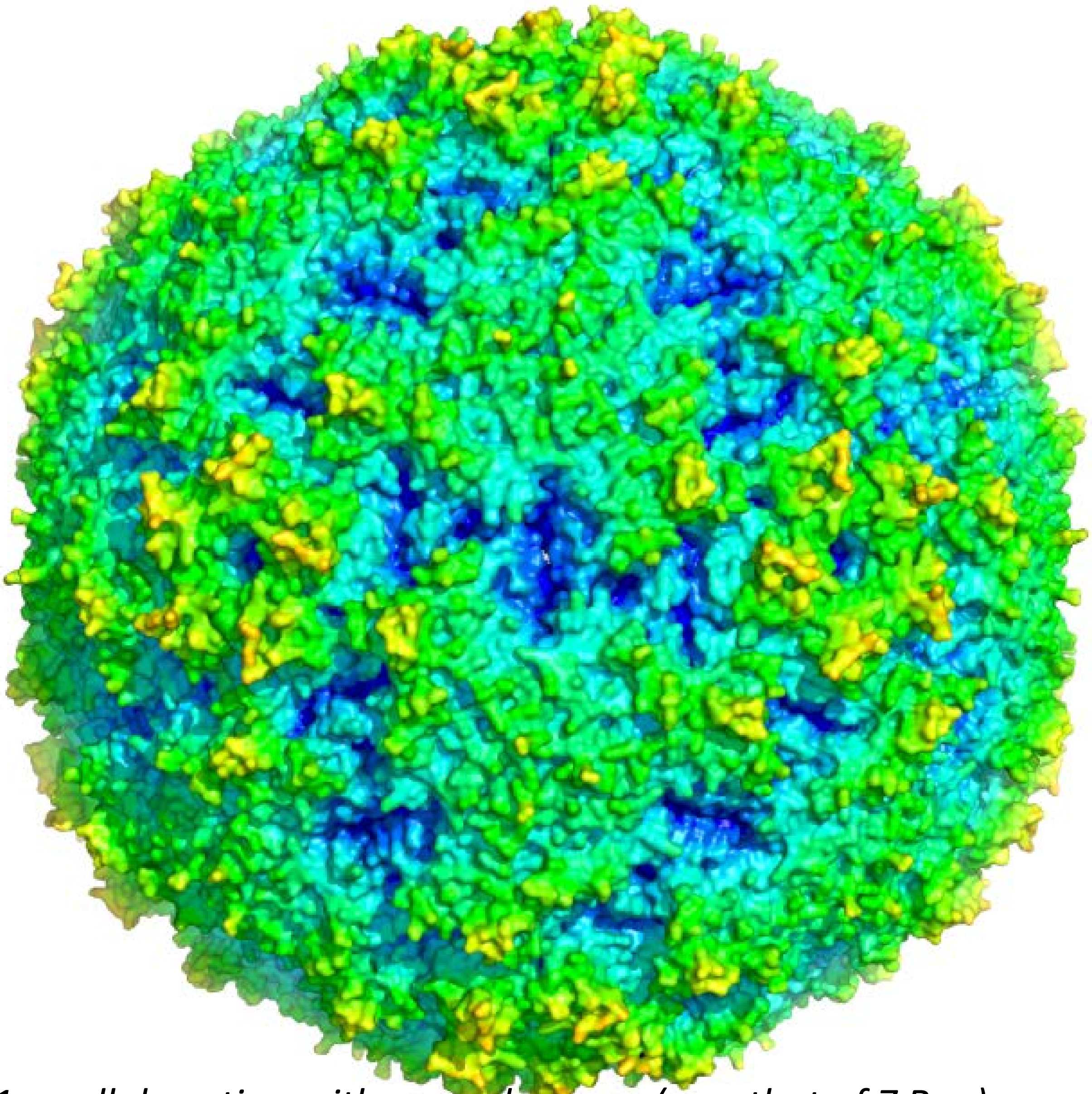
0.05°per 0.05 s. 10^{12} photons / s into 20 μ beam – crystal lifetime ~0.4 s

Focus towards the detector

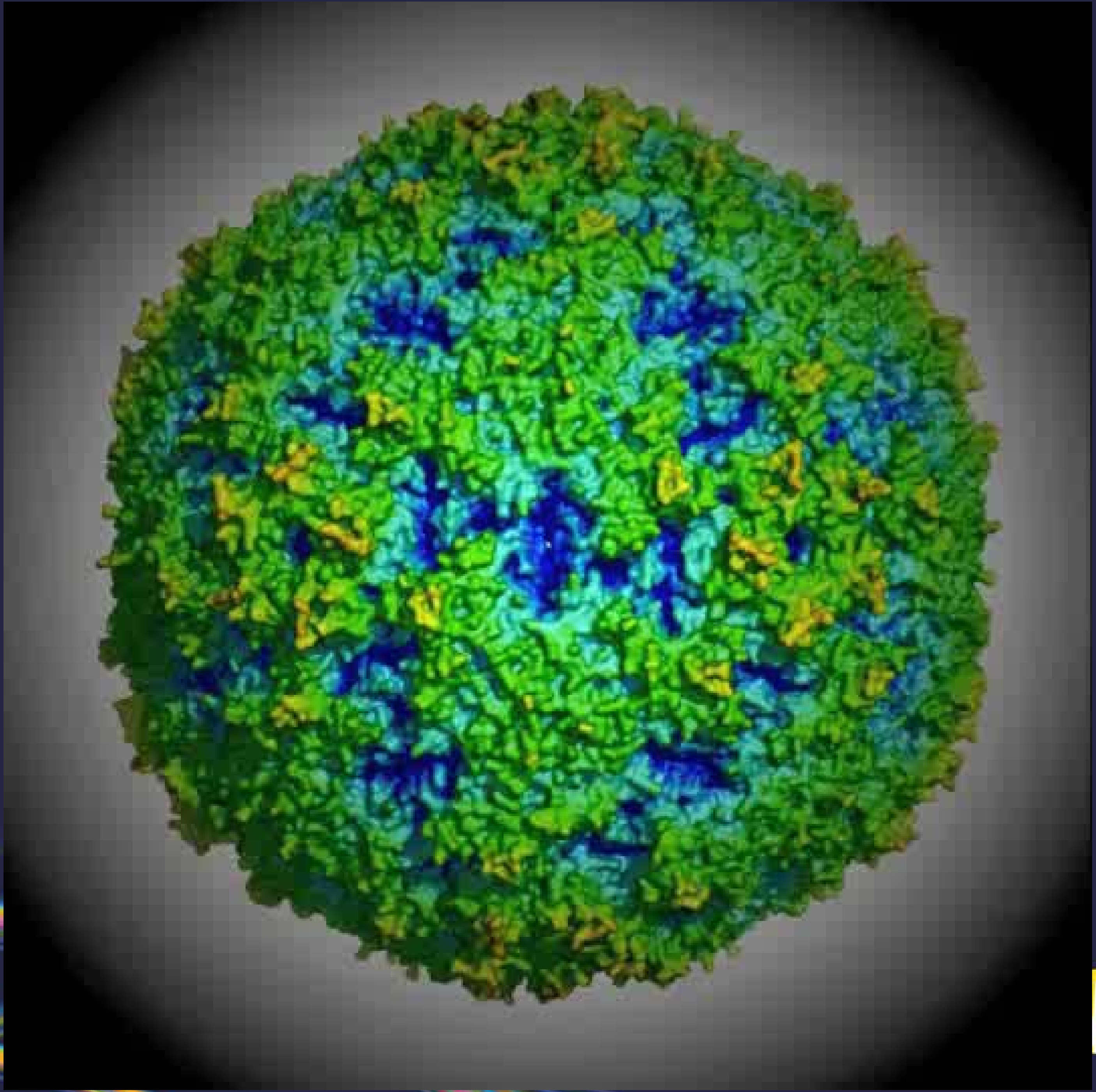
I24 staff, plus E Fry, JS Ren, A Kotcha DIS, Oxf



Dave Stuart group (March 2012 in Nature)



Structure of EV71 – collaboration with several groups (esp. that of Z Rao)
(11 structures determined at Diamond, I24 – one frozen, other RT)



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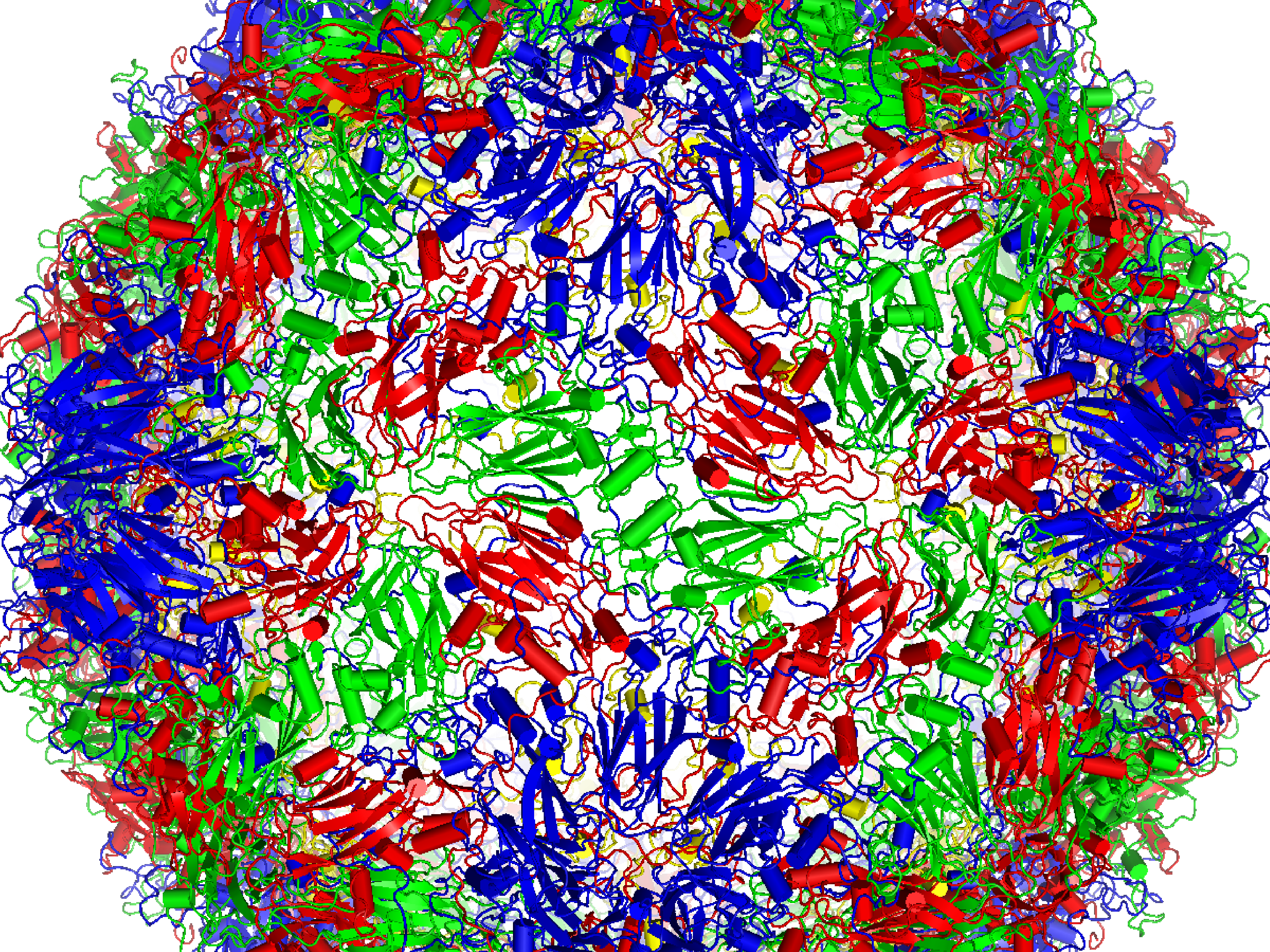
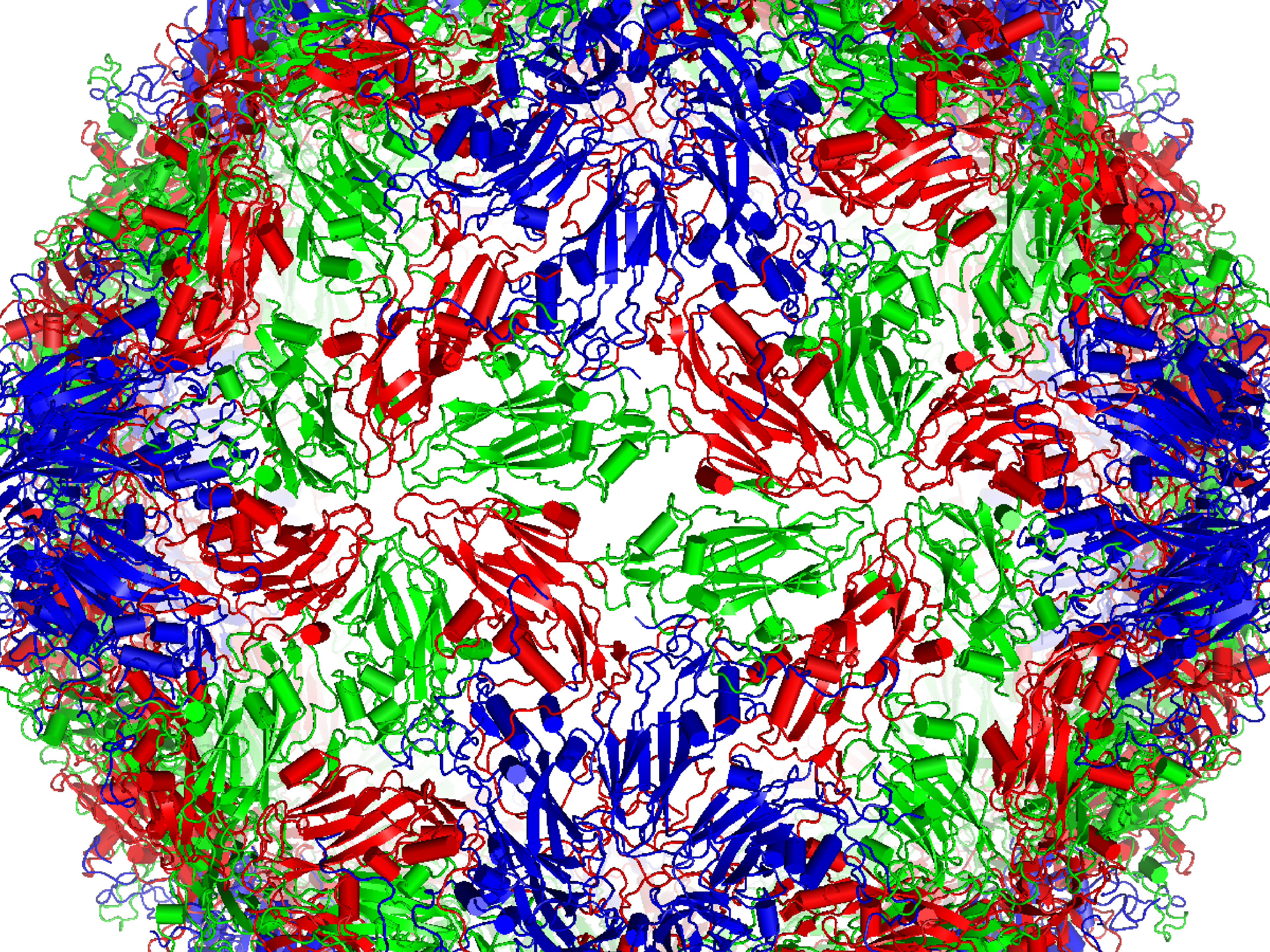




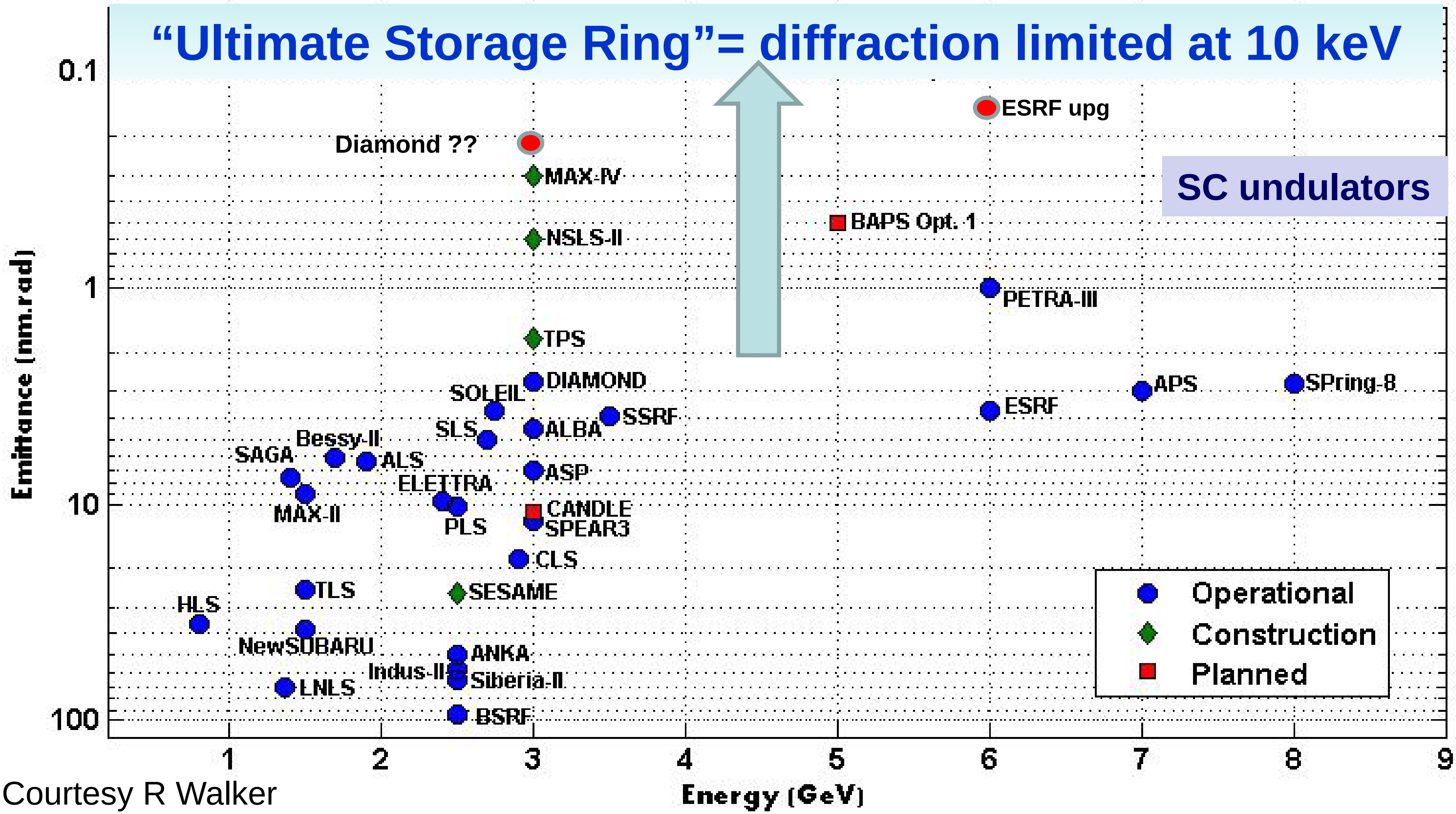
So what about the future of SXR from storage rings?

It's not the end of the road for storage ring light sources …!

$\varepsilon_0 \propto E^2$

$\varepsilon_0 \propto \theta^3$

damping wigglers



Courtesy R Walker

Design challenges for low emittance sources:

⇒large number of bending magnets

⇒low dispersion function, good for low emittance, but ..

⇒high quadrupole strengths

⇒high sextupole strengths

⇒highly non-linear beam dynamics

⇒small ”dynamic aperture” (area in which particle motion is stable)

⇒ poor lifetime and injection difficulties

Courtesy R Walker

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What about the future?

- Diffraction limit for 10 keV is ca 10 pm rad. Vertically already easily reached today, horizontally new MBA lattices reach 100 pm rad and design exist for the USR.
  - ERLs no real advantage…so far?
  - do we need 100 keV diffr. limited photons ???
- Tailor made affordable storage rings would enable specific methods with high user/sample throughput (medical applications, phase contrast microscopy…)
- "Table top"?
  - a beamline is very long in any case (stability!!!)
  - User mode more efficient in larger facilities

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Crazy ideas

- Change bunch structure on demand

  eg short bunches down into the fs regime with high current and low emittance

FELs

complementary to storage rings

The 4th generation of SR sources

Or

The first generation of X-ray lasers

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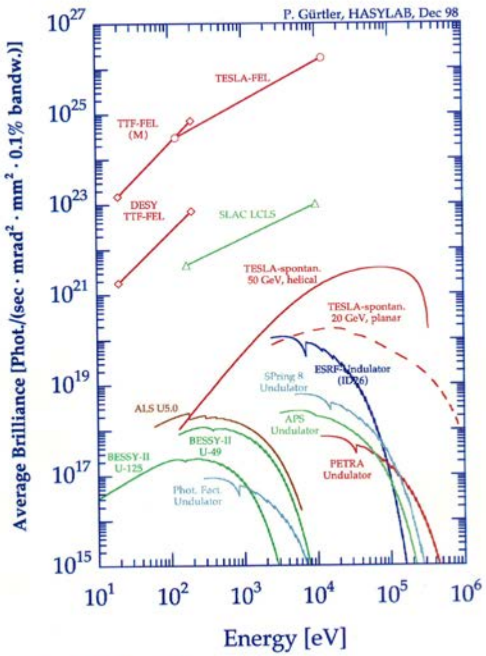
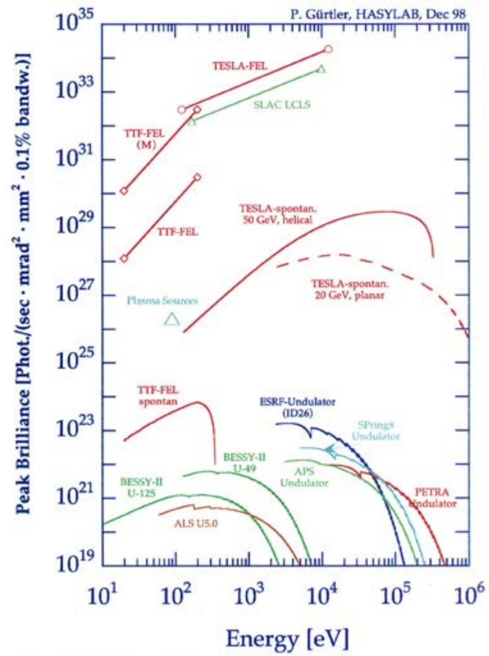
XFELs – the straight line into the future!



Spectral Brilliance (SB):

partially coherent source : $SB = \dfrac{spectral\ Flux}{4\pi^2 \Sigma_x \Sigma_{x'} \Sigma_z \Sigma_{z'}}$ $\quad \Sigma = \sqrt{\sigma_e^2 + \sigma_p^2}$

fully coherent source : $SB = \dfrac{spectral\ Flux}{(\lambda/2)^2}$ $\quad \Sigma' = \sqrt{\sigma_e'^2 + \sigma_p'^2}$



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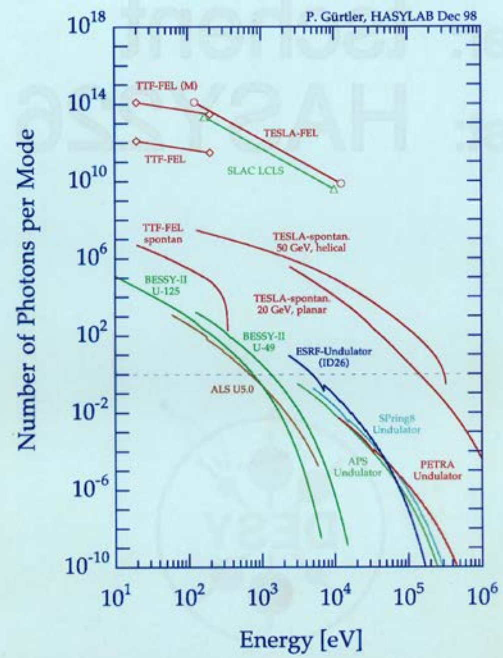
fully coherent source : $SB = \dfrac{spectral\ Flux}{(\lambda/2)^2}$ $\quad \Sigma' = \sqrt{\sigma_e'^2 + \sigma_p'^2}$

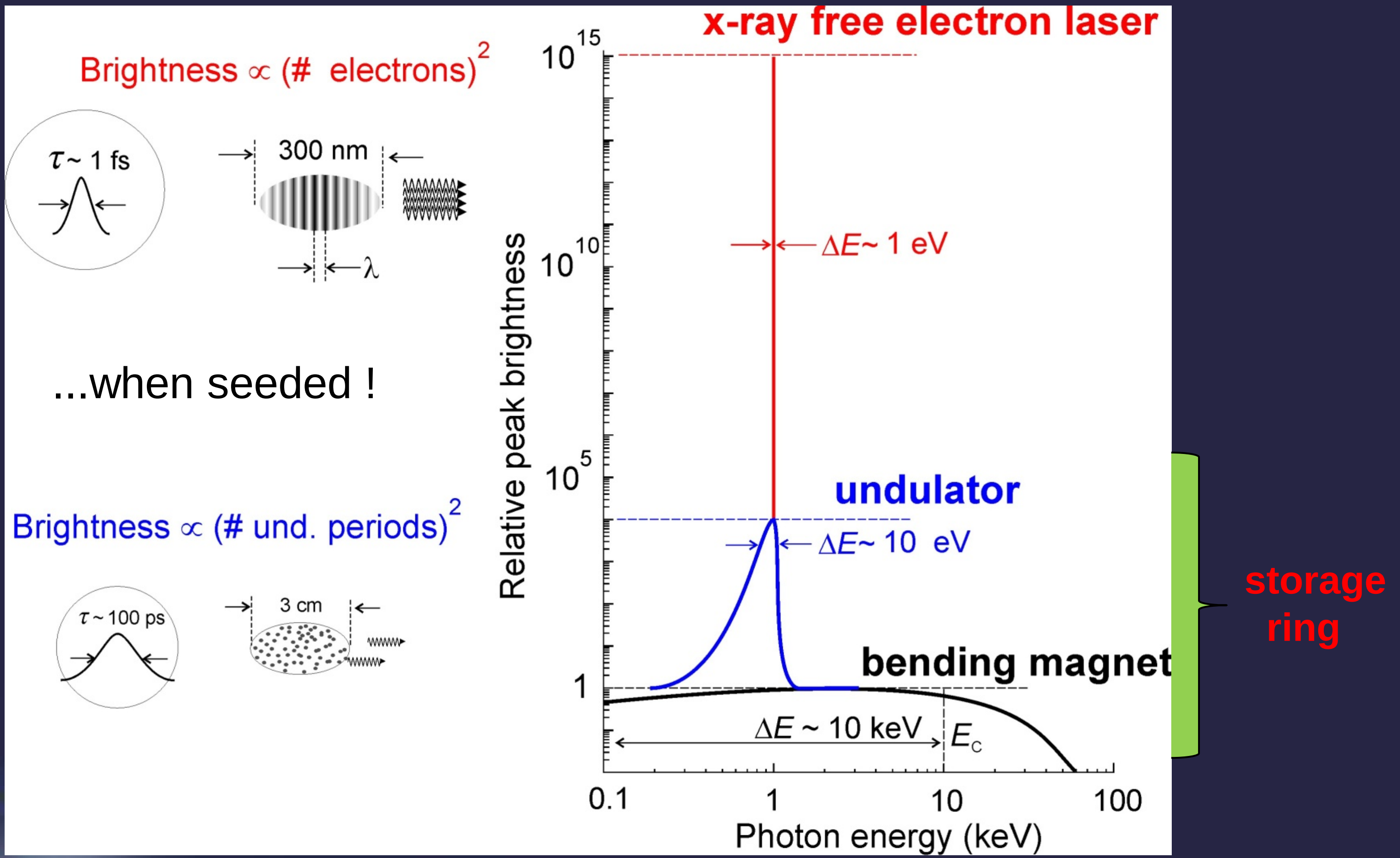


Number of Photons per Mode N :

$$N \equiv \frac{Peak\ Brilliance \cdot \lambda_{ph}^3}{4 \cdot c} \equiv$$ *average # photons which can interfere being in one quantum state ≡ "mode"*

(Gaussian beam, not FT - limited)

X-ray properties: storage ring versus FEL

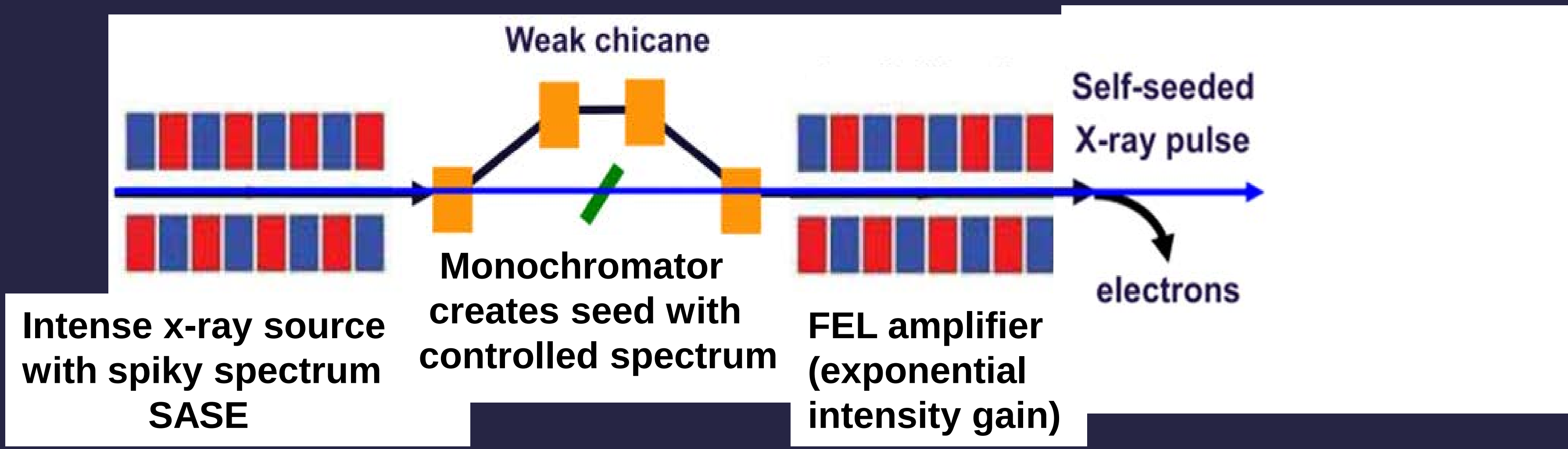


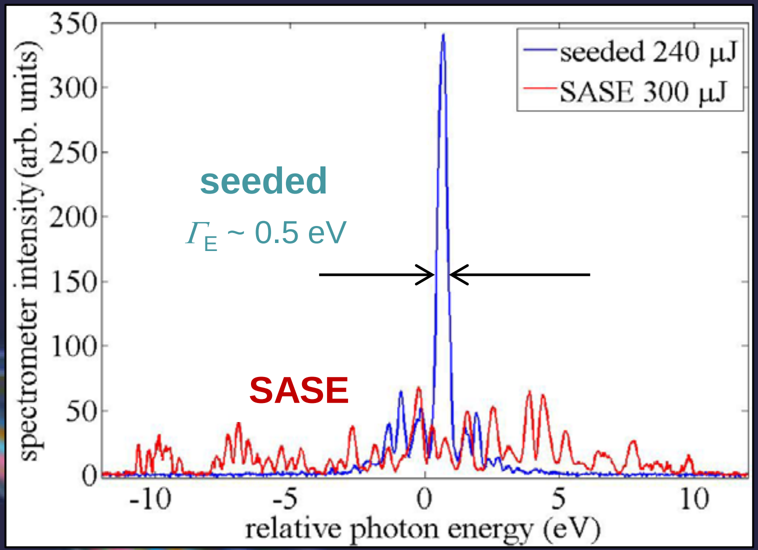
Assume energy bandwidth of 1eV

- **XFEL photons per pulse ≈ storage ring photons in 1 s**
- **XFEL photons are coherent (indistinguishable)**

courtesy J Stoehr

SASE versus self seeded x-ray beam (LCLS)

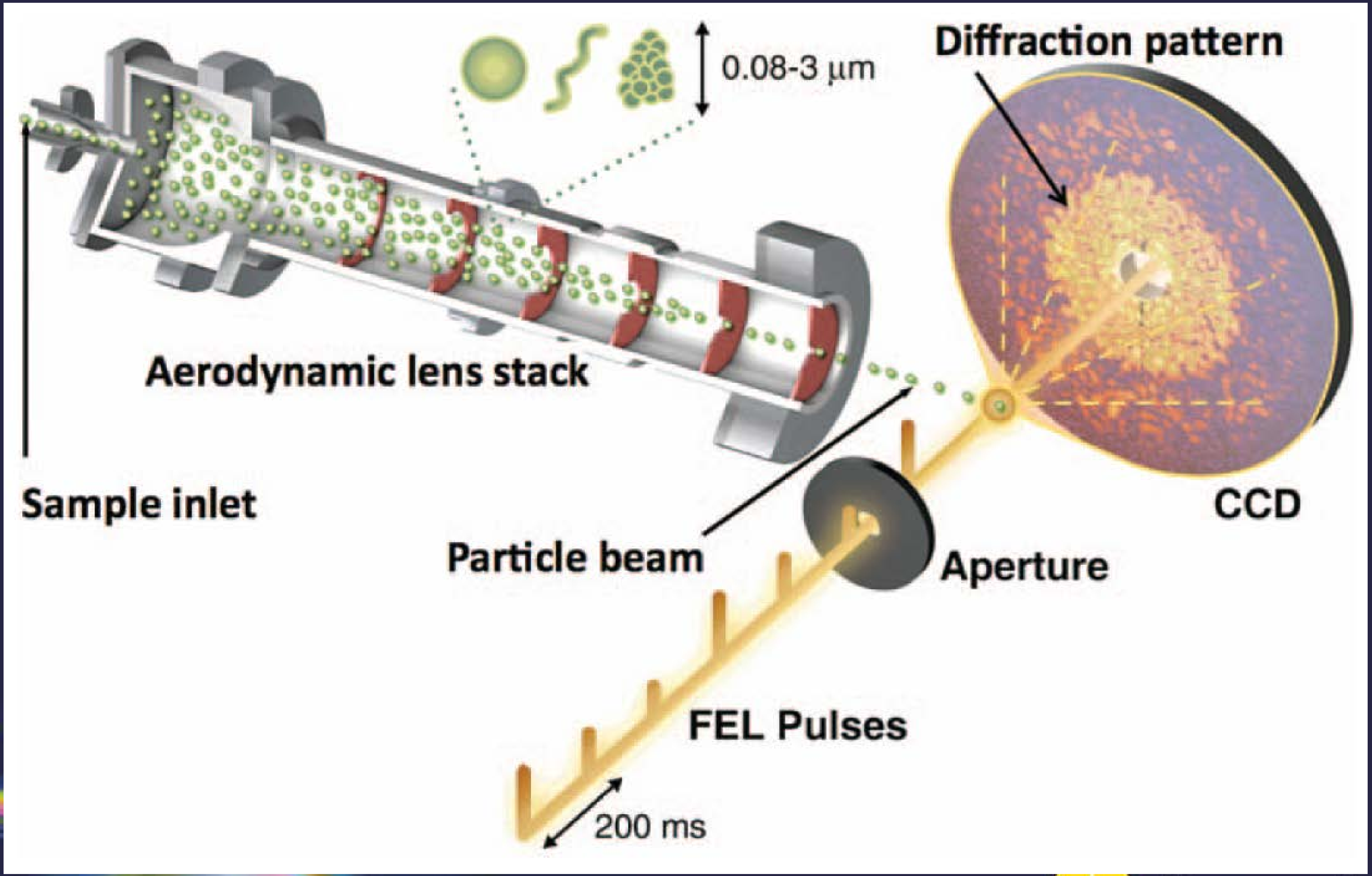




8.3 keV
40 pC

Courtesy:
J Stoehr

Single-shot X-ray diffraction with injected particles
(H.Chapman, J.Hajdu et al.)



M.J. Bogan et al., Aerosol Science and Technology, 44:i–vi (2010)

Courtesy: J Stoehr

First X-FEL solved protein structure

Cathepsin B enzyme protein - part of the African sleeping sickness parasite

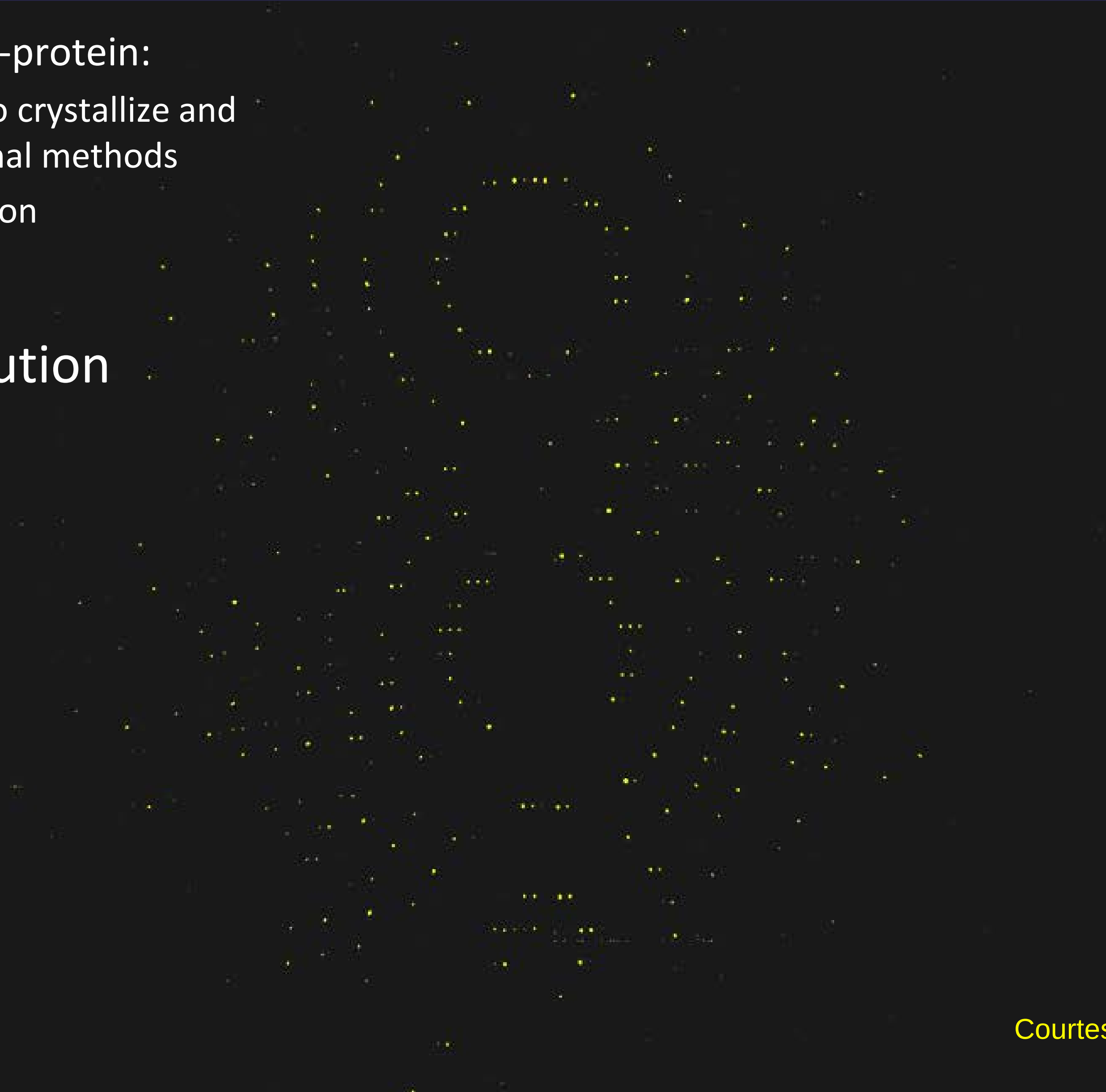
Cathepsin B glyco-protein:

Famously difficult to crystallize and solve by conventional methods

shots: 4 million

of hits 10%

2Å resolution



Courtesy: J Stoehr

First results: room temperature study of S_1 state

Room temperature femtosecond X-ray diffraction of photosystem II microcrystals

Jan Kern[a,b], Roberto Alonso-Mori[b], Julia Hellmich[c], Rosalie Tran[a], Johan Hattne[a], Hartawan Laksmono[d], Carina Glöckner[c], Nathaniel Echols[a], Raymond G. Sierra[d], Jonas Sellberg[e,f], Benedikt Lassalle-Kaiser[a], Richard J. Gildea[a], Pieter Glatzel[g], Ralf W. Grosse-Kunstleve[a], Matthew J. Latimer[e], Trevor A. McQueen[h], Dörte DiFiore[c], Alan R. Fry[b], Marc Messerschmidt[b], Alan Miahnahri[b], Donald W. Schafer[b], M. Marvin Seibert[b], Dimosthenis Sokaras[e], Tsu-Chien Weng[e], Petrus H. Zwart[a], William E. White[b], Paul D. Adams[a], Michael J. Bogan[b,d], Sébastien Boutet[b], Garth J. Williams[b], Johannes Messinger[i], Nicholas K. Sauter[a], Athina Zouni[c], Uwe Bergmann[b,1], Junko Yano[a,1], and Vittal K. Yachandra[a,1]

[a]Physical Biosciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720; [b]Linac Coherent Light Source, SLAC National Accelerator Laboratory, Menlo Park, CA 94025; [c]Max-Volmer-Laboratorium für Biophysikalische Chemie, Technische Universität Berlin, D-10623 Berlin, Germany; [d]PULSE Institute, SLAC National Accelerator Laboratory, Menlo Park, CA 94025; [e]Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, Menlo Park, CA 94025; [f]Department of Physics, AlbaNova, Stockholm University, S-106 91 Stockholm, Sweden; [g]European Synchrotron Radiation Facility, BP 220, F-38043 Grenoble Cedex, France; [h]Department of Chemistry, Stanford University, Stanford, CA 94025; and [i]Institutionen för Kemi, Kemiskt Biologiskt Centrum, Umeå Universitet, S-901 87 Umeå, Sweden

Edited by* Edward I. Solomon, Stanford University, Stanford, CA, and approved May 2, 2012 (received for review March 20, 2012)

- 50 fs pulses, 3.4×10^{11} photons/pulse at 9 keV
  - ➢ undamaged room temperature atomic/electronic structure
  - ➢ future studies will reveal reaction dynamics

Courtesy:J Stoehr

Chemical structure: Understanding Photosynthesis

- Has created our **atmosphere** and ozone layer
- Only fundamental source of **food** on earth
- Has created **fossil energy** sources (crude oil, coal, gas)

Courtesy:J Stoehr

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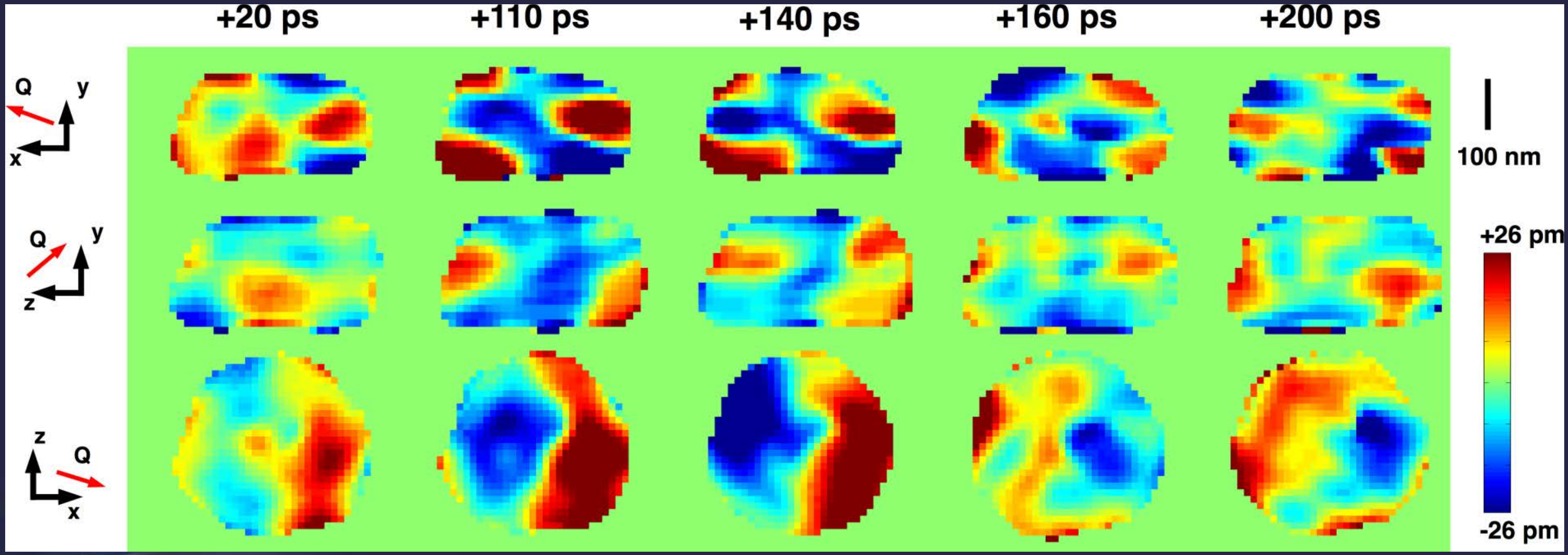
Ultrafast three dimensional imaging of lattice dynamics in gold nanocrystals

J. N. Clark1, L. Beitra1, G. Xiong1, A. Higginbotham2, D. M. Fritz3, H. T. Lemke3, D. Zhu3, M. Chollet3, G. J. Williams3, M. Messerschmidt3, B. Abbey4, R. J. Harder5, A. M. Korsunsky6,7, J. S. Wark2 & I. K. Robinson1,7

Science, May 2013



Courtesy: I Robinson

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The Future of X-FEL Science

- **Through experiments:**
  - nanocrystal diffraction (towards single molecules???)
  - Structure of whole proteins and reaction centers
  - Function through pump-probe studies of dynamics
  - Explore transient atomic structure of matter (e.g. liquids)
  - Understand electronic and spin structure of excited states
  - Hot dense matter equation of states

Through accelerators advances:

- Develop terawatt, femtosecond seeded pulses (towards attosecond pulses);
- **lower cost linacs and undulators !!!!**
- **stable** XFEL beams

How can we make fs-ps X-ray movies?

How does the future of synchrotron radiation look like?

Storage Ring Sources

will provide high average brilliance to study matter down to sub nm, psec and meV resolution

Free Electron Lasers

will provide fsec, ultra high power (peak brilliance)

Both will in the future be complimentary sources for science

diamond

Thanks a lot for your attention

and

I hope some of you will make some of that come true…

wellcome trust

Science & Technology Facilities Council