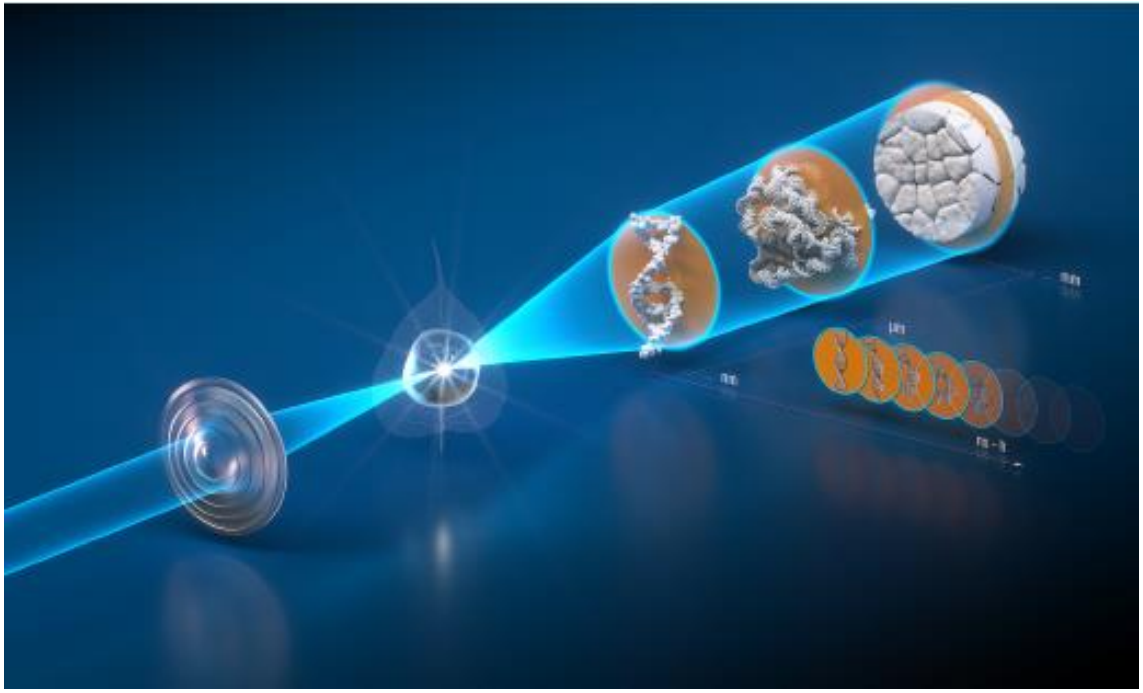
Extreme pressure and temperature research at PETRA IV.



Extreme Conditions Research with a 3D X-ray Microscopes

H. P. Liermann, R. Farla, I. Sergeev, K. Glazyrin

HELMHOLTZ RESEARCH FOR GRAND CHALLENGES

DESY

Extreme pressure and temperature research at PETRA III.

Where can you create high-P and high/low-T at PETRA III:

Dedicated Beamlines:

- **P02.2 => Extreme Conditions Beamline** => dedicated to high-pressure high/low-temperature x-ray diffraction in the DAC => **oversubscribed by a factor of 3 in the last year**
- **P61B Large Volume Press - Extreme Conditions (LVP-EC)** => dedicated to high-pressure -temperature x-ray diffraction in the multi anvil press => starting operation (only 50 %) => already **oversubscribed by a factor of 1.8** (which will certainly increase)

Beamline that have High-Pressure Capabilities (mostly in the DAC):

- **P01 => High Resolution Dynamics Beamline** => Nuclear Resonant Scattering Station & Inelastic X-ray Scattering Station => 15 % high-pressure DAC work
- **P09 => Resonant Scattering and Diffraction Beamline** => resonant scattering capabilities at high-P in the DAC
- **P24 => Chemical Crystallography** => some single crystal diffraction capabilities at high-P in the DAC

Beamlines capable of high pressure, but without own high pressure program

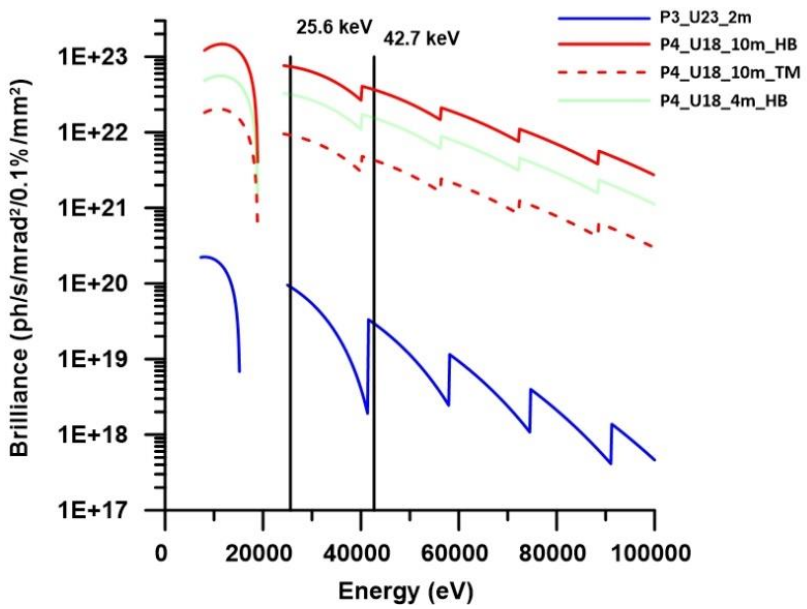
- **P10 => Coherence Application Beamline** => small angle scattering, diffraction at high resolution (large sample-detector distance)
- **P06 => Hard X-ray Micro/Nano-Probe** => scanning for density determination, potentially fluorescence and EXAFS

If we want to meet the ever increasing demands of our user community then we need improve capabilities to conduct Extreme Conditions Research in the future and especially at PETRA IV!

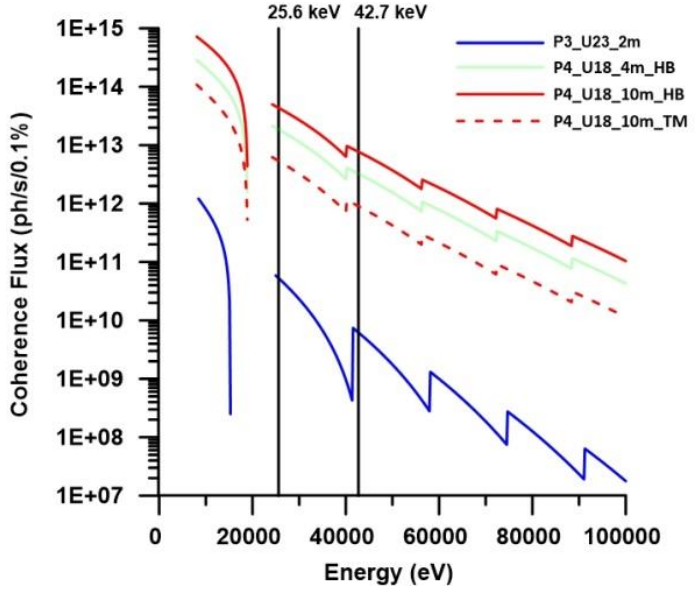
Improved Capabilities for Extreme Pressure and Temperature Research at PETRA IV.

What will the new light source offer: Example P02.2

Brilliance



Coherence



PETRAIII (ε_x=1000pm.rad ε_y=10pmrad) => PETRAIV (ε_x=20pm.rad ε_y=4pm.rad)

Improvements when going from PETRA III to PETRA IV

- Brilliance higher by a factor of 500
- Flux higher by a factor of 30 (U23 2m => PMCU18 4m)
- Coherence higher by a factor of 1000

X-ray techniques relevant to extreme pressure and temperature research that will benefit from the improve properties of PETRA IV.

How the new machine properties transfer into the X-ray techniques!

- **Smaller source size and x-ray beam divergence**
  - ➢ Improved focusing (smaller x-ray beam)
  - ➢ More flux in a smaller x-ray beam (higher brilliance)

All X-ray diffraction and spectroscopic techniques will benefit:

X-ray diffraction (high Energies)
- Powder X-ray Diffraction
- Single Crystal X-ray Diffraction
- Non Crystalline Diffraction

Inelastic Scattering
- Nuclear forward scatteri
- Nuclear Inelastic S
- Synchrotron M ing

scopy
- -ray Fluorescence
- X-ray Absorption Near Edge
- Extended X-ray Absorption Fine Structure
- X-ray Emission Spectroscopy
- X-ray Raman Spectroscopy

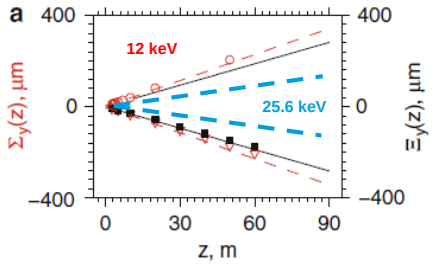
- **More coherent X-ray beam**
  - ➢ Improved transfer coher izontal ~ vertical)
  - ➢ Particular true for

All X-ray imaging benefit

Imaging ticular at high energies)
- Phase aging
- Absorp ontrast Imaging (Radiography)
- Time resolved Micro-tomography
- Near field and far field high energy diffraction microscopy
- Coherent I
- Scanning transmission microscopy
- Ptychography

Combining X-ray Diffraction & Spectroscopy with X-ray Imaging will enable the exploration of several length scales simultaneously (atomistic to meso)

Horizontal ≃ Vertical



Approximation L_{coh} ~ (λ* L)/source size
=> scales linearly with the wavelength

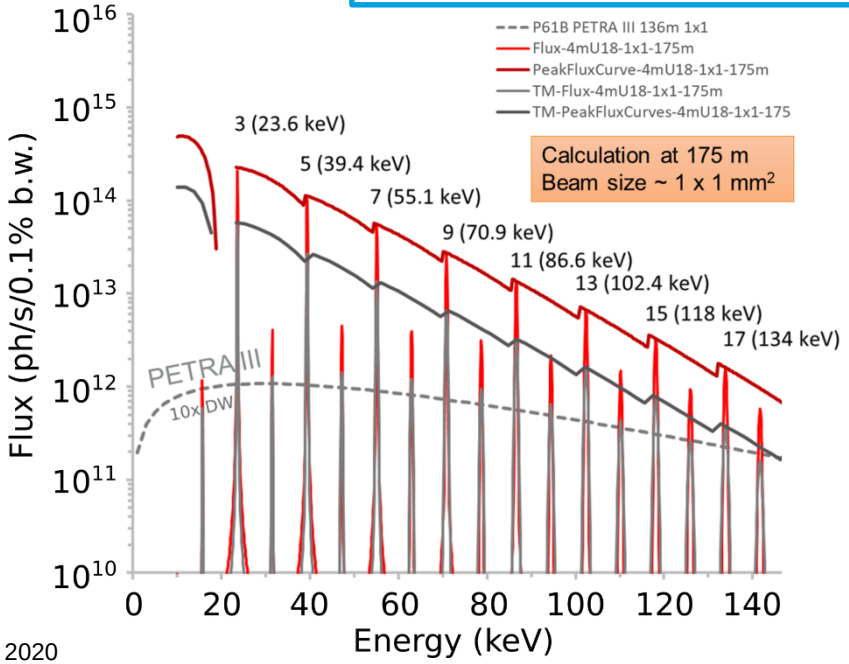
From Vartanyants & Singer (2015)

Proposals for the future P61.B

Scientific Instrument Proposals (SIP) to improve and expand the LVP beamline P61.B

In-situ XRD & imaging at high pressure and temperature using the 6-ram LVP at PETRA IV
(X-ray diffraction and imaging in existing multi anvil technique)
PI: Melanie Sieber / Tomoo Katsura

Planetary melt and liquid studies using a wide-open LVP at high P-T at PETRA IV
(X-ray diffraction & imaging in Paris Edinburgh Press, etc.)
PI: Melanie Sieber / Jean-Philippe Perrillat

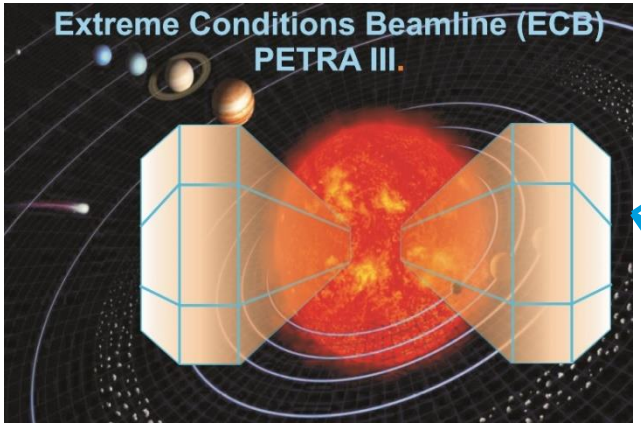


PETRA IV photon flux at 175 m distance in 1 x 1 mm^2 aperture.
- Brightness Mode (200 mA – 1600 bunch)
- Timing Mode (80 mA – 80 bunch).

By tuning the undulator strength parameter, K the **peak flux curve** is obtained for each harmonic.

Proposals for future P02.2

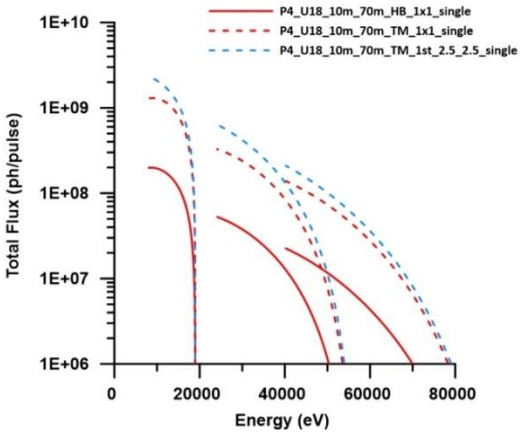
Scientific Instrument Proposals (SIP) to improve and expand the Extreme Conditions Beamline P02.2



High-Pressure High-Temperature X-ray Diffraction and Imaging Microscope
(high energy x-ray diffraction and imaging in the existing high-P & -T DACs)
PI: C. Prescher

Dynamic Compression Microscope
(time resolved high energy x-ray diffraction and imaging in existing dynamic DAC & new laser shock/ramp compression)
PI: D. Kraus

Multiprobe Extreme Conditions Instrument
(x-ray spectroscopy, diffraction and imaging existing high-P & high/low T DAC techniques)
PI: D. Laniel & T. Meier



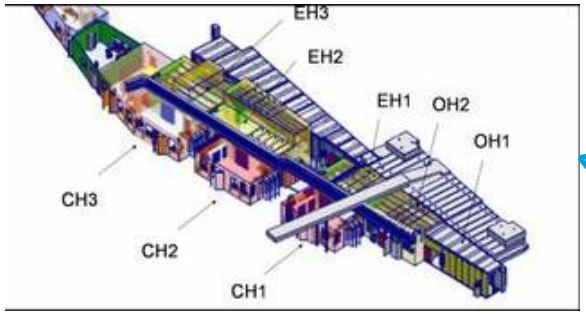
Flux in a single bunch
=> time resolved high energy diffraction in the MHz

PETRA IV for the ECB follow ups

- Brilliance higher by a factor of 500
- Flux higher by a factor of 30 (U23 2m => PMCU18 4m)
- Coherence higher by a factor of 1000

Proposed for future P01

Scientific Instrument Proposals (SIP) to improve and expand the high-pressure and –temperature research at the High Resolution Dynamic Beamline P01.



Electronic structure and bonding properties of light-element compounds under extreme conditions using X-ray Raman scattering and X-ray emission spectroscopy

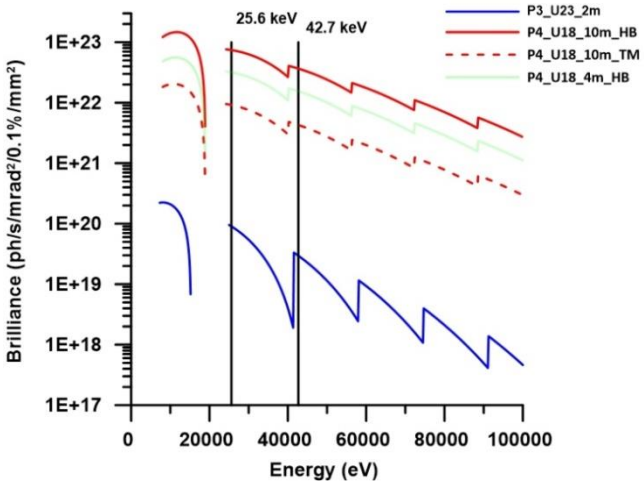
(x-ray Raman and X-ray emission spectroscopy with existing high-P & -T DAC setups)

PI: S. Petitgirard, C. Sternemann, M. Wilke, G. Spiekermann

Nuclear Resonance Scattering at extreme conditions - implications for Earth Sciences

(Nuclear Resonance Scattering with high-P setup)

PI: I. Kupenko



Talks will be in the **"PETRA IV Workshop: Earth, Environment, and Materials for Nanoscience and Information Technology"** (2.-4. Nov. 2020)!

What did we forget?

This is what was suggest for the upgrade of the existing beamlines/instruments but maybe we have overlooked an area of research that should also be included in the existing SIP or that would require an additional SIP!

We are very much interested in synergies

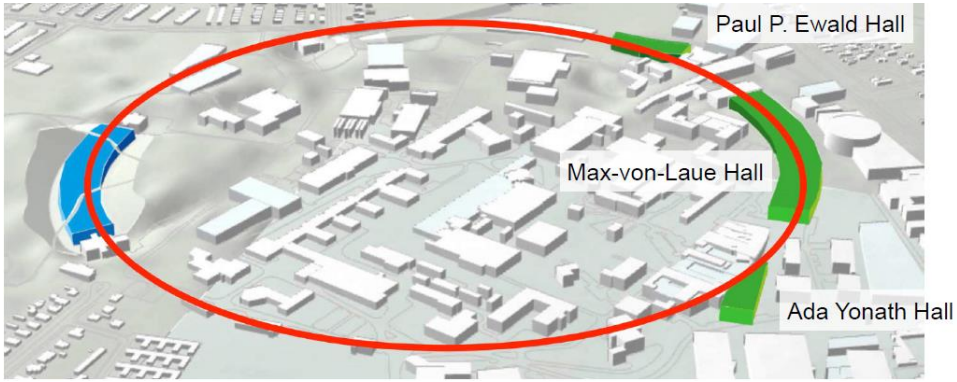
What techniques or sample environments can interact with our proposed SIPs and what communities would be interested in exploring research at the proposed SIPs that are not already covered!

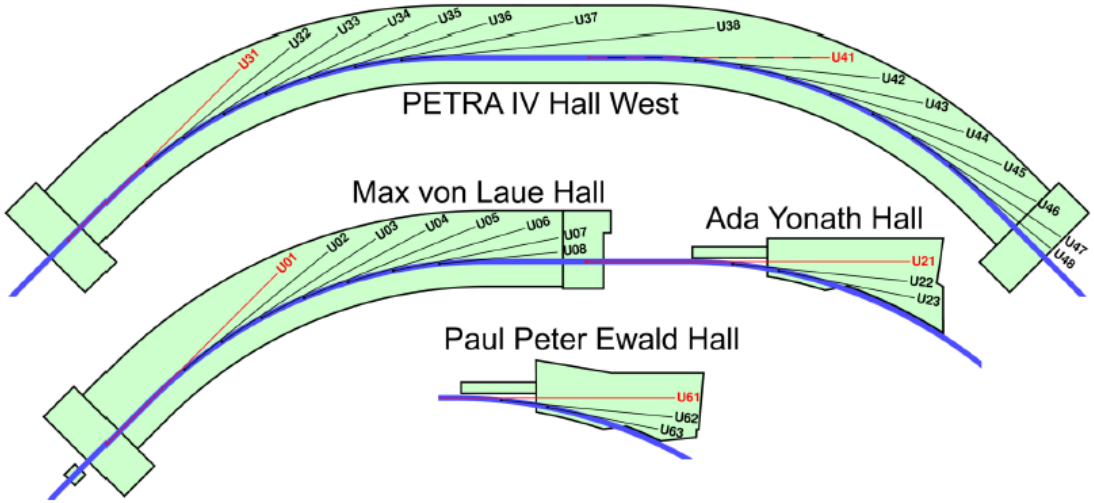
More to come!

There will be another session on extreme pressure and temperature research in the workshop with the area of Earth, Environment, and Materials for Nanoscience and Information Technology (Nov. 2nd-4th). In addition we will have a Satellite Workshop On Scientific Instrument Proposals for Extreme Pressures and Temperatures Research at PETRA IV (Nov. 5-6th) were we will present the SIP (both scientific and instrumental aspects in more detail)

Thank you for your attention!

Proposing SIP for the future research at extreme pressures and temperatures is a real community effort. We thank everyone their contribution.





Total of 30 beamlines