Frontiers of High Pressure Research at the European Synchrotron Radiation Facility

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OUTLINE

- Static High Pressure Research: status and trends
- Dynamic Compression: recent developments, future plans
- The EBS
- Extreme Conditions Science at EBS
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High Pressure at ESRF Today

**ID06, ID15B, ID27:** X-ray Diffraction – Structure, Crystallography, Strain, Deformation, …

**ID18:** Nuclear Resonance Scattering - Magnetism, Phonons

**ID20:** Resonant Inelastic X-ray Scattering - Electronic and Magnetic Structure

**ID28:** Inelastic X-ray Scattering, Diffuse Scattering – Phonons

**ID12, BM23, ID24:** XAS, XMCD - Local and electronic structure, Magnetism, …

**ID02, ID26, ID11, ID16B, BM01, BM30, ID09B, ID19, …**

ID20: 72 Analysers and Panoramic DAC
Static High Pressure Facilities

- Diamond Anvil Cell - $P < 300 \text{ GPa} \ (1 \text{ TPa})$
- Paris-Edinburgh Press (ID27 and BM23) – $2 \text{ mm}^3$ – $P < 17 \text{ GPa}, T < 1800 \text{ K}$
- Large Volume multi-anvil Press (ID06) – $50 \text{ mm}^3$ – $P < 20 \text{ GPa}, T < 2500 \text{ K}$
STATIC HIGH PRESSURE FACILITIES

Static field - 8 T

Pulsed Magnetic field - 30 T

Low T - 2 K

Resistive heating - 1300 K

Laser heating - 5000 K

Gaston Garbarino
Tuesday 18 June 12h00

Jeroen Jacobs
Thursday 20 June 11h00
1. The quest for metallic solid Hydrogen

2. Pressure-induced reactivity of rare gases

3. Superplumes at the Core-Mantle Boundary
NRS observes appearance of superconductivity in H$_2$S at HP

Direct observation of Meissner effect in H$_2$S compressed to 153 GPa

Troyan Science 2016

Expulsion of magnetic field in H$_2$S by monitoring NRS from $^{119}$Sn sensor
Synthesis of FeH$_5$: A layered structure with atomic hydrogen slabs

C. M. Pépin,$^{1,2,6}$ G. Geneste,$^1$ A. Dewaele,$^1$ M. Mezouar,$^3$ P. Loubeyre$^{3,*}$

- Planes of atomic H
- Potential high Tc superconductor

Pépin Science 2017
Chemistry of Xenon at Megabar Pressure

Synthesis and stability of xenon oxides Xe₂O₅ and Xe₃O₂ under pressure

Agnès Dewaele*, Nicholas Worth², Chris J. Pickard³, Richard J. Needs⁴, Sakura Pascarelli⁵, Olivier Mathon⁶, Mohamed Mezouar⁷ and Tetsuo Hirunek⁸

Xe [Kr] 4d¹⁰s² 5p⁶

Stability of xenon oxides at high pressures

Dewaele Nature Chemistry 2016
STRUCTURAL CHANGES IN $\text{SiO}_2$ DOWN TO THE CORE MANTLE BOUNDARY

Magma properties at deep Earth’s conditions from electronic structure of silica

S. Petitgirard$^{1*}$, C.J. Sahle$^2$, C. Weis$^3$, K. Gilmore$^2$, G. Spiekermann$^4$, J.S. Tse$^5$, M. Wilke$^4$, C. Cavallari$^2$, V. Cerantola$^2$, C. Sternemann$^3$

Petitgirard Geochemical Research Letters 2018
STATIC COMPRESSION AT SYNCHROTRONS TODAY

XRD 1.3 Mbar 4300K

Intensity (arbitrary units) vs 2θ (degree)

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XMCD 2 Mbar

Normalized XANES vs Energy (eV)

---

XRD 7 Mbar

Normalized XMCD *10^-3 vs Energy (eV)

---

Single Crystal XRD

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Nuclear Resonance Scattering

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Anzellini Science 2013

Torchio PRL 2011

Dubrovinsky Nature 2015

Spaulding Nature Comm. 2014

Troyan Science 2016
Static compression with LH–DAC covers Earth’s core conditions

~ 360 GPa, 5500 K

1. What is the stability limit of hcp phase in solid Fe?
2. What is the local structure in the liquid?
3. What is the nature of ion-ion correlations in the WDM regime?

Can we create and probe WDM at the synchrotron, with data quality as “at ambient”?
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Go more extreme → TPa & eV

- Conditions beyond those existing in our planet → Input for planetary models
- Synthesis of novel materials
- Reveal new physical chemistry

Al @ 1TPa

Explore the time scale of high pressure phenomena → ns

Dynamic behavior of matter and materials under high strain rates
- Mechanisms and nucleation of phase transitions
- Yield strength (dynamics of dislocations)
- Nanostructuration, amorphisation, metastable phases

Particle ejection

Heterogeneous media

Ensemble Poitiers

ISP Imperial London
A synergetic approach to dynamic compression at ESRF

Probing local and electronic structure in Warm Dense Matter: single pulse synchrotron x-ray absorption spectroscopy on shocked Fe

Olbinado J. Phys D 2018

Probing the early stages of shock-induced chondritic meteorite formation at the mesoscale

M. Mezouar

O. Mathon

R. Torchio

A. Rack

multi-technique approach

M. Wulff
HPLF-I (2018-2021)
Couple a 100 J (upgradable to 200 J) ns-shaped laser to XAS on ID24

In Construction

HPLF-II (from 2023)
Extend to XRD, XRI, XES on ID23
Laser upgrade

EBS Beamline program
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DIFFRACTION LIMITED STORAGE RINGS

MBA

DBA

Advanced Photon Source

ESRF

SACLA

MAXIV

LNLS

DESY

Page 20  Frontiers of High Pressure Research at the ESRF | Hands on ! High-pressure techniques at the ESRF-EBS | 17 June 2019 | Sakura Pascarelli
**GOAL: REDUCE EQUILIBRIUM HORIZONTAL EMITTANCE**

\[ \varepsilon \propto \frac{E_e^2}{(N_{sect} \cdot N_{dipole})^3} \]

<table>
<thead>
<tr>
<th>Field Strength</th>
<th>ESRF today</th>
<th>EBS</th>
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<tbody>
<tr>
<td>0.85 T</td>
<td>0.67</td>
<td>0.18</td>
</tr>
<tr>
<td>0.39 T</td>
<td>0.55</td>
<td>0.2</td>
</tr>
</tbody>
</table>

**EBS lattice**

- Hybrid 7 Bend Achromat = (4 dipoles + 3 dipole-quad + 24 quad., sext., oct.) per cell
- ID length = 5 m

31 magnets per cell instead of currently 17

32 cells (arcs) with 4 girders each
Brilliance

Horizontal emittance

$\varepsilon_x = 4 \text{ nm}$

$\varepsilon_x = 0.15 \text{ nm}$

Coherent Fraction

Pink beams
THE ESRF EXTREMELY BRILLIANT SOURCE (ESRF-EBS)

- photon source **brilliance** (x100)
- coherent fraction of the photon beam (x50)

![Before and after EBS]

![Graph showing photon source brilliance and coherent fraction over years]

**Photons/s/mm²/mrad²/0.1%BW**

- **Ultra low emittance storage ring**
- **4th generation ESRF-EBS**
- **ESRF (2014)**
- **3rd generation ESRF (2014)**
- **2nd generation**
- **1st generation**
- **X-ray tubes**

Frontiers of High Pressure Research at the ESRF | Hands on! High-pressure techniques at the ESRF-EBS | 17 June 2019 | Sakura Pascarelli
# THE EBS PROGRAMME

## SCHEDULE:

<table>
<thead>
<tr>
<th>Year</th>
<th>Event</th>
</tr>
</thead>
<tbody>
<tr>
<td>2017-2018</td>
<td>Delivery of the components, testing, and pre-assembly</td>
</tr>
<tr>
<td>10(^{th}) Dec 2018</td>
<td>End of USM and start of the shutdown</td>
</tr>
<tr>
<td>Jan – March 2019</td>
<td>Dismantling of the storage ring</td>
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<tr>
<td>April – Nov 2019</td>
<td>New storage ring installation</td>
</tr>
<tr>
<td>Dec 2019 – March 2020</td>
<td>Accelerator commissioning</td>
</tr>
<tr>
<td>March – Aug 2020</td>
<td>Beamline restart and commissioning</td>
</tr>
<tr>
<td>25(^{th}) August 2020</td>
<td>Back to full User Operation</td>
</tr>
</tbody>
</table>
Dismantling the historical ESRF storage ring
TEMPORARY STORAGE OF THE ESRF HISTORICAL RING

1700 TONS OF MATERIAL AND 200 KM CABLES
CIVIL WORK AND PREPARATION OF THE TUNNEL

[Images of civil work and preparation of the tunnel]
INSTALLATION OF THE NEW GIRDERS
THE EBS STORAGE RING STARTS TO TAKE ITS SHAPE
EBS – SCIENCE CASE(S) IN BRIEF

- In-situ or operando characterisation
- Coherence based techniques
- Spatial resolution
- Temporal resolution

- New focusing/collimation schemes
- Horizontal diffraction/scattering planes
- Penetration
- Radiation damage

FROM AVERAGED TO SINGLE OBJECT INFORMATION

DYNAMICS

REAL SYSTEMS
EXPERIMENTAL PROGRAM OVERVIEW: 3 INTERCONNECTED SUB-PROGRAMS

EBS Beamlines
- EBSL3: High throughput large field phase-contrast tomography beamline
- EBSL8: Serial crystallography beamline
- EBSL1: Beamline for coherence applications
- EBSL2: Beamline for hard X-ray diffraction microscope

Refurbishment Programme
- CDR4: Surface science
- CDR5: Extreme conditions
- CDR7: High brilliance XAS
- ID21, ID23-2
- ID17, ID18 → ID14
- ID26 optics

Instrumentation Programme
- Detectors
- Monochromators
- BL control system

Data Analysis as a Service
- Data Policy
- Data storage and archiving
- Scientific programming

User Platforms
- Cryo-EM Facility
- High Power Laser Facility

EBS + BL Refurbishment + BL readiness for EBS
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EBSL5:
High flux nano-XRD beamline for science at extreme conditions (ID27)

NRS-EBS:
Pushing the limits of NRS in energy and spatial resolution (ID14)

CDR6:
A worldwide unique facility for XRD, XRI, XES, XAS dynamic compression studies (ID23 and ID24)

EBSL7:
Towards sub-μm, high brilliance EXAFS (ID24)

Horizontal emittance

$\varepsilon_x = 4 \text{ nm}$

$\varepsilon_x = 0.15 \text{ nm}$
Super-Earth planets interiors

New EH4
KB system: 0.2 μm × 0.2 μm

x-ray spectrograph:
energy resolution of 40 μeV

New OH3

Alexander Chumakov
Thursday 20 June 9:45

Elastic properties, sound velocity at Megabars
EBSL5 - SCIENCE UNDER EXTREME CONDITIONS (ID27)

- Materials at and beyond the current limits of static P and high T
  - Double stage Diamond Anvil Cell
  - Solving the fluid H₂ to fluid H transition
  - Fast melting, kinetics of chemical reactions at extreme conditions

Mohamed Mezouar
Tuesday 18 June 9:45

- Structure and chemistry of low Z melts and glasses
  - Exploring extreme temperature states using laser heating

- Rheology of materials at extreme conditions

In situ chemical analysis by nano-XRD and XRF
EBSL7 – Time Resolved and Extreme Conditions XAS

Time resolved & extreme conditions XAS (ID24_ED)

- extreme conditions for geophysics, planetary science, new materials
- magnetic response in the MegaGauss regime
- 3D spatially resolved chemical speciation

Sub-μm, high brilliance EXAFS (ID24_DCM)

- in situ and operando time resolved chemistry
- environmental science
- high pressure, earth and planetary science

Angelika Rosa
Tuesday 18 June 12:15
CONCLUSIONS

• High Pressure Research is, since 25 years, a very important part of the scientific program at ESRF

• Static compression methods are now offered on more than half of the beamlines.

• ESRF offers highly specialized beamlines for studies of matter at extreme P and T, allowing to probe long range order, local environment, electronic, magnetic vibrational properties, charge ordering, …

• We are observing a trend from our user community to push towards dynamic compression, to go to higher P, T values & to start exploring the time scale of high pressure phenomena.

• Dynamic compression methods are being developed on several beamlines, including ID24 (XAS), ID19 (XRI) and ID09 (XRD).

• The EBS will offer orders of magnitude higher flux and brilliance, and will allow us to address outstanding questions in high pressure research that are out of reach today.
ACKNOWLEDGMENTS

M. Wulff (ID09)
A. Chumakov (ID18)
M. Olbinado, A. Rack (ID19)
C. Sahle (ID20)
O. Mathon, A. Rosa, N. Sevelin, R. Torchio (BM23&ID24)
G. Garbarino, M. Mezouar, V. Svitlyk (ID27)
Thank you for your attention