The High Energy Materials Science Beamline (HEMS) at PETRA III

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Abstract. The HEMS Beamline at the German high-brilliance synchrotron radiation storage ring PETRA III is fully tunable between 30 and 250 keV and optimized for sub-micrometer focusing. Approximately 70 % of the beamtime will be dedicated to Materials Research. Fundamental research will encompass metallurgy, physics and chemistry with first experiments planned for the investigation of the relationship between macroscopic and micro-structural properties of polycrystalline materials, grain-grain-interactions, and the development of smart materials or processes. For this purpose a 3D-microsctructure-mapper has been designed. Applied research for manufacturing process optimization will benefit from high flux in combination with ultra-fast detector systems allowing complex and highly dynamic *in-situ* studies of micro-structural transformations, e.g. during welding processes. The beamline infrastructure allows accommodation of large and heavy user provided equipment. Experiments targeting the industrial user community will be based on well established techniques with standardized evaluation, allowing full service measurements, e.g. for tomography and texture determination. The beamline consists of a five meter in-vacuum undulator, a general optics hutch, an in-house test facility and three independent experimental hutches working alternately, plus additional set-up and storage space for long-term experiments. HEMS is under commissioning as one of the first beamlines running at PETRA III.

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INTRODUCTION

PETRA III is the new high-brilliance synchrotron radiation source on the DESY site in Hamburg-Bahrenfeld, Germany. For a total investment of 225 million € , shared by the German Federal Government (90 %) and the City of Hamburg (10 %), the former storage ring PETRA II has been converted into one of the future most brilliant x-ray sources worldwide with 14 new beamlines and up to 30 experimental stations [1]. After starting the conceptual design in 2002 and the final approval of the project in May 2005, the reconstruction of the storage ring began July 2, 2007, with first positrons in it by April 2009. It is currently commissioned into the final design parameters [2].

Several national and international organisations collaborate to build various beamlines and, thus, enhance the infrastructure at the site. Design, construction, operation and main funding of the High Energy Materials Science Beamline HEMS is the responsibility of the German Research Center Geesthacht, GKSS [3]. Approximately 70 % of the beamtime will be dedicated to Materials Research, the rest reserved for “general physics” experiments covered by DESY. *Fundamental research* will be done in the fields of metallurgy, physics, chemistry, and biology with experiments planned for the investigation of the relation between macroscopic and micro-structural properties of polycrystalline materials, grain-grain-interactions, re-crystallisation processes, and the development of new and smart materials or processes. *Applied research* for manufacturing process optimization will benefit from high flux/high brilliance in combination with ultra-fast detector systems allowing highly dynamic *in-situ* studies of micro-structural transformations, e.g. during laser and friction stir welding. Experiments targeting the *industrial user community* will be based on well established techniques with standardised evaluation, allowing "full service" measurements. Environments for grain and strain mapping will be provided as well as automated investigations of large sample numbers, e.g. for texture determination and tomography.

BEAMLINE CHARACTERISTICS

The infrastructure of HEMS (lead shielded hutches, control cabins, cabling, tubing, access safety system, monochromators, shutters, air-conditioning) has been installed. The beamline is currently being commissioned. In the following we describe the expected characteristics, the updated beamline layout [4] and the current status of various planned experiments and already installed major equipment, respectively.

The Source

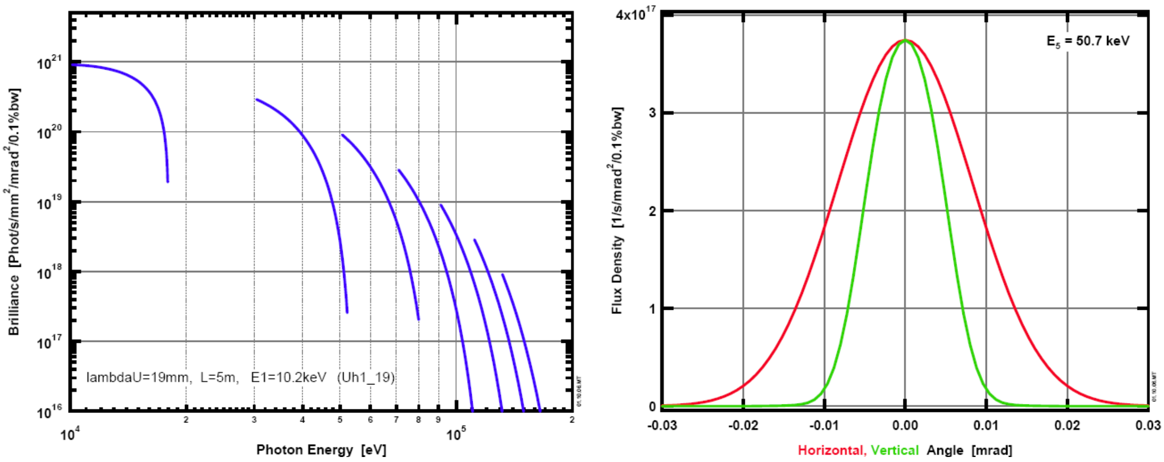
The basic design parameters of the storage ring PETRA are an energy of 6 GeV, a current of 100 mA, and an emittance of 1 nmrad (horizontally) and 0.01 nmrad (vertically), respectively. The source for HEMS will be a *4.5 m long in-vacuum undulator* (U19-5) at a high-β position optimized for full tunability from 30 keV onwards. The key parameters chosen are shown in Fig. 1 together with the resulting spectra [5]. As the planned undulator is not yet manufactured, the commissioning takes place with a substitute standard DESY 2m-undulator.

σ_h = 140 μm σ_h' = 7.0 μrad
σ_v = 4.9 μm σ_v' = 2.0 μrad
σ_r = 1.2 μm σ_r' = 1.6 μrad

(a)

gap_{min} = 7.0 mm E_1 = 10.2 keV
λ_U = 19 mm   L = 4.5 m
B_o = 0.70 T   K = 1.24
$dP/d\Omega$ = 0.25 W/μrad^2 P_{tot} = 5.6 kW

(b)



(c)   (d)

FIGURE 1. Source sizes and divergences (a), technical undulator specifications (b), resulting brilliance (c), and 5th harmonics flux density (d) for HEMS, respectively – calculated for a high-β location.

Beamline Design

Due to quite detailed demands for future experiments expressed in two previous HEMS workshops and confirmed by an international supervisory review panel, the final design for the beamline (P07 in sector 5 of the 280 m long experimental hall) consists now of one main optics hutch (OH1), an in-house test facility (EH1) and three independent experimental hutches (EH2, EH3 and EH4) working alternately, plus additional focussing optics hutches (OH2, OH3) with set-up and storage space for long-term experiments as sketched in Fig. 2. Two near-by side laboratories (machine shop and cleaning facility), four control cabins, a temperature lock room for EH4, and some office space in a 1st floor hall gallery complement the beamline infrastructure.

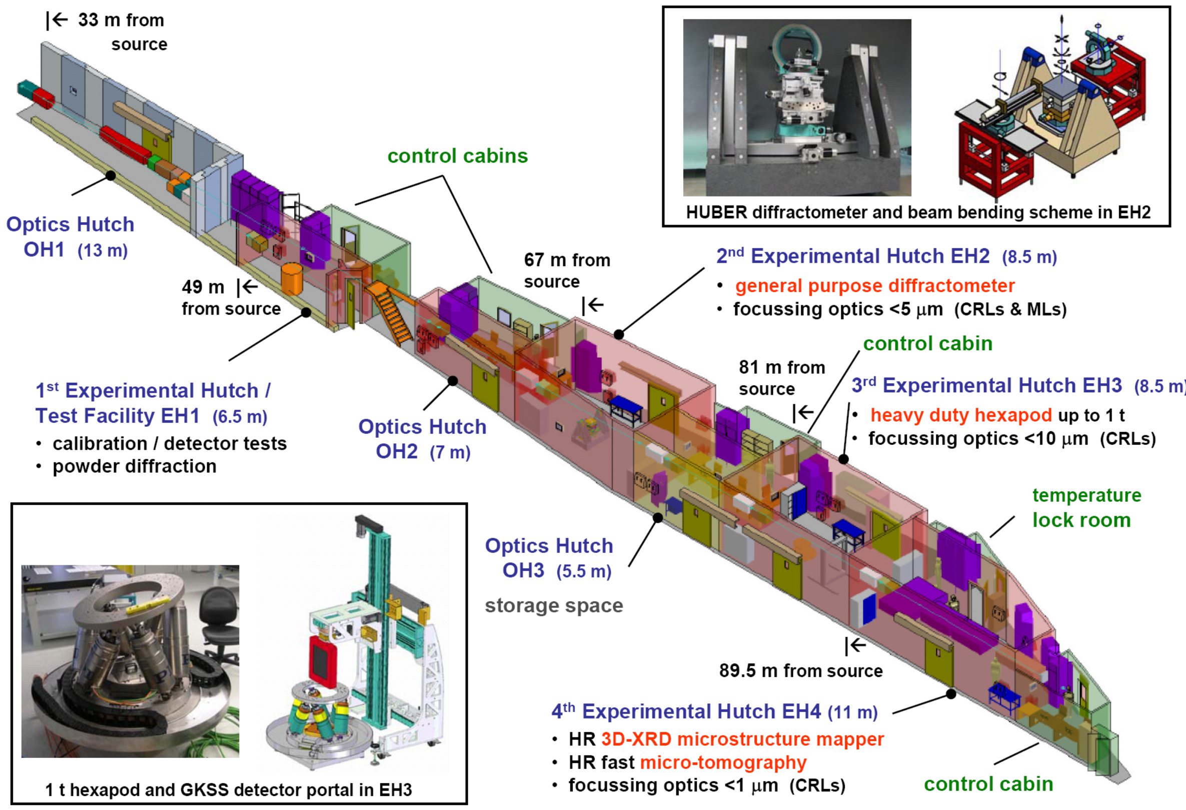


FIGURE 2. 3D-design with main experimental stations of HEMS.

Optics

The 1st optical element inside the concrete shielded main optics hutch OH1 is an indirectly water-cooled single bounce monochromator (*SBM*) allowing to choose either a Si(111) or Si(220) Laue single-crystal, both with 35.36 degrees asymmetric cut lattice planes and of dimension 15 x 20 x 1.5 mm^3. As the scattering angle is fixed to 4.25 degrees horizontally by the floorplan, one can, thus, choose (only) two different energies of 53.3 keV or 87.1 keV, respectively, for scattering in the Test Facility EH1.

The 2nd optics consists of an again indirectly water-cooled double crystal monochromator (*DCM*) with bent Si(111) Laue crystals (40^o asymmetric cut) in fixed exit geometry (horizontal deviation 21 mm) keeping the beam at 1.4 m height above the floor. Both SBM and DCM are custom-built by FMB-Oxford [6] with standardized sub-components, the SBM already installed in July 2009, the DCM factory test accepted in September 2009 and to be inserted in October 2009.

A *multilayer filter box* inside the ring tunnel (4 mm glassy carbon + 0.1 mm Cu, designed by DESY) cuts out the low-energy harmonics (allowing cooling by water instead of standard liquid nitrogen). A lens change box for *Compound Refractive Lenses* [7] will allow variable in-line focusing with easy handling. It should be installed in 2010 and will be positioned variably either in OH1, OH2 or OH3 as likewise possible future ML focussing mirrors.

Experiments

All experimental stations have their neighbouring independent control cabins, allowing one group to set up their experiment while another one, further up the beam, is still experimenting with life beam. The in-house *Test Facility EH1* permits general testing, detector calibration, *etc*., but also the set-up of minor experiments. This can be done while other experiments are being performed. However, the energy is restricted to only two possible values (comp. above). Any user experiment further down in the direct branch must not be influenced (both crystals can be taken out of the beam by a lateral translation).

Experimental Hutch EH2 allows "general physics" experiments. Since July 2009 it is equipped with a versatile diffractometer from HUBER [8] in an improved design as set-up by Reichert et al. [9] at ID15A at ESRF, Grenoble, for the study of deeply buried interfaces. An additional beam bender will enable precise structural investigations of free liquid surfaces [10]. The hardware, including heavy load tables and a scintillation detector, wait on site for final installation, see top inset in Fig. 2.

Experimental Hutch EH3 will satisfy the engineering community with its demand for handling large and heavy samples or sample environments (e.g. turbine blades, welding and fatigue-loading machines, furnaces or cryostats). Due to the large penetration length of hard x-rays, this community can methodically profit from its experience in neutron scattering. The much higher brilliance at HEMS, however, will facilitate the construction of special sample environments, emphasizing *in-situ* investigations of structural transformations during manufacturing processes. The work-horse will be a prototype hexapod for heavy load of 1 t custom-built by Physik Instrumente [11] according to demanding specifications (travel ranges tens of cm, tilt angles 15^o, resolution 1 μm). It was factory test accepted in October 2008 and is ready for installation on site. As 2D-detectors, a mar345 image plate is already on stock, a mar555 selenium based flat panel direct conversion detector has been tested at ESRF and is – as a specially customer-modified prototype – expected for delivery by November 2009 [12], see bottom inset of Fig. 2.

In the last *Experimental Hutch EH4* two specialized instruments (currently designed) will share the space (accessible also via a temperature lock room): a strain and stress mapper for polycrystalline materials, flexible enough to perform both 3D-XRD and DCT (diffraction contrast tomography) [13], and a dedicated micro-tomography set-up that will complement to higher energies the future Imaging Beamline P05 at PETRA (which is operating in the range 5-50 keV) [1]. All stations will use rotary air-bearing stages with a wobble of sub-micro-radians. The location and separate air conditioning should allow a stable focus down to the 100 nm range.

SUMMARY

The HEMS beamline at PETRA III – currently being commissioned – is optimized for hard x-rays in the fully tuneable range 30-250 keV in order to investigate non-destructively bulk properties or deeply buried structures and interfaces mainly in the context of Materials Research, but versatile enough to allow experiments in the merging fields of physics, chemistry and biology. Fast 2D-detectors together with varying focus spots down to 200 nm will allow highly dynamic *in-situ* experiments of micro-structural transformations in the future. It can handle large and up to 1 t heavy user provided equipment. Two specialized experiments, designed in-house at GKSS, will allow the detailed characterization, as well as tomographic imaging, of grains, their interaction and their stress and strain states with sub-micrometer resolution.

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