



| The European Synchrotron



Next Generation X-ray Analyses and the ESRF Upgrade Programme

Low Emittance Workshop
INFN-LFN
Frascati 17-19 September 2014

Francesco Sette – sette@esrf.fr

Major synchrotrons in the world

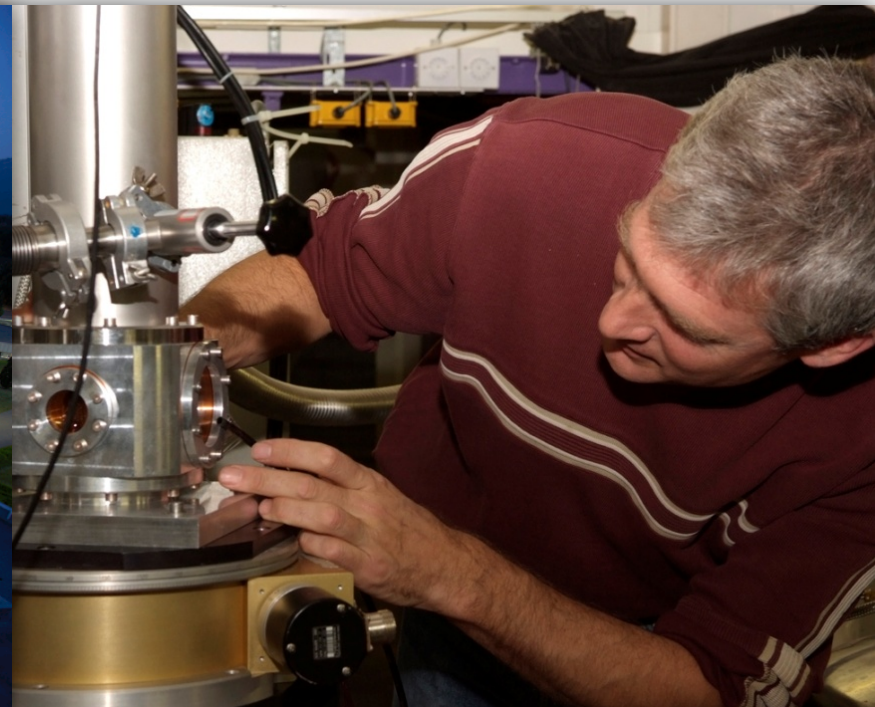


ESRF is the world's first 3rd generation hard X-ray source

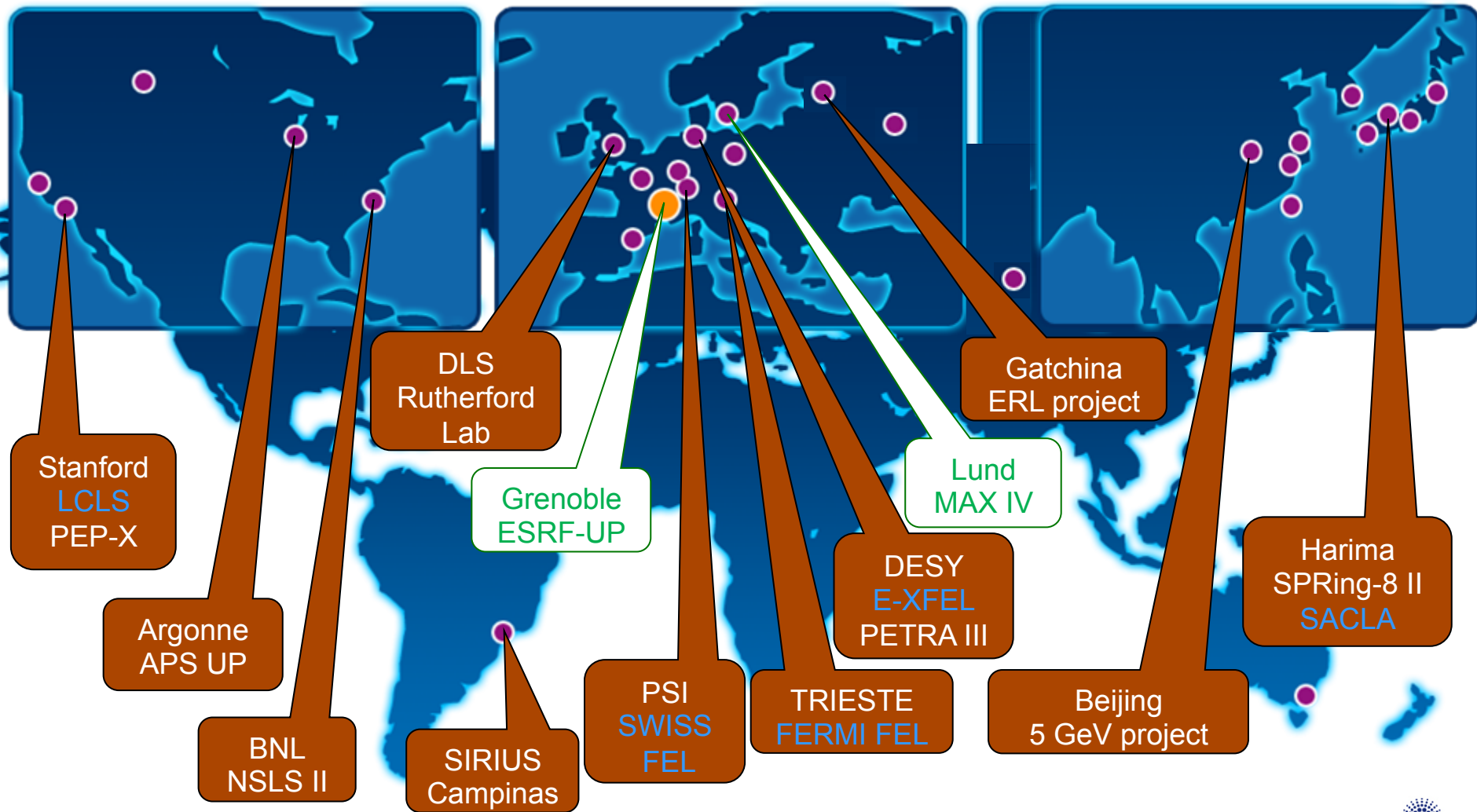


Upgrades of existing sources and future storage rings for new synchrotron science (**ESRF**, PETRA III, APS, Spring-8, ...)

New, better science



Major new projects in X-ray science 2012





Low Emittance Rings 2014 Workshop 17 -19 September 2014 INFN - LNF – FRASCATI - ITALY

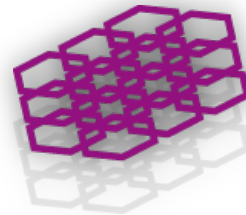
- MAX-IV, ESRF-II, APS-II, SPRING-8-II (SPRING-6?)
- DIAMOND-II, ELETTRA-II, ANKA-II, SLS-II, etc.
- SIRIUS, BAPS, etc.

ESRF Upgrade Programme: *X-ray nano-beams for science*

Objective: a new generation of instruments for *frontier and applied science* in condensed matter, materials, and living matter.

New beam lines and a brighter, and more coherent and stable source

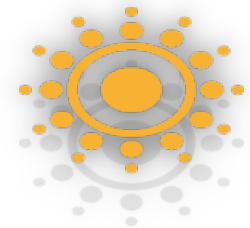
Advanced materials



Health & life sciences



Energy research



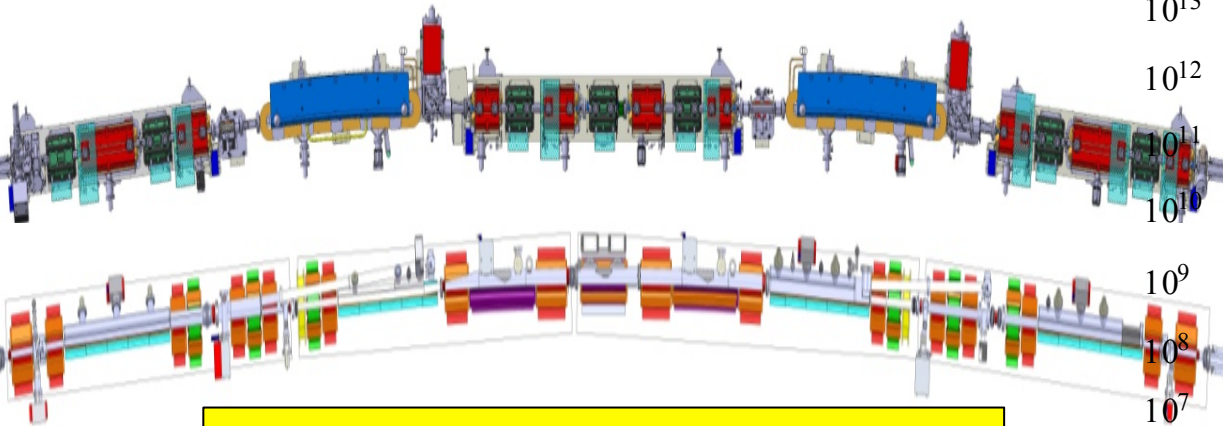
2007

- ❖ Science and technology at the atomic scale
- ❖ Biology and time-resolved science
- ❖ Soft matter and imaging of biological samples
- ❖ Materials and chemistry
- ❖ Earth environment and extreme condition science

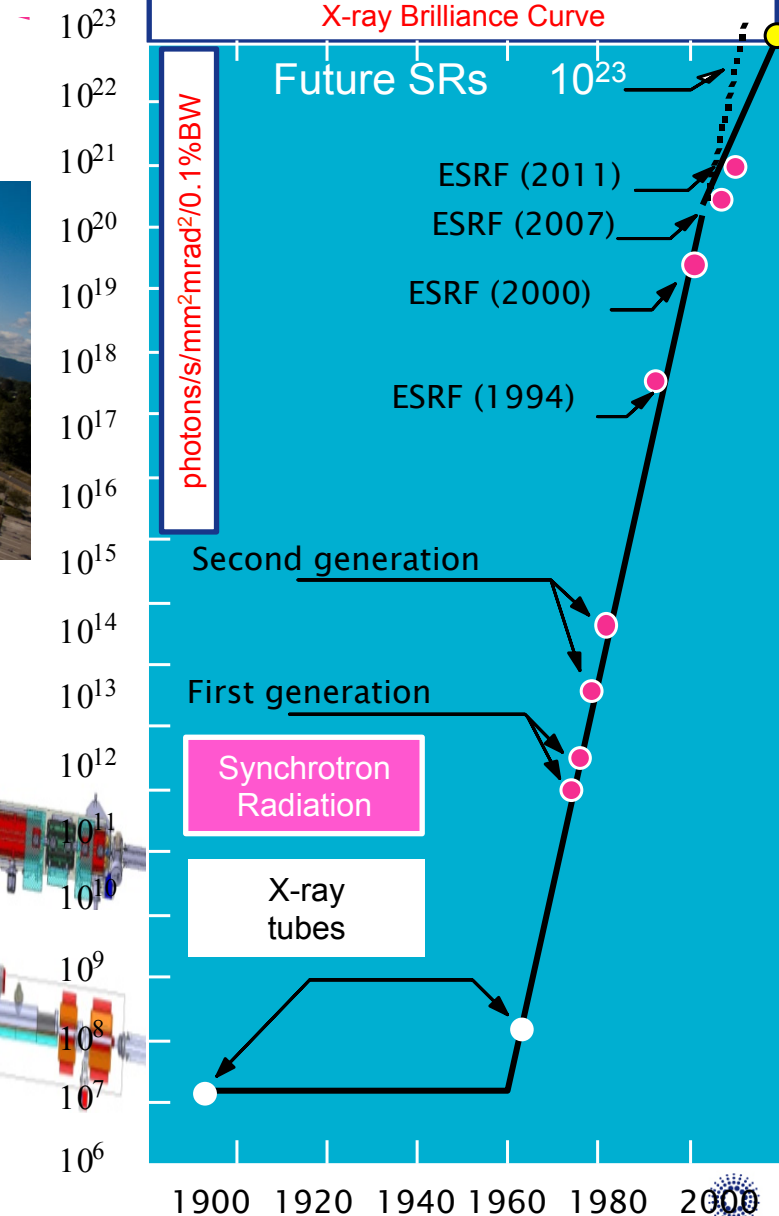
ESRF Upgrade Programme Phase II (2015-2022)



Present ESRF Lattice: $\epsilon_x = 4 \text{ nm}$

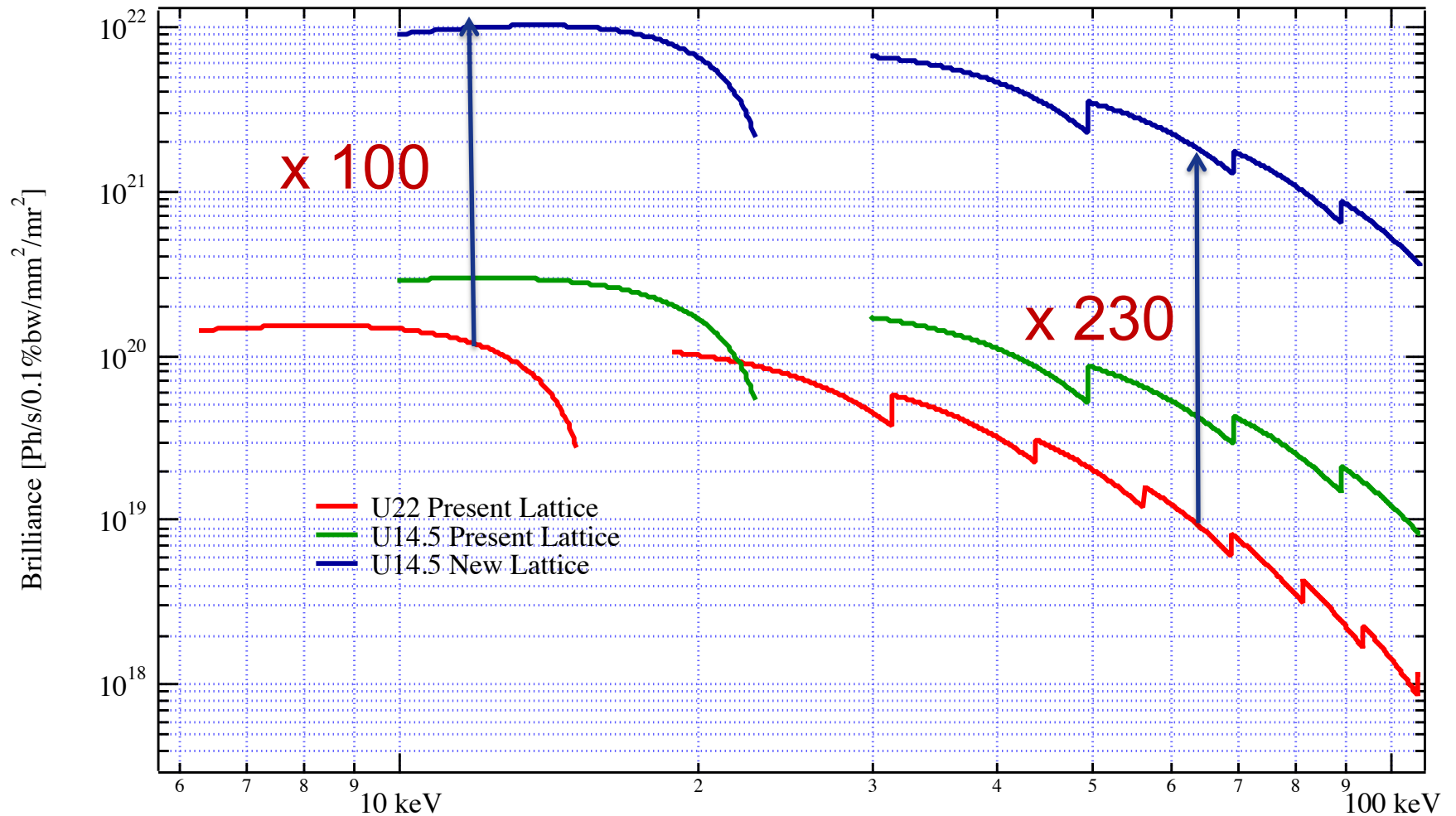


Low Emittance Lattice: $\epsilon_x = 0.15 \text{ nm}$



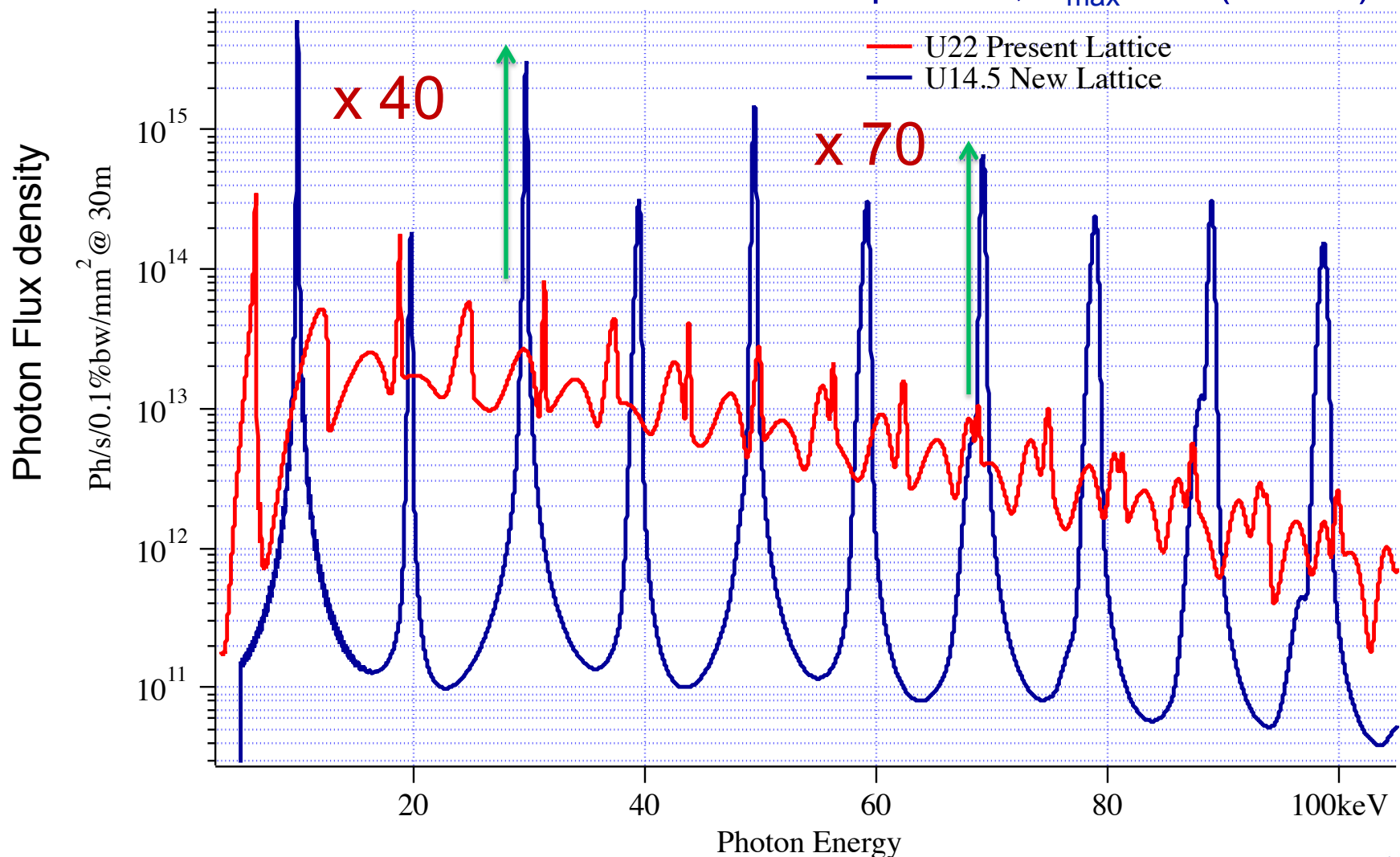
2 m IVUs & CPMUs: U22 Min. Gap 6 mm, $K_{max}=1.7$

U14.5 Min. Gap 4 mm, $K_{max}=1.7$ (CPMU)



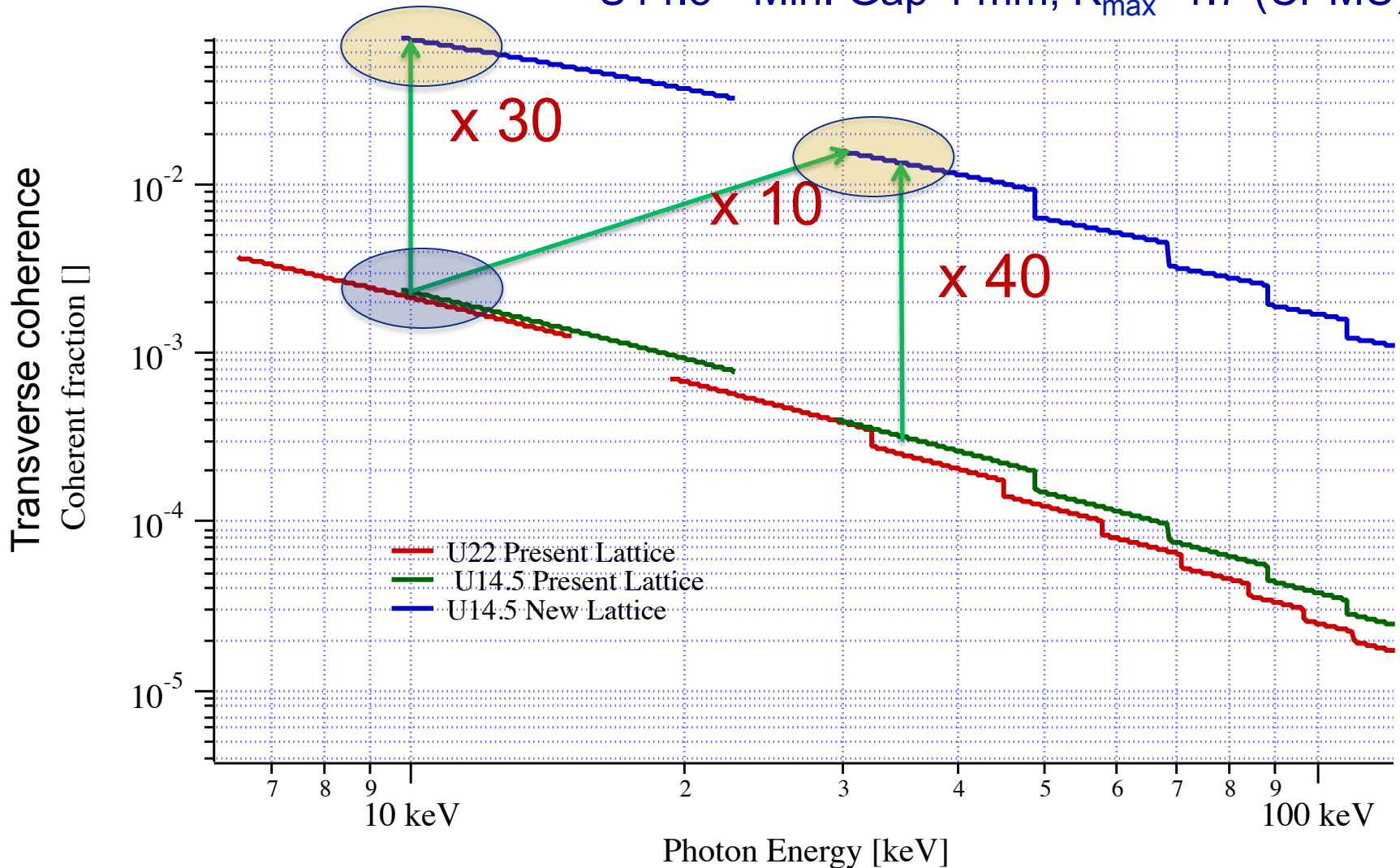
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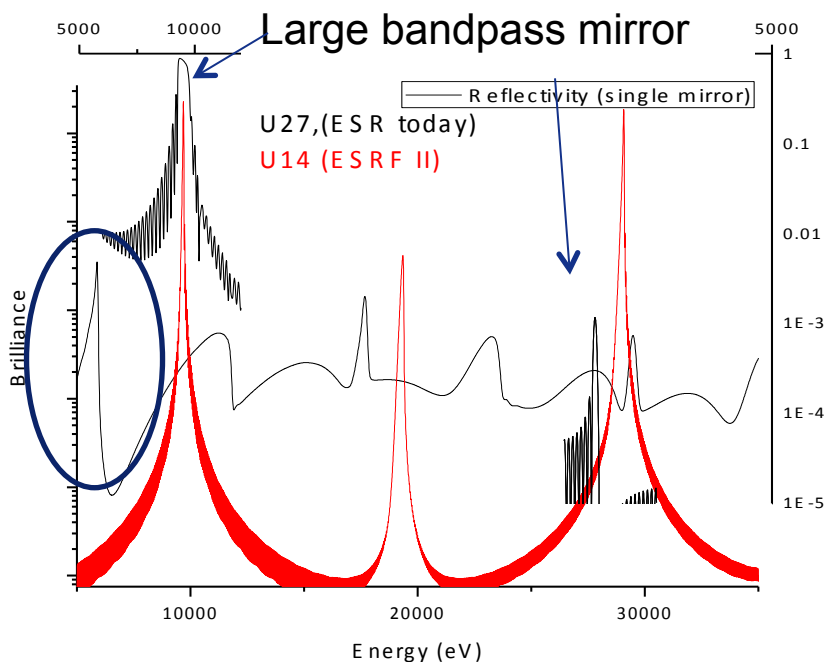
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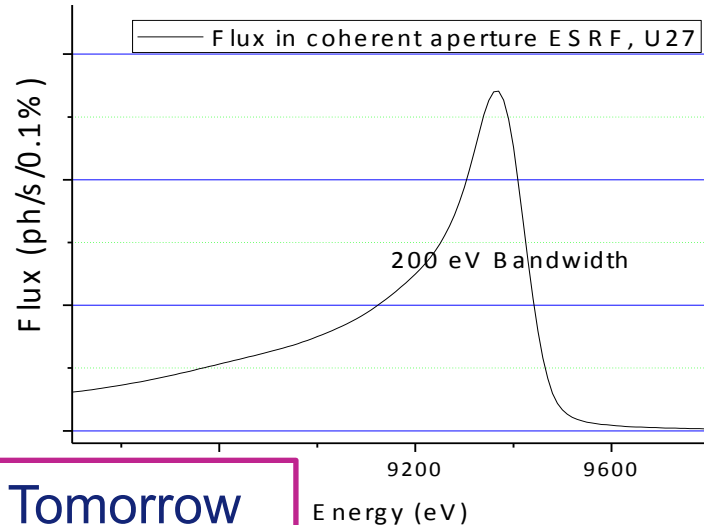


COHERENT FLUX FOR SHORT COHERENCE LENGTHS (NANO PARTICLES!):

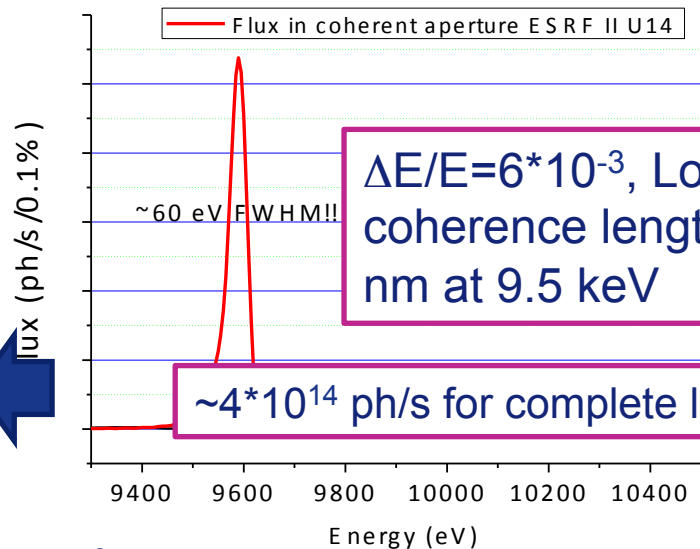
Today's flux inside the coherent aperture at 9.5 keV:



Pink beam (20 nm long. coh. length)
coherent flux x2000 !!



Tomorrow



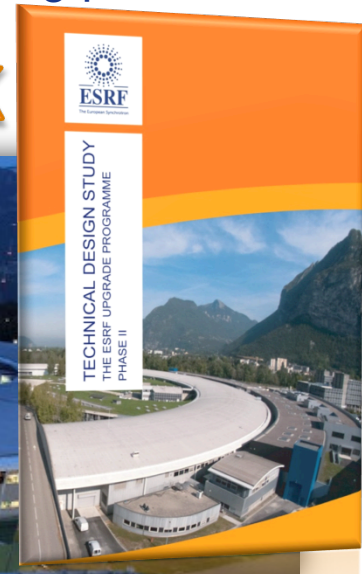
ESRF UP Phase II

A NEW LOW-HORIZONTAL-EMITTANCE LATTICE

from 4 *nm* to ~0.1 *nm*

- Increased brightness and coherent fraction (*x40 ++ on IDs and x60 on BMs*)
- Substantial reduction of the total power on beam line optics
- Power density increase by not more than a factor of ~2 (IDs) and ~6 (BMs)
- Possibility of substantial increase in (coherent) flux using pink beams

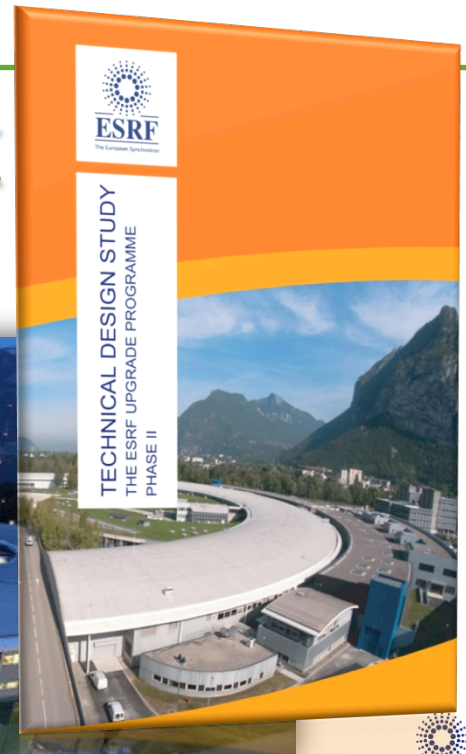
Orange Book



ESRF Upgrade Programme Phase II (2015-2022)

- New lattice for the storage ring (2015-2020)
- Four new beamlines (2018-2022)
- Scientific Instrumentation (2015-2022): New detector programme; IT infrastructure for handling large data volumes

Orange Book



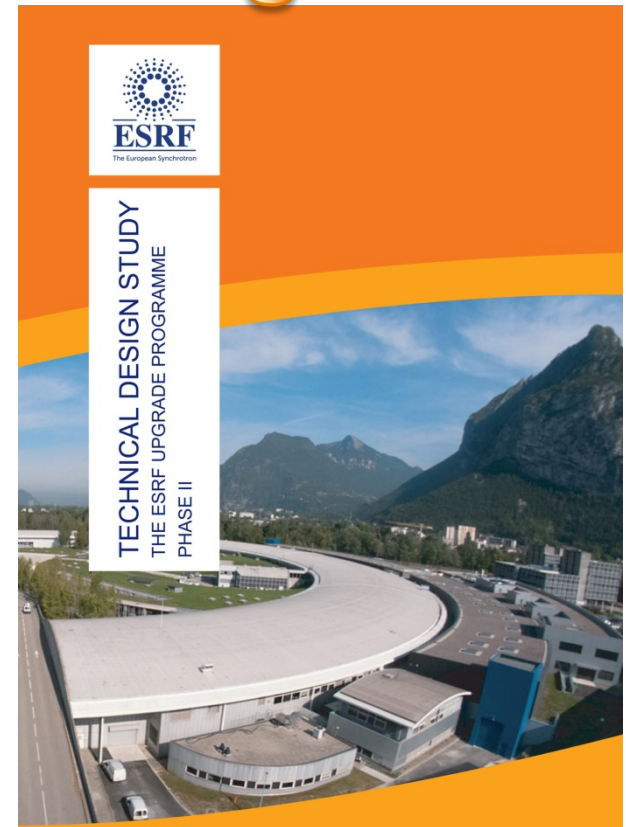
ESRF Upgrade Programme Phase II (2015-2022) – Preparation

Orange Book

13 September 1976 1st meeting of a working group on "Synchrotron Radiation" created by the European Science Foundation (ESF)

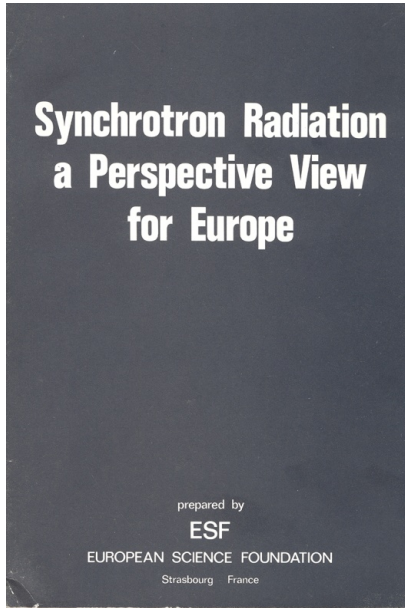
Chairman: H. Maier-Leibnitz

1. December 1977: **BLACK BOOK**
2. May 1979: **BLUE BOOK** (Ed. Y. Farge)
3. December 1982: **YELLOW BOOK** (Ed. J. Als-Nielsen)
4. October 1984: **GREEN BOOK** (Eds. B. Buras, S. Tazzari)
5. February 1987: **RED BOOK** (Foundation Phase Report) submitted to the Council
6. October 2007: **PURPLE BOOK** (2009-2019 ESRF Science and Technology Programme)
7. June 2014: Draft **ORANGE BOOK** (ESRF UP Phase II)

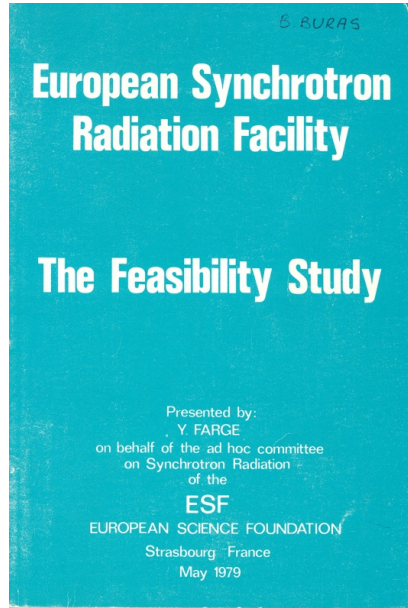


2014

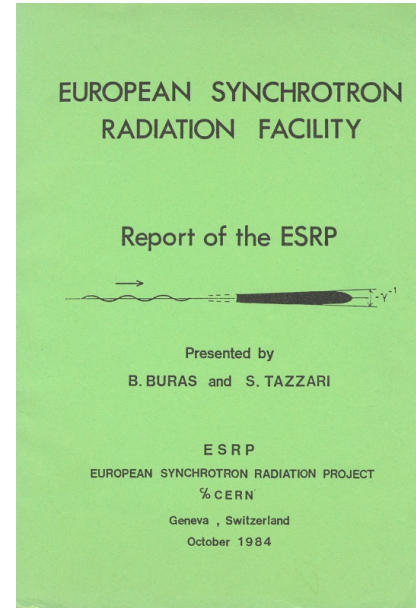
38 YEARS OF ESRF HISTORY



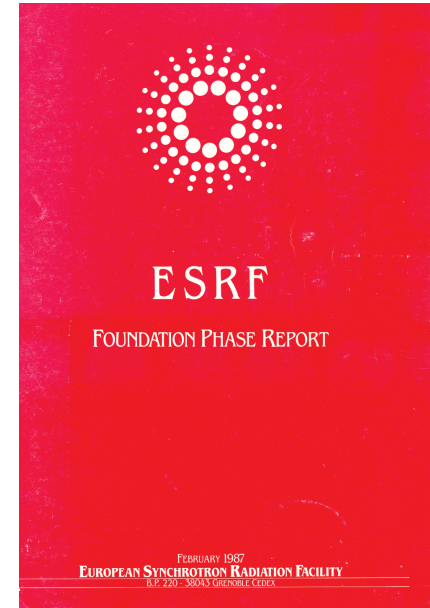
1977



1979



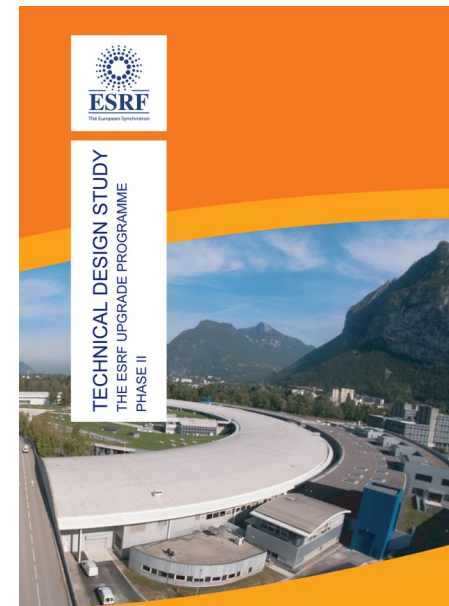
1984



1987



2007



2014

Complement to the Council Resolution of 17 June 2008
on the Upgrade Programme: **APPROVED on 24 June 2014**

The ESRF Council
- at its 61st meeting -
launched
the UP PHASE II

Complement to the Council Resolution of 17 June 2008 on the Upgrade Programme: **APPROVED** on 24 June 2014

➤ DELIVERABLES:

The second part of the Upgrade Programme (“UP Phase II”) shall include, as specified in the ESRF UP Phase II Technical Design Study Report (the “Orange Book”):

- A new hybrid multiple bend achromat lattice for the ESRF storage ring;
- 4 new beamlines;
- Scientific instrumentation for a new detector programme; IT for Large Data Handling

➤ TIMELINE:

The UP Phase II shall be completed by the end of 2022

➤ COST:

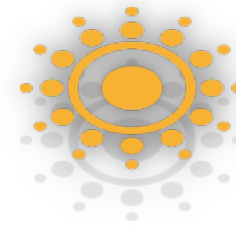
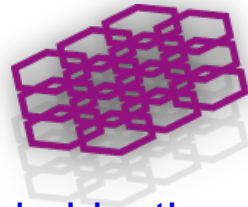
The UP Phase II will cost 149.1 M€

➤ ANNUAL CONTRIBUTIONS:

The total annual Members’ contributions during the UP Phase II (2015-2022) should be stable and remain constant at the level of 2014 (at 2014 prices)

ESRF Upgrade Programme

X-rays for science in the mesoscopic regime
beyond optical imaging – approaching e-microscopy



Challenges and objectives:

- enhancing human health
- developing a sustainable economy with new tools
- exploring unknown territories



Understanding (embedded) structures
down to the atomic level
within multiscale structural hierarchies

Phase I of the ESRF Upgrade Programme has
prepared many beamlines for this task

- with limitations in
- Brightness (~95% loss in nanobeams)
 - Coherence (0.2% at 10 keV)

Structure and Dynamics of Functional Biological Units

From serial crystallography to molecular machines in functional biological cells

Bio-regeneration, Evolutionary Biology, Hierarchical (composite) Materials

Time-resolved bio-response of organisms to exogenous materials



Earth & Planetary Science Novel states of matter

Revealing hidden stories of Nature with a diffraction-limited X-ray Source

Energy Science Catalysis, Materials Processing

Diffraction-limited sources: opportunities for in-situ studies

Nanotechnology, Information technology, Quantum computing
5D diffraction imaging of electronic devices and nanostructures

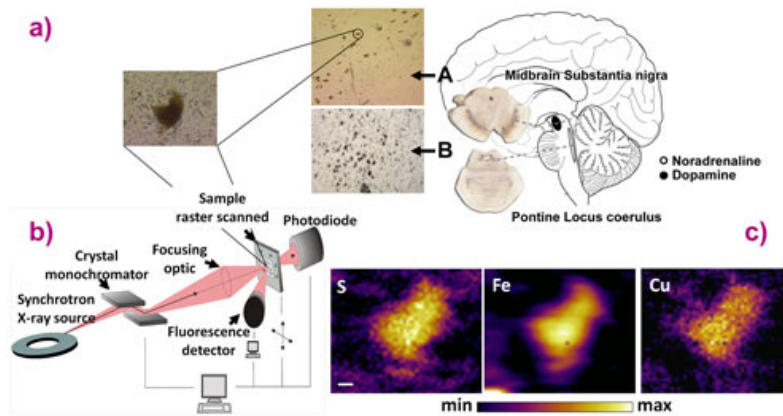
Interactions between biological systems

Opportunities

- Probing the bioresponse to exogenous materials with ultimate sensitivity and resolution
- Multiscale analysis of heterogeneous materials
- Low-dose *in vivo* tomography of living organisms

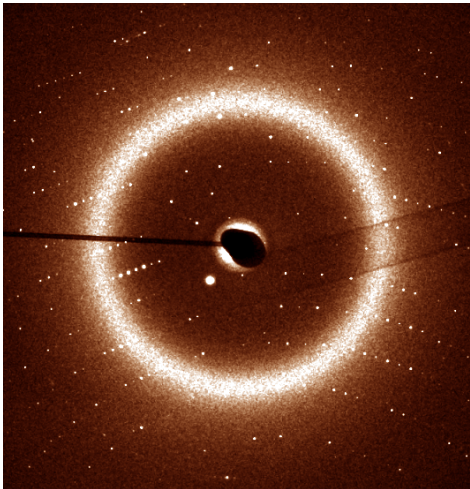
One of the big challenges for our aging societies: Degenerative diseases
Alzheimer's disease, Parkinson's disease

Copper pathology in vulnerable brain regions in Parkinson's disease



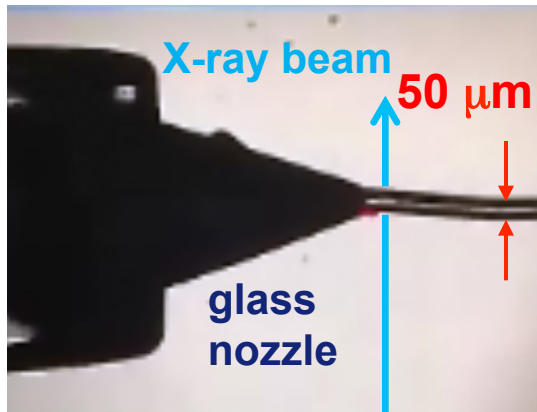
Davis *et al.* 2014, Neurobiology of Aging

Limitations	Solution
spatial resolution	higher brightness
detection limit	higher brightness
radiation damage	better detectors
data analysis	IT and software



Membrane-Protein Serial Micro-Crystallography using Synchrotron Radiation and a Liquid Cubic Phase Injector

MICRO-BEAM LCP-INJECTOR SETUP AT ID13

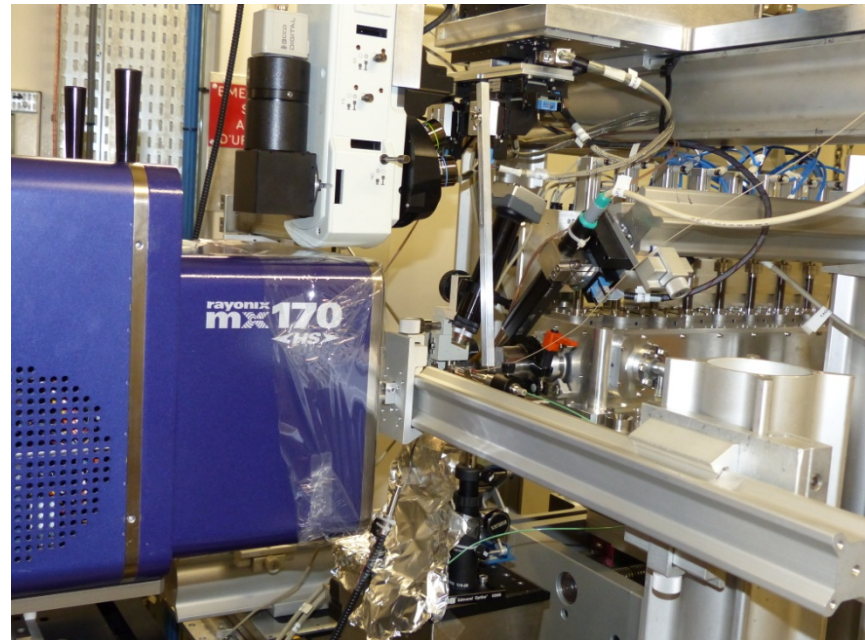
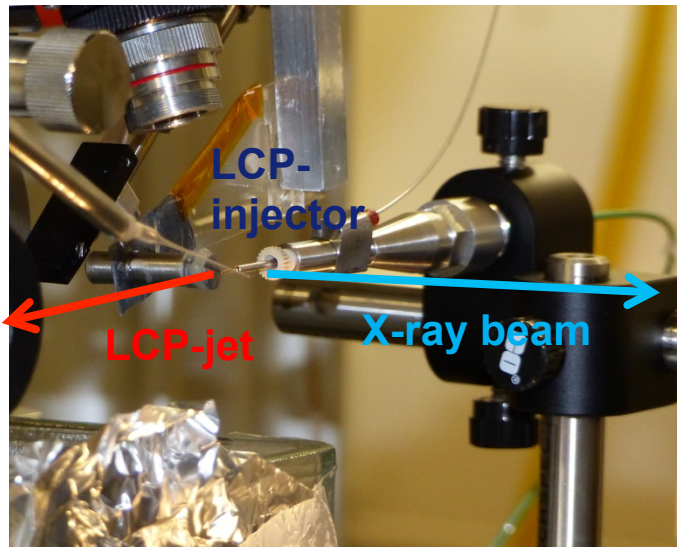


liquid cubic phase (LCP) injector in operation

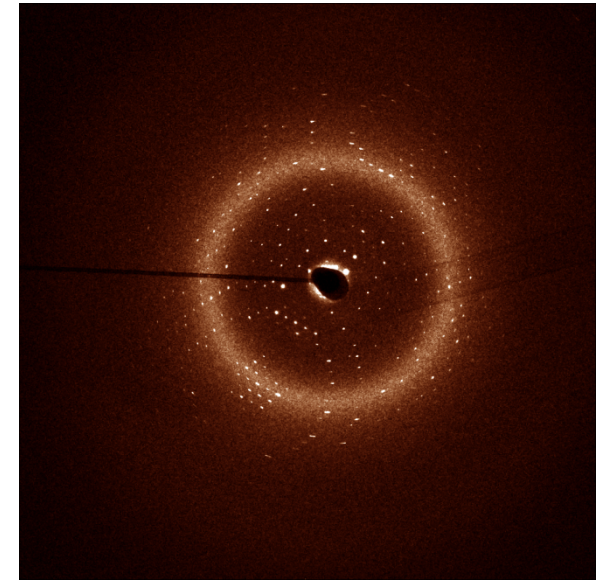
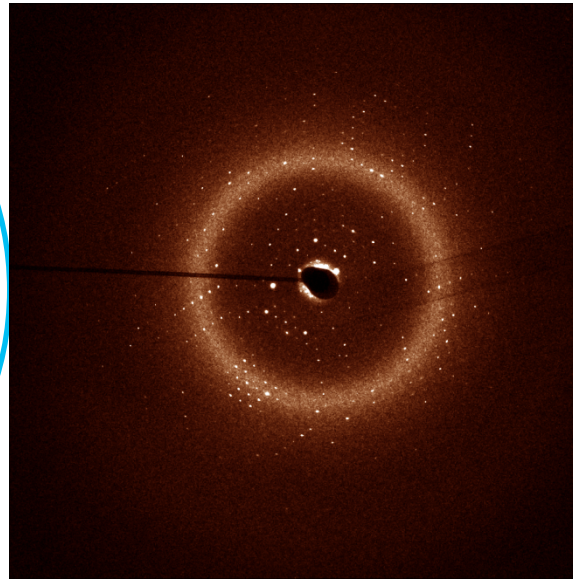
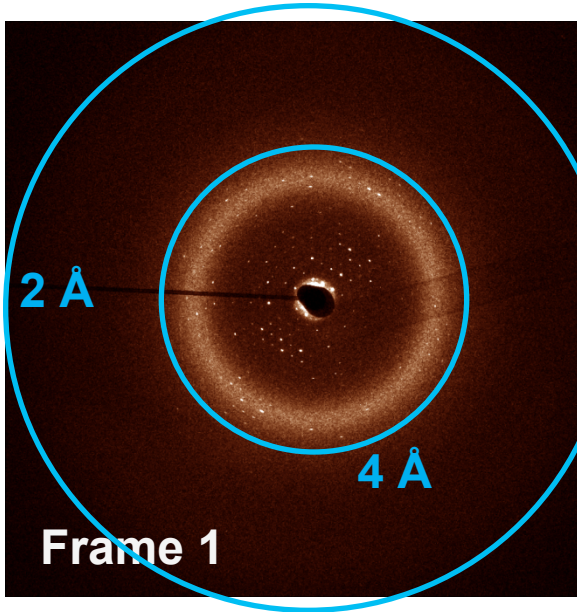
- pressurized via HPLC pump
- helium mantle stream
- LCP-jet with 50 μm diameter
- velocity of LCP-jet: 100 $\mu\text{m}/\text{sec}$

Weierstall et al.: Nature Communications (2014) 5, 3309

micro-beam 13 keV, 8×10^{11} ph/sec
3x2 μm^2 (FWHM HxV)



BACTERIORHODOPSIN MICRO-CRYSTAL FLY-BY IN 3 SUBSEQUENT FRAMES



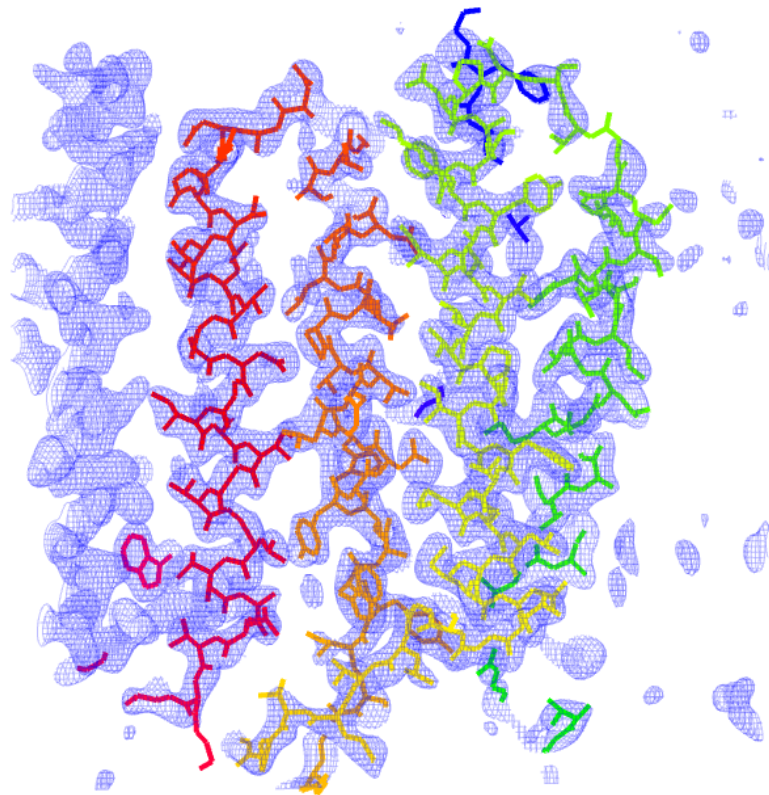
exposure: 25 ms

overhead: 75 ms

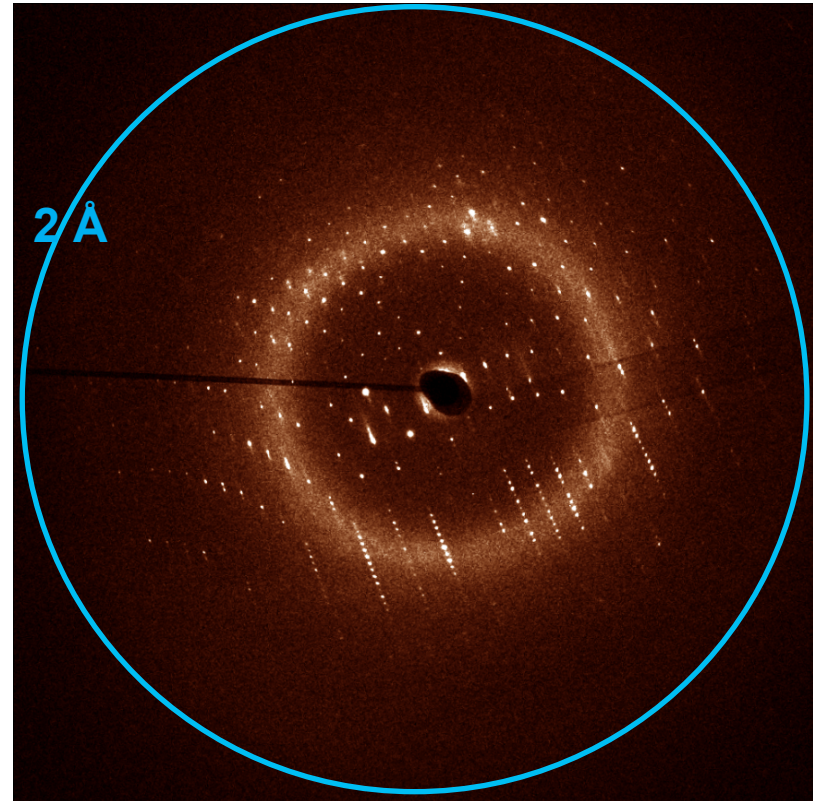
EIGER 4M
(3 μs overhead)

Average travel per 25 ms exposure: 2.5 μm
Crystal detected in 3 subsequent frames
>> crystal size ~ 30 μm
(preliminary evaluation:
Typical hit rate in the percent range limited
by overhead and crystal concentration)

foreseen for Spring 2015 at ID13:
EIGER 4M pixel array detector for
quasi-continuous exposure @ 750 Hz
80-90 % of the sample could be used
ESRF storage ring upgrade (white paper)
>> μs exposure possible



Preliminary data analysis and structure refinement of **Bacteriorhodopsin membrane protein test crystals from synchrotron LCP-jet serial data at ID13 (electron density map current resolution 2.7 Å)**

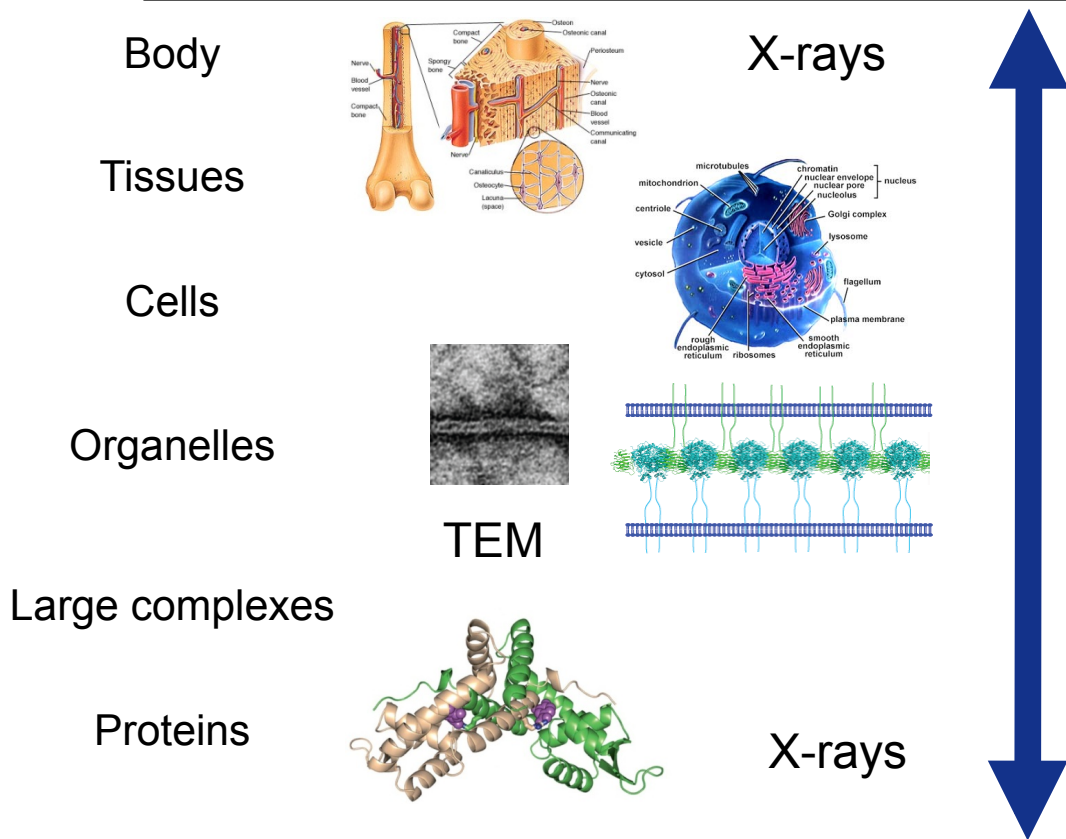


Acknowledgement:

*R. Neutze (Gothenburg univ., S): main proposer and coordinator of Marie-Curie ITN “NanoMem”
Moraes I. (Imperial college, diamond light source, UK): scientific coordination of MI-1178 beamtime
Weierstall et al. (Arizona State University, USA): LCP-injector
Schertler G., Standfuss J., et al. (PSI, CH): structure refinement, BR-sample preparation
Chapman H., White T., et al (Desy/Petra/C-FEL , D): serial crystallography data reduction*

Structural and functional biology: New opportunities at cellular and molecular levels

- Opportunities
- *Ab initio* crystal structure determination of large protein complexes
 - Room temperature serial protein crystallography of microcrystals
 - High resolution imaging of cells and probing protein structural dynamics during physiological activity

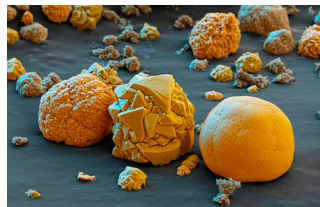


Limitations	Solution
spatial resolution	coherence
radiation damage	better detectors
data analysis	IT and software

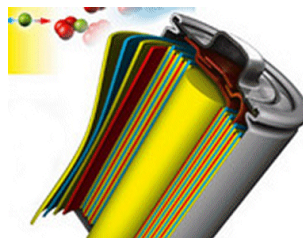
In situ materials chemistry

Opportunities

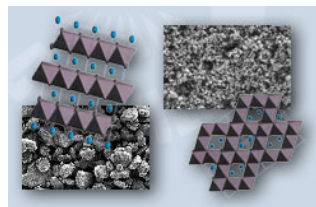
- Materials chemistry of devices to solve grand challenges in clean energy provision and transport
- A 'chemically resolved X-ray vision' on working catalysts and devices for a green energy economy
- Understanding and optimising complex devices on realistic time scales



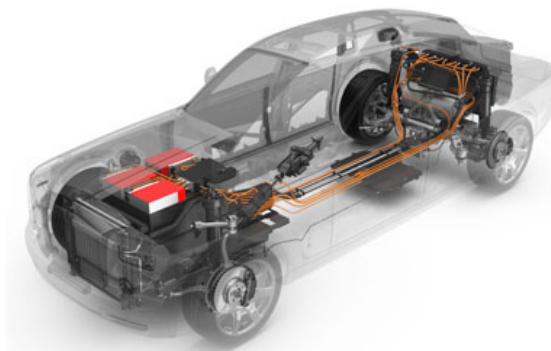
new materials:
characterisation



Ni-Co-Ma compounds for electrodes



device development:
in-situ studies



LiFePO₄ cathode material

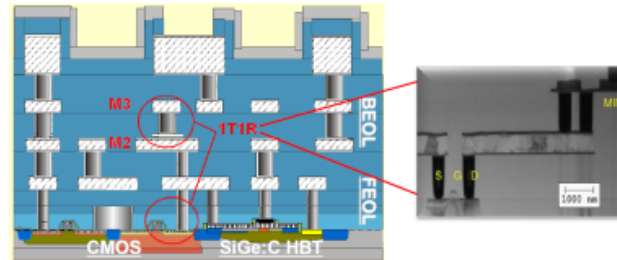
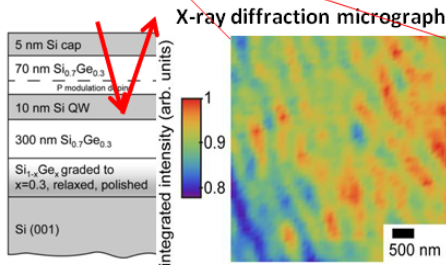
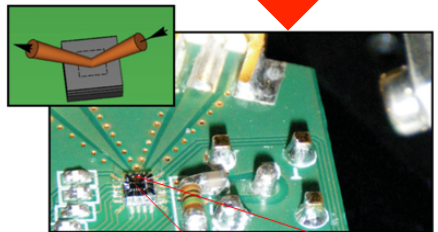
Limitations	Solution
spatial resolution	brightness
time resolution	brightness
penetration	high energy
data analysis	IT and software

Nanomaterials for technology

Opportunities

- *In situ* imaging of strain and chemical composition in biocompatible sensors
- Device imaging and failure analysis under operating conditions: from solar cells to quantum computers
- Three dimensional imaging of nano-electronic building blocks

Strategy for European Semiconductor Industry: more than Moore



back-end of line integration of non volatile RRAM into a SiGe BiCMOS chip technology for system on chip solutions

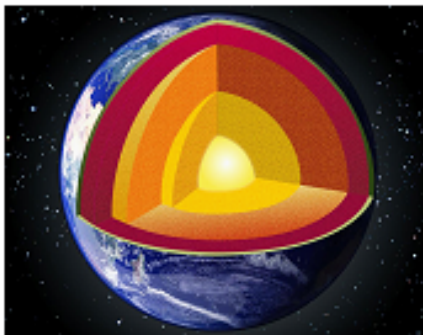
quantum computing device
Evans et al. (2012)
Advanced Materials

Limitations	Solution
spatial resolution	coherence
strain resolution	coherence
time resolution	brightness
data analysis	IT and software

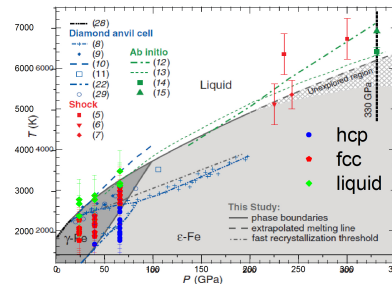
Matter at extreme pressures and temperatures

Opportunities

- Probing structural complexity and its relation to, e.g. superconductivity and quantum phenomena
- Imaging materials complexity in the TPa regime at the nanoscale
- Understanding the structure and dynamics of Earth's and Exo-planets deep interiors



Phase diagram



Creating thermodynamic conditions that exist only in a very small volume and/or for a very short time

Limitations

beam size

time resolution

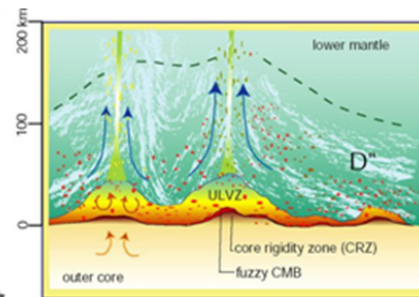
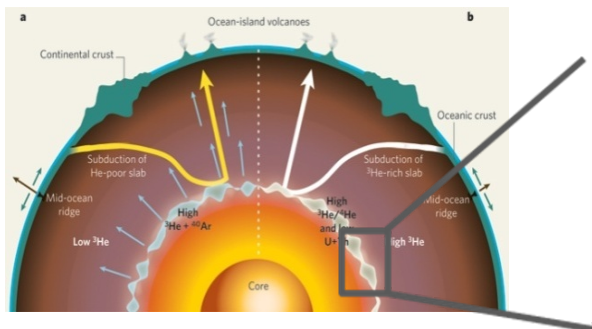
data analysis

Solution

brightness

brightness

IT and software



Experimental Challenges

Managing Radiation Damage:

- New Detector Technologies
- Smart automation and data collection strategies
- Data management: flow control, collection, storage, analyses

Enabling Technologies:

- *nano*-mechanics, -positioning, -optics, etc.
- Software, software and software





ESRF: preparing the next 20 years of excellence in synchrotron science

- A new page in X-ray science:
 - intense – stable – coherent X-ray nano-beams to unveil the mysteries of materials and living matter in the lengthscale gap between optical and electron microscopies: 1-1000 nanometers*
- An ambitious Upgrade Programme delivering by 2022:
 - a new low-emittance storage ring for a qualitatively brighter source*
 - a new portfolio of revolutionary instruments*
 - an extraordinary scientific instrumentation programme*
- Continue to serve the scientific community of the Partner Countries on the analytical characterization of materials and living matter:
 - new generations of efficient, sustainable materials*
 - new pharmaceutical products and medical treatments*
 - new understanding of the world surrounding us*



ESRF: preparing the next 20 years of excellence in synchrotron science

- A new page in X-ray science:
intense – stable – coherent X-ray nano-beams to unveil the mysteries of materials and living matter in the lengthscale gap

An exciting context for the next 15-20 years!!

an extraordinary scientific instrumentation programme

- Continue to serve the scientific community of the Partner Countries on the analytical characterization of materials and living matter:
 - *new generations of efficient, sustainable materials*
 - *new pharmaceutical products and medical treatments*
 - *new understanding of the world surrounding us*



Thank you for your attention!

A Light for Science

