PETRA III:
A Low Emittance Synchrotron Radiation Source

Technical Design Report

– Executive Summary –

Editors:
K. Balewski, W. Brefeld, W. Decking, H. Franz, R. Röhlsberger, E. Weckert
DESY, Hamburg, Germany

February 29, 2004

Contents

Chapter 1

Introduction

During the past 30 years, research carried out at synchrotron radiation facilities has made significant contributions to basic as well as applied sciences. The development of experimental techniques answering a wide variety of scientific questions is progressing at an unprecedented pace. These improvements have always been strongly correlated to the advances in source brilliance. In the very beginning, scientists, mainly physicists, investigated the basic properties of synchrotron radiation. However, soon its unique properties were recognized: tunability over a large range of the electromagnetic spectrum, extreme collimation, very high intensity, polarization properties and a pulsed time structure. Synchrotron radiation experiments at the synchrotron of the Deutsches Elektronen-Synchrotron (DESY) were among the first and played a key role for the following developments. First experiments in 1967 concentrated on spectroscopic investigations of atoms in the VUV energy range for which no laboratory sources were available. Already in 1970 first small angle scattering experiments using X-rays were carried out on biological samples exploiting the small divergence of the beam. Today, the spectral range used for experiments extends from the infrared to the very hard X-ray range at several 100 keV. Since these early days when only few experts took on the effort to carry out pioneering experiments, the situation has changed dramatically and many synchrotron radiation techniques have reached a considerable state of maturity and a high degree of automation, thus, making these techniques available for a wide user community. The developments in many fields such as surface and interface physics, magnetism, absorption and fluorescence spectroscopy, or diffraction and scattering experiments at high photon energies would be unthinkable without synchrotron radiation. Another very successful field is structural biology, where meanwhile the fraction of protein crystal structures newly deposited in the Protein Data Base (PDB), and measured using synchrotron radiation, is approaching 90%.

Worldwide about 40000 scientists are using synchrotron radiation very often in an interdisciplinary approach. The operational German sources serve about 3000 users per year, 2000 of them using DESY facilities. The applications stretch over such different fields as atomic and cluster physics, condensed matter physics, chemistry, materials science, structural biology, crystallography, geo- and environmental science and medical science. In the beginning, scientists used in a ‘parasitic’ mode the radiation emitted from the bending magnets of synchrotrons and later of storage rings, built for particle physics research. These so-called first generation sources were soon followed by the 2^{nd} generation providing radiation from linear, periodic magnetic arrays of small dipoles, so-called wigglers, in addition to the radiation emitted by bending magnets. Such wigglers provide a 30–100 fold flux of a bending magnet. All these machines have in common relatively large particle beam cross sections of the order of one millimeter. They provide rather large photon beams, which are very well suited for studies of samples of milli- to centimeter sizes such as whole work pieces common in materials science.

For the 3^{rd} generation of synchrotron radiation sources a further, rather dramatic improvement of the photon beam quality has been achieved by exploiting the constructive interference of the radiation emitted from the individual poles of periodic magnetic structures called undulators. For these devices to function efficiently rather small and parallel particle beams are needed. These very demanding requirements and the fast growth of the user community led to the construction of dedicated synchrotron radiation sources specialized for serving undulators with particle energies matching the photon energy range needed for the main applications, e.g. BESSY II in Berlin for the VUV and soft X-ray regime and the European Synchrotron Radiation Facility (ESRF) in Grenoble for hard X-rays.
The main domain of undulator beams is the investigation of small samples or sample regions in the sub-millimeter to sub-micrometer range. The most suitable parameter to compare 3^{rd} generation sources is brilliance, that means the flux per second in a given energy range normalized to the size of the source and to the solid angle under which the radiation is emitted. In Fig. 1.0.1 the brilliance as a function of photon energy is compared for a number of synchrotron radiation sources. The dramatic increase in brilliance from 2^{nd} to 3^{rd} generation facilities has triggered a large number of new techniques and experiments unthinkable before. Meanwhile, focussing of hard X-rays down to a spot size of $< 100\,\mathrm{nm}$ has been demonstrated at ESRF providing the possibility to analyze samples at very high spatial resolution. A high brilliance beam contains a considerable fraction of coherent photons enabling techniques like phase contrast imaging and X-ray photon correlation spectroscopy (XPCS) to become practical tools for the investigation of the static and dynamic properties of matter. The same holds for a number of other techniques where the basic feasibility was demonstrated at 2^{nd} generation sources but applications to scientifically interesting samples need the high brilliance of 3^{rd} generation sources.

At present, DESY is operating the storage ring DORIS III, a 2^{nd} generation synchrotron radiation source, at a positron energy of 4.45 GeV. The relatively high particle energy provides a considerable flux also at photon energies in the hard X-ray regime beneficial to a number of applications that require penetration into or through larger bulk specimen. The large positron beam at DORIS III provides relatively large photon beams which are ideally suited for the investigation of milli- to centimenter size samples. The corresponding beamlines are robust and easy to operate by users. However, small samples, extremely small foci, experiments at extremely high resolution in reciprocal space or in energy, or coherence experiments are beyond the capability of the radiation provided by this storage ring. For that reason DESY decided to rebuild its 2.304 km long storage ring PETRA II into a 3^{rd} generation synchrotron

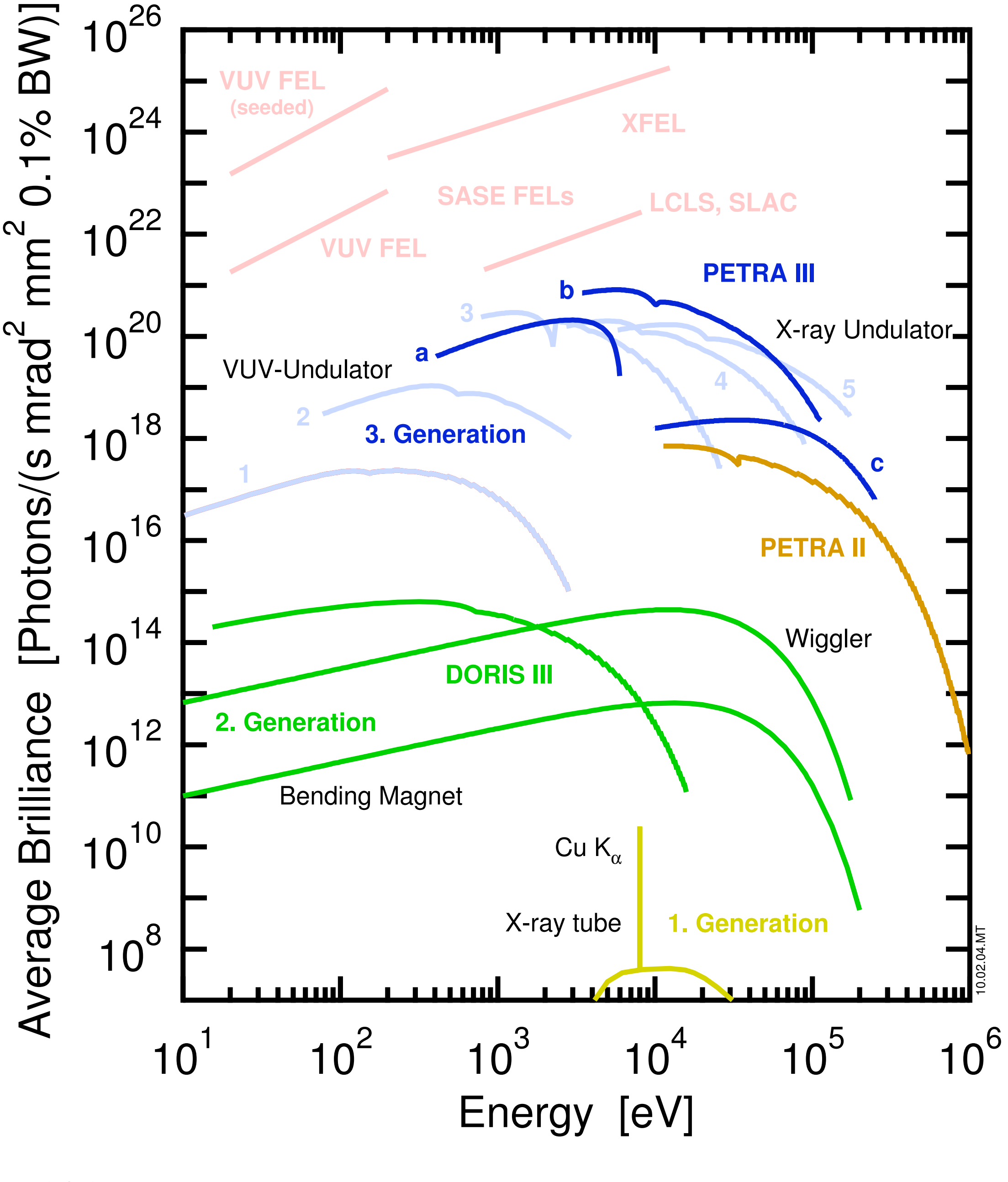

Figure 1.0.1: Average brilliance of synchrotron radiation and free-electron laser (FEL) photon sources available or planned at DESY compared with the actual performance of other 3^{rd} generation storage rings and the FEL for hard X-rays under construction at SLAC, Stanford. The tuning curves of the DORIS III sources are colored in dark green including the BW2 and BW3 wiggler. The other labels apply as follows: 1. BESSY II U125, 2. ALS U5, 3. DIAMOND U46, 4. ESRF ID16, 5. SPring-8 BL46; PETRA III: a. soft-X-ray undulator (4 m, high-β), b. standard $K_{\max} \approx 2.2$ undulator (5 m, high-β), c. hard X-ray wiggler ($K_{\max} \approx 7$, 5 m, high-β).

radiation source called PETRA III. The conversion of PETRA will start in 2007. The particle energy of this new source will be 6 GeV at an initial current of 100 mA. Present plans feature 13 independent undulator beamlines for experiments. The emittance of PETRA III will be 1 nmrad which is a so far unrivaled value for storage rings operated at a comparable high particle energy for the production of hard X-rays. PETRA III will provide a maximum brilliance of the order of 10^{21} ph/s/mm^2/mrad^2/0.1% BW with a considerable fraction of coherent photons also in the hard X-ray range. With a coupling ratio of 1% PETRA III will be diffraction limited in the vertical direction up to a photon energy of about 10 keV.
The choice of a particle energy of 6 GeV was motivated by an optimization for a small beam emittance, which scales with the square of the energy, and a sufficiently high particle energy which is needed to provide tunable high-energy photon beams with sufficient flux and brilliance.

After the conversion of PETRA, a number of unique sources will be available for the research with synchrotron radiation at DESY: (i) the high energy storage ring PETRA III for the investigation of matter with sub-millimeter to sub-micrometer spatial resolution, (ii) the storage ring DORIS III for applications that need high flux and that can use beams of millimeter size dimensions, (iii) the VUV-Free Electron Laser (VUV-FEL) for research with extremely intense and coherent photon beams in the VUV and soft X-ray regime down to 6 nm wavelength and pulses of $\approx$ 50 fs duration. In 2012, the planned European X-ray Free Electron Laser Laboratory (XFEL) should provide very short, extremely intense, coherent hard X-ray pulses up to about 12–14 keV photon energy with a peak brilliance about nine orders of magnitude higher than available today. This unique ensemble of X-ray sources will offer most attractive opportunities for photon science.

Today, the ESRF is serving the European synchrotron radiation community with brilliant photons mainly in the hard X-ray regime. However, the ESRF is heavily overbooked and can not fulfil all user requests for beamtime. In the somewhat softer energy range a number of medium particle-energy storage rings like SOLEIL close to Paris, DIAMOND near Oxford and the Spanish light source in the vicinity of Barcelona are planned or under construction in Europe in addition to the existing facilities ELETTRA, MAXLab, BESSY II and the Swiss Light Source (SLS). These facilities attract communities using the photons in the VUV as well as in the soft X-rays regime from undulators and X-ray photons up to about 10–20 keV from wigglers, wavelength shifters, and small gap in-vacuum undulators. With its particle energy of 6 GeV and the future upgrade possibilities for beamlines providing even extremely hard X-ray radiation, PETRA III fits very well into the whole scenario of European sources in order to serve the community with very brilliant X-ray beams at photon energies also well beyond 20 keV photon energy.

Furthermore, with its design parameters (see Sec. 2.2) and future upgrade possibilities the PETRA III storage ring represents a development about half way in between presently operating 3rd generation X-ray sources and what is, according to a theoretical study by the ESRF machine group, considered to be the ultimate storage ring. Especially the very small horizontal emittance is expected to provide significantly better conditions than presently available for the realization of very small focal spot sizes and for experiments exploiting the coherence properties of the beam. Therefore, the PETRA III upgrade represents a unique possibility to strengthen the research infrastructure in the harder X-ray regime and, probably more important, to provide a significant improvement for all techniques that require a low emittance source.

The design study presented in this report has been developed since year 2000 in close collaboration with the synchrotron radiation community and a large number of international experts in the field of beamline instrumentation and synchrotron radiation storage rings. Ten workshops were organized to exchange and discuss ideas.
The technical design concerning the conversion of the storage ring has already been preliminary reviewed by a panel consisting of the DESY machine advisory committee (MAC) and external machine experts from 3^{rd} generation synchrotron radiation sources. According to their first judgement the conversion of PETRA is '…considered to be a cost effective solution …and …a very clever design …'. This panel is expected to accompany the storage ring part of this project.

Experiments requiring the high brilliance of PETRA III were discussed in a series of user workshops which led to a larger number of proposed experiments for PETRA III than the number of available undulator ports. After publication of this report, an external, international advisory board will be established to assist DESY in prioritizing these beamline proposals.

The next chapter in this technical design report will give a comprehensive overview of the PETRA III project including a short description of the proposed experimental stations. The following chapters describe in detail the conversion of the storage ring and the refurbishment of its infrastructure, the proposed insertion devices, the beamline vacuum system, the X-ray optics, and a detailed description of the science case as well as technical issues of the proposed experimental stations. The last chapters of this TDR deal with civil engineering, project costs and personnel requirements, schedule, and future upgrade possibilities.

Chapter 2

Executive Summary

2.1 Science at Low Emittance High-Energy Synchrotron Radiation Sources

Synchrotron radiation science experienced a tremendous boost during the past 10–15 years after the advent of 3^{rd} generation low emittance synchrotron radiation sources like ESRF (Grenoble), APS (Argonne) and SPring-8 (Harima) in the hard X-ray regime and ELETTRA (Trieste), BESSY II (Berlin), SLS (Villingen) and MAXLab (Lund) in the somewhat softer energy range. While the sources of first and 2^{nd} generation operating in parasitic or dedicated mode deliver intense X-ray beams from bending magnets and wigglers, 3^{rd} generation facilities use undulators as their main radiation sources. The total flux of a wiggler at a 2^{nd} generation source like DORIS III at DESY is not significantly smaller than the flux of an undulator beamline at a 3^{rd} generation source but it is distributed over a considerably larger solid angle, thus providing ideal conditions for the investigation of samples of about millimeter to centimeter size. In comparison, the source size of an undulator beam of a 3^{rd} generation source is about two orders of magnitude smaller providing ideal conditions for the investigation of much smaller samples or for micro- to nano-focussed beam. The commonly used quantity to characterize synchrotron radiation sources is the well known brilliance B[1]

$$B = \frac{F}{4\pi^2 \sigma_{Tx}\sigma_{Ty}\sigma_{Tx'}\sigma_{Ty'}} \tag{2.1.1}$$

where F is the spectral photon flux in photons/(s·0.1% BW); σ_{Tx} and σ_{Ty} are the total (index: T) photon source sizes in horizontal and vertical direction, respectively; $\sigma_{Tx'}$ and $\sigma_{Ty'}$ are the total beam divergence in horizontal and vertical direction[2]. Usually, all flux and brilliance values are given for a 0.1% energy bandwidth (BW) which is about seven times larger than the average intrinsic energy bandwidth behind a Si (1 1 1) monochromator. The total photon source size and divergence are given by the convolution of the sizes ($\sigma_{x,y}$) and divergences

---

[1] Brilliance is often called brightness in American literature. The definition of all quantities in this TDR are according to (Kim, 1995).

[2] All source sizes and divergences will be characterized by their RMS values assuming Gaussian shaped distribution functions.

$(\sigma_{x',y'})$ of the electron beam with the intrinsic radiation characteristics $(\sigma_r, \sigma_{r'})$ of a single electron. For that reason the horizontal emittance

$$\epsilon_x = \sigma_x \cdot \sigma_{x'} \tag{2.1.2}$$

of a storage ring is of crucial importance for the photon beam parameters. The vertical emittance is given by $\epsilon_y = \kappa \cdot \epsilon_x$ with the so-called coupling factor κ that depends mainly on the precision of the alignment of the storage ring. Typical values for κ at present synchrotron radiation storage rings are in the range of 1 %. The brilliance is usually given in units of photons/(s mm^2 mrad^2 0.1%BW) and characterizes the number of photons per unit phase space volume. Undulator sources at modern 3^{rd} generation storage rings are very well suited to produce high brilliance due to the small source size and the low divergence of the emitted radiation.
To a certain extent it is also possible to focus the relatively large beam of a wiggler of a 2^{nd} generation source onto a small sample area at the expense of an increased divergence in the focus. However, due to limitations in the achievable demagnification ratio and the small aperture of X-ray optical elements the large source size of 2^{nd} generation storage rings imposes a lower limit for the smallest achievable focal spot size. If an experiment requires both, high flux on a very small sample area and a beam as parallel as possible, then only 3^{rd} generation sources are able to fulfill these demands.

High brilliance is mandatory for a number of experimental techniques:

- Protein crystallography: For many proteins it is extremely difficult to grow large crystals. At the same time interesting structures get more complex, leading to weakly diffracting crystals with large unit cells and a very densely populated reciprocal space which requires a parallel and intense beam to resolve different diffraction orders.
- High resolution diffraction from small sample areas, especially from surfaces and interfaces: These techniques require a very parallel beam conditioned by slits to an appropriate size. Providing a high intensity beam under these conditions is not possible at a 2^{nd} generation source.
- Spectroscopy with sub-μm spatial resolution: These experiments require the smallest possible source size due to the achievable demagnification ratio and the limited aperture of the available X-ray optical elements.
- Small angle scattering with μm spatial resolution or very small samples: This technique requires a micro-focus beam but a divergence small enough to obtain sufficient resolution in the scattering pattern.

A low emittance storage ring operated in the 6–8 GeV range allows to generate well collimated undulator radiation up to quite high X-ray photon energies which have significant advantages in materials science applications where

- very small but intense photon beams can be generated for hard X-rays that are needed to penetrate large samples and components for 3D microscopy with sub-μm spatial resolution.

- Extremely small foci of hard X-rays will also allow for cone beam tomographic techniques for 3D imaging in the 100 nm resolution range.

The spectral flux F of such an undulator is significantly higher than that of a wiggler. Yet, since an undulator emits discrete energy bands the total heat load on the optical elements compared to the flux density available for the experiment is significantly lower than for a wiggler. For this reason an extremely high flux at the sample position can be generated with sufficient stability. This is a prerequisite for experiments that use only a very small wavelength bandpass of the incident radiation such as:

- Inelastic scattering: This technique only became a standard technique due to the availability of 3^{rd} generation synchrotron radiation sources. Experiments on μm-size samples like those used for high pressure studies are still a challenge and need very long data acquisition times.
- Nuclear resonant scattering: Since only a very small part of the energy spectrum of the incident photons can be used, experiments are flux limited at present 3^{rd} generation sources.

Every incoherent source like an undulator at a storage ring provides a certain fraction of coherent photons. The transversely coherent flux F_c is given by

$$F_c = B\left(\frac{\lambda}{2}\right)^2 = \frac{F\lambda^2}{16\pi^2\sigma_{Tx}\sigma_{Ty}\sigma_{Tx'}\sigma_{Ty'}}, \tag{2.1.3}$$

with λ being the photon wavelength. At a PETRA III undulator with a brilliance above 10^{20} ph/(s mm^2 mrad^2 0.1% BW) F_c will be about $4 \cdot 10^{10}$ ph/s in a monochromatic beam[3] at 12 keV photon energy. The transverse coherence length $\xi_{t(x,y)}$ of a beam from an incoherent source of size $\sigma_{T(x,y)}$ at distance L for a particular wavelength is given by

$$\xi_{t(x,y)} = \frac{\lambda \cdot L}{2 \cdot \sqrt{2\ln 2} \cdot \sigma_{T(x,y)}}. \tag{2.1.4}$$

The longitudinal coherence length ξ_l is determined by the monochromaticity of the beam:

$$\xi_l = \frac{\lambda^2}{\Delta\lambda}. \tag{2.1.5}$$

For the intrinsic line of an undulator the relative bandwidth is given by

$$\Delta\lambda/\lambda = 1/nN, \tag{2.1.6}$$

with N being the number of poles and n the harmonic number[4]. Thus the longitudinal coherence length of an undulator line is given by $\xi_l = nN\lambda$. These coherence properties promoted the development of new experimental techniques during the last years:

---

[3] Behind a Si (1 1 1) monochromator.

[4] In principle $1/nN$ has to be convoluted with the particle energy spread of the storage ring in order to obtain the true $\Delta\lambda/\lambda$. The energy spread contribution, however, is only significant for higher harmonics of very long undulators.

- X-ray photon correlation spectroscopy (XPCS): This technique allows to gain insight into the dynamics of materials on time and length scales that are not accessible with other methods like inelastic neutron scattering or laser correlation spectroscopy using energies in the visible spectral range.
- Phase contrast imaging: In samples where differences in absorption contrast are very small, the interference contrast of neighboring rays that experience slightly different phase shifts due to inhomogeneities of the index of refraction can clearly be detected. This experimental technique provides a totally new, non destructive imaging method mainly for low-Z materials.

The advantages mentioned above hold more or less for all 3^{rd} generation high-energy synchrotron radiation sources such as ESRF, APS and SPring-8. The emittance of PETRA III will be 1 nmrad. This is by a factor of three to four smaller than that of present sources. The smaller emittance translates directly to a smaller source size which results in a higher brilliance and a higher coherent fraction. The experiments that benefit most from the smaller emittance are:

- Micro- or nano-focus experiments; the smaller source size allows the realization of very small focal spots. Since at the same time the divergence of the radiation is also smaller, a significantly larger part of the total beam can be collected by optical elements leading to a higher focal flux density.
- High resolution diffraction experiments for the investigation of fine details in momentum space that derive from long range correlations in real space, because they need extremely high resolution in energy ($\Delta\lambda/\lambda$) and Q-space.
- Coherence applications like XPCS as mentioned before.

In addition to ‘standard’ size insertion devices that are available at most other synchrotron radiation sources, the geometry of PETRA III allows to install a number of very long (> 20 m) insertion devices. One of them will be implemented already in the first stage. Therefore, very high photon flux can be provided for some of the flux ‘hungry’ experiments mentioned above.

2.2 PETRA III Conversion Overview

2.2.1 Storage ring

The conversion of the PETRA storage ring will include the total rebuilding of one eighth of the storage ring to provide the electron beam optics for nine straight sections. Eight of them will provide space for one 5 m or two 2 m long insertion devices (ID). The two 2 m IDs will be inclined towards each other by 5 mrad. This scheme allows to operate two independently tunable undulators in a single straight section with beam paths sufficiently separated for individual beamline optics. The ninth straight section will be suitable for the installation of an insertion device up to a length of 25 m. From the present point of view and taking into a

	ϵ_x [nmrad]	E [GeV]	ϵ_x/E^2		ϵ_x [nmrad]	E [GeV]	ϵ_x/E^2
USR	0.3	7	0.006	SLS	4.4	2.4	0.763
PETRA III	1	6	0.027	ELETTRA	7	2.4	1.215
SPring-8	3.4	8	0.053	BESSY II	6	1.9	1.66
APS	3	7	0.061	Spear III	18	3	2
ESRF	3.9	6	0.108	MAX II	9	1.5	4
Diamond	2.5	3	0.2	ANKA	41	2.5	6.56
Soleil	3	2.5	0.48	DORIS III	450	4.5	22.2

Table 2.2.1: Emittance ϵ_x, particle energy E and normalized emittance ϵ_x/E^2 of a number of operating and planned storage rings. 'USR' denotes a study about an ultimate storage ring carried out by the ESRF machine group (Ropert et al., 2000). 'PETRA III' denotes the upgraded PETRA storage ring. Planned sources or feasibility studies are colored in green, sources under construction in blue and operational facilities in black.

account the available space in the experimental hall, a number of 13 insertion devices (one with 20 m, four with 5 m and eight with 2 m) are planned.

Due to the large radius of PETRA III, the angle between the beams of neighboring straight sections will be 5°. This angle does not allow to have large experimental stations using the radiation from the bending magnets between the undulator beams. However, depending on the exact layout of the undulator beamlines, the option to use radiation from the bending magnets downstream of each undulator will be kept open.

The design values for the new storage ring will be 6 GeV for the particle energy and 100 mA for the current. However, all components handling heat load or dealing with radiation safety will be dimensioned for a current of at least 200 mA in order to leave room for further upgrades. The envisaged particle energy of E = 6 GeV is a compromise between a small horizontal emittance $\epsilon_x \propto E^2$ and a particle energy E sufficiently high to provide also tunable beams of high photon flux in the energy range of 50–150 keV.

In addition to the straight sections located in the converted eighth of the storage ring, four straight sections with 64.8 m and another four with about 108 m length exist at PETRA. These straight sections will in part be used for damping wigglers with a total length of 80 m in order to reduce the emittance of the particle beam to its design value of 1 nmrad. Since the emittance of a storage ring scales quadratically with the particle energy, the quantity ϵ_x/E^2 can be used to compare different storage rings. In Tab. 2.2.1 the quantity ϵ_x/E^2 is listed for a number of storage rings that are in operation, under construction or planned. It is obvious that PETRA III compares favorably with present sources at higher particle energies. Only the parameters of a theoretical ESRF study for an ultimate storage ring (USR) would provide a lower emittance beam.

In order to ensure a reliable operation of the storage ring almost all magnet coils of the remaining 7/8 of the storage ring will be replaced as well as the whole vacuum system. In addition, further upgrades are necessary for the RF system of the storage ring, the magnet power supplies and the cooling system.

The Touschek lifetime is decreasing with the emittance of a storage ring. For this reason the

	β_x [m]	β_y [m]	σ_{Tx} [μm]	σ_{Ty} [μm]	$\sigma_{Tx'}$ [μrad]	$\sigma_{Ty'}$ [μrad]	ID-length [m]
low-β 5 m	1.3	3	36	6.0	28	3.7	5
high-β 5 m	20	2.4	141	5.5	7.7	3.8	5
low-β 2×2 m	1.4	3	37	5.7	27	5.4	2
high-β 2×2 m	16.2	2.6	127	5.3	9.3	5.5	2
20 m-ID	16	5	126	7.9	8.2	2.7	10
DW-drift	16	16	127	13	8.5	3.3	5
ESRF low-β	0.5	2.73	59	8.3	90	3	5
ESRF high-β	35.2	2.52	402	7.9	10.7	3.2	5
SPring-8	22.6	5.6	277	6.4	13	5	4.5
APS	15.9	5.3	217	12.6	15.3	5.7	4

Table 2.2.2: Overview of typical β functions, photon source sizes $\sigma_{x,y}$ and divergences $\sigma'_{x,y}$ for various ID positions at different storage rings compared to PETRA III. The photon source parameters are given in RMS values for a photon energy of 12 keV. '2×2 m' indicates the inclined undulator insertion device positions at PETRA III. 'DW-drift' denotes possible undulator positions in the straight sections outside the new, converted eighth of the PETRA storage ring. For this position, $\alpha_x = -0.7$ and $\alpha_y = 0.7$. The α values of all other PETRA III insertion device positions are zero which holds also for the dispersion in the straight ID sections. To calculate the values for PETRA III, SPring-8 and APS an emittance (coupling) of 1 nmrad (1%), 3.4 nmrad (0.2%) and 3 nmrad (1%) was assumed, respectively. All values are calculated from published β-functions and emittances using SPECTRA (Tanaka & Kitamura, 2003). ESRF values were taken from *ESRF Highlights 2003*.

standard bunch filling pattern will consist of a large number (960 bunches corresponding to 8 ns bunch distance) of equally spaced bunches with comparatively low charge. The lifetime for higher charged bunches for timing modes of operation (e.g. 40 bunches with 192 ns bunch distance) at 100 mA will be as low as 2 h compared to about 24 h for the 960 bunch mode. Considering the very good experience of SLS and APS in terms of thermal stability of the storage ring as well as the X-ray optical elements, a topping-up injection mode of operation is foreseen. Since the time between top-up injections can be as small as 70 s for a 40 bunch filling pattern in order to keep the current constant within 1%, a very high availability for the injector and pre-accelerator systems is required demanding also significant refurbishments of these systems. The RMS-bunch length at PETRA III will be about 40 ps.

In Tab. 2.2.2 the planned β-functions ($\beta_{(x,y)} = \sigma_{(x,y)}/\sigma_{(x',y')}$, see also Eq. 2.1.2) as well as photon source sizes and divergences in the straight sections of PETRA III are compared to those at other high energy synchrotron radiation sources. Similar to the ESRF there will be the option to have either a low or a high-β value in a straight section of the converted eighth of the storage ring. According to present plans the possibility to switch between these two β-function values during a short shut down period is envisaged. The vertical beam parameters of present high-energy 3^{rd} generation SR sources are very similar since all of them are close to the diffraction limit in this direction. Therefore, the improvement provided by PETRA III is mainly for the beam parameters in the horizontal direction.

The experiments can only benefit from the small source sizes if the beam stability is very high. For this reason a suitable diagnostics and beam position control system will be established.

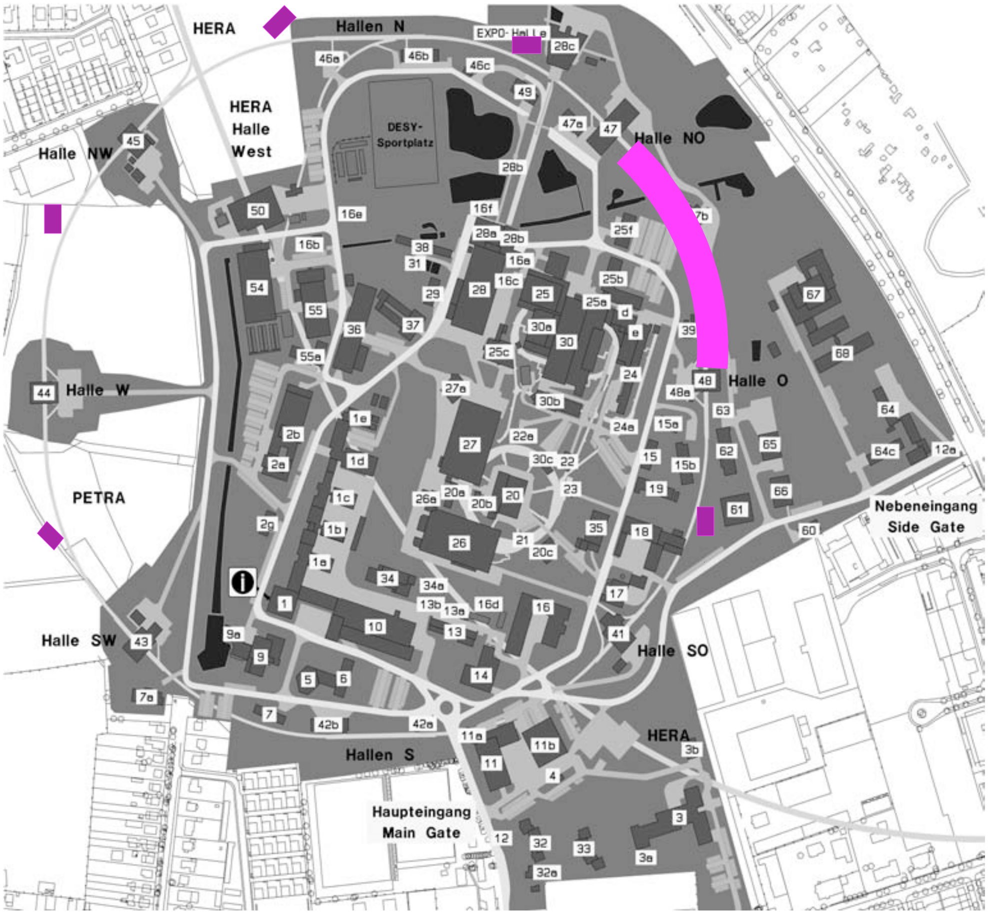

Figure 2.2.1: Schematic position of the new experimental hall (magenta) situated between buildings 47 and 48. Additional buildings for experiments are sketched in dark magenta at positions where further undulator beamlines could be placed in future.

2.2.2 Experimental hall

A new experimental hall will be built at the rebuilt eighth of the storage ring. Its location is schematically indicated in Fig. 2.2.1. Designs for the experimental hall are based on the experience at other synchrotron radiation facilities. The requirements for the floor stability of a synchrotron radiation facility of very low emittance are extreme. Therefore, the whole ring tunnel in the new eighth of the storage ring will be rebuilt and located inside the experimental hall. Both shielding walls will be of 1 m thickness and cast out of heavy concrete. The tunnel roof will consist out of 0.5 m thick removable concrete blocks.

The experimental hall will be equipped with a crane able to lift up to 20 tons. The present planning foresees to cast the floor in the experimental hall as one concrete slab about 1 m in thickness which will carry the ring tunnel and the experiments. This slab will be vibrationally decoupled from the experimental hall super structure and the auxiliary buildings. Other possibilities for the design of the experimental hall floor are still under investigation.
The dimensions of the hall are such that beamlines can be up to 103 m long inside the experimental hall. For experimental hutches outside the main hall the following options exist:

- The first undulator (20 m ID, counting starts at hall 47) has space for a 210 m long beamline.
- The beamlines of the second and third ID can be extended up to 150 m length.

The air conditioning of the hall will be designed for a temperature stability of ± 1 K. Along the outer perimeter of the experimental hall there will be laboratory and workshop space in the ground floor and office space in the first floor among other necessary infrastructure and facilities. The total space for laboratories and offices amounts to about 1800 m^2. The hall will be accessible from both ends by doors large enough for trucks. In addition there will be four entrances along the outside of the hall large enough for smaller fork lifters.

2.2.3 Expected photon beam performance

The characteristics of the electron beam have already been shortly described above (see Sect. 2.2.1). The vacuum chamber inside the undulators will have an internal aperture of 7 mm. This means that the minimum magnetic gap of the undulators will be limited to a value of about 9.5 mm. In Fig. 2.2.2 the tuning curves of typical PETRA III undulators as well as the flux at higher photon energies through a 1 mm^2 pinhole in 35 m distance from the source are compared with those of existing 3^{rd} generation synchrotron facilities. The majority of the undulators will be designed to be tunable over the whole wavelength regime ($\mathrm{K}_{\mathrm{max}} \approx 2.2$). The highest brilliance available will be above $10^{21}\,\mathrm{ph/(s\,mm^2\,mrad^2\,0.1\%BW)}$. The maximum brilliance of a 2 m insertion device is about 3.2 times less than the one of a 5 m ID while a 20 m ID provides about 2.7 times the brilliance of a 5 m device. This relatively small increase is due to the necessary change in β-function in order to be able to operate such a long device. The increase in flux scales approximately with the length.
The transverse coherence lengths (Eq. 2.1.4) calculated from the values in Tab. 2.2.2 are listed in Tab. 2.2.3. The total coherent flux (Eq. 2.1.3) at about 12 keV is $4 \cdot 10^{10}, 10^{11}$ and $2.5 \cdot 10^{11}$ ph/s/0.01%BW for a 2 m, 5 m and a 20 m insertion device, respectively. With a horizontal and vertical emittance of $\epsilon_x \approx 1$ nmrad and $\epsilon_y \approx 0.01$ nmrad, PETRA III will be a diffraction limited source up to photon energies of about 10 keV in vertical direction and up to 100 eV in the horizontal direction, i.e. $\epsilon_x \epsilon_y \leq (\lambda/4\pi)^2$.
Fig. 2.2.2b shows that the photon flux of a high flux wiggler at PETRA III at photon energies around 100 keV through a 1 mm^2 pinhole is higher than that of a standard $\mathrm{K}_{\mathrm{max.}} \approx 2.2$ undulator. Very likely both devices will be outperformed by superconducting undulators if the development advances so far that these devices can be manufactured with a phase error small

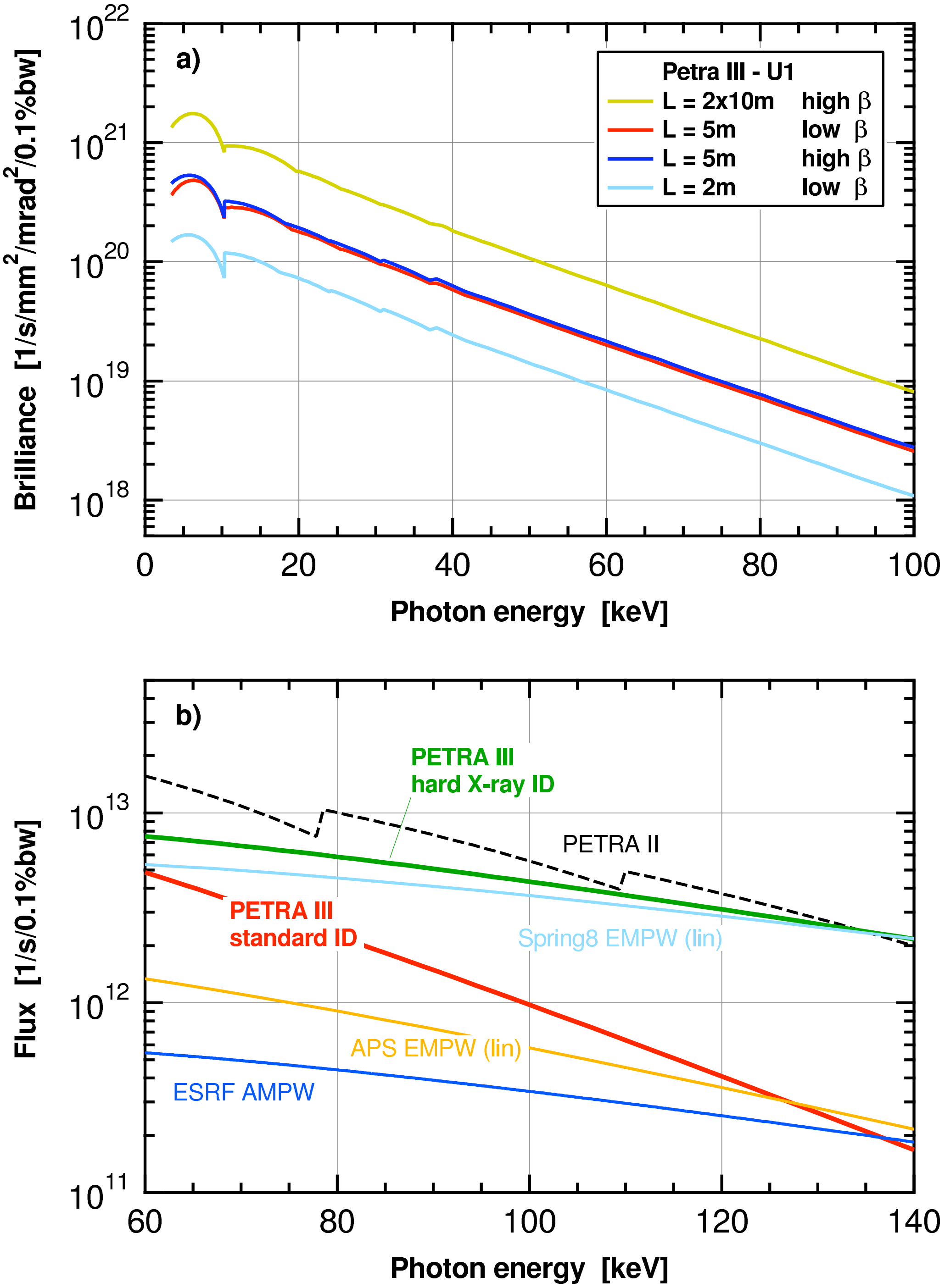

Figure 2.2.2: a. Comparison of the brilliance of typical PETRA III K_{max}=2.2 undulators for different length and β functions (according to Tab. 2.2.2) for the following parameters: 1 nmrad emittance, 1% coupling, 100 mA current, 9.5 mm minimum gap and 29 mm period. b. Flux through a $1 \times 1\,\mathrm{mm}^2$ pinhole at 40 m source distance for a number of high-energy radiation insertion devices. The source distance for the PETRA II undulator is 100 m. Note, this comparison is only relevant for apertures <1 mm.

	$\xi_{t,x}$	$\xi_{t,y}$
high-β	18 μm	500 μm
low-β	72 μm	460 μm

Table 2.2.3: Horizontal and vertical coherence lengths at PETRA III in FWHM calculated for 1 nmrad emittance and 1% coupling at 12 keV photon energy and at 60 m distance from the source.

enough for the effective use of the higher harmonics of the spectrum. Another interesting and new development that should be kept in mind are variable period undulators (Shenoy et al., 2003a; Shenoy et al., 2003b).

It should be emphasized that the brilliance calculations above are based on the assumption of a 1% horizontal/vertical coupling. A smaller coupling value would further increase the brilliance especially at higher photon energies due to a smaller vertical source size. However, it will also further reduce the Touschek lifetime. The main difference between PETRA III and current high-energy, 3^{rd} generation synchrotron radiation sources will therefore be in horizontal emittance which results in a smaller horizontal source size and therefore a larger total fraction of coherent photons or a higher number of photons in a given microfocus.

For photons in the VUV and XUV range, a high-energy storage ring has significant advantages for experiments needing circular polarized photons in the 200–2300 eV range with a high degree of polarization, which can only be obtained in the first undulator harmonic of a helical undulator.

2.3 Proposed Experimental Stations

In order to define the experimental stations to be proposed for PETRA III a number of user workshops were organized in the years 2002 and 2003 at DESY and the following criteria have been applied for beamline proposals:

1. Exploitation of the unique properties of the X-ray beams provided by PETRA III.
2. Implementation of innovative developments and techniques.
3. Consideration of the requirements of the specific HASYLAB user community.
4. Complementarity to other existing opportunities at large scale synchrotron radiation facilities in Europe and at upcoming X-ray free-electron lasers.

In the following a list of the titles of beamlines or experimental stations proposed for PETRA III is given:

- X-ray diffraction and imaging
    - High energy X-ray diffraction

  - Coherence applications
  - High resolution diffraction
  - Micro- and nano-tomography

- High energy resolution spectroscopy
  - Inelastic scattering
  - Nuclear resonant scattering

- Materials science
  - High energy X-rays for materials science
  - Powder diffraction
  - Small angle scattering
  - Microfocus applications

- X-ray absorption and resonant scattering
  - Absorption spectroscopy
  - High-energy photoelectron spectroscopy
  - Hard X-ray microprobe
  - Resonant scattering
  - Variable polarization XUV beamline

- Structural biology
  - Macromolecular crystallography (EMBL proposal for three stations, MPG proposal for two stations)
  - Biological absorption spectroscopy
  - Biological small angle scattering

In the following sections each proposed station will be described briefly. For the final layout of the experimental hall it is assumed that in many cases more than one experimental station can be operated in time sharing mode on a single undulator beamline if the requirements for the beamline optics are similar.

2.3.1 X-ray diffraction and imaging

2.3.1.1 High energy X-ray diffraction

With the development of high-energy 3rd generation synchrotron radiation sources, high-energy X-ray diffraction became a powerful tool for the analysis of bulk materials and buried interfaces by the use of extremely collimated and small beams. Since the absorption lengths above 100 keV for most materials lie in the range of 0.1 mm to several cm, studies on thick samples become feasible. For the same reason, thick window materials for sample environments as cryostats or furnaces become less critical or even negligible. Moreover, difficult corrections for absorption, extinction and multiple scattering effects can be avoided in many cases. Another important feature of high-energy X-rays is that reciprocal space can be mapped up to large momentum transfers such as 30–50 Å^{-1}, which is crucial for precise structure determination of liquids and amorphous materials. Up to now most applications of hard X-rays have addressed bulk properties of thick samples. However, the application of high-energy diffraction methods becomes particularly attractive if combined with microfocusing techniques. The high penetration depth allows one to directly access ordering phenomena and phase transitions at buried interfaces that are not accessible with any other technique. It is expected that such studies can be extended into new areas by using high-brilliance X-ray beams delivered at PETRA III.

Using a particle energy of 6 GeV the flux density at 100 keV photon energy delivered by a PETRA III undulator or wiggler is one or two orders of magnitude and the brilliance is more than four orders of magnitude larger than the most powerful hard X-ray insertion device at DORIS III. Upcoming new insertion device techniques, like superconducting in-vacuum undulators, and the very small emittance of PETRA III will provide an even more brilliant beam at higher photon energies. The beam will be further concentrated by refractive lenses and/or bent monochromator crystals. The beamline will be optimized for an energy range of 50–100 keV. A minimum focal spot size in the micrometer range is envisaged for the investigation of buried layers or small volume elements inside larger bulk samples. The beamline will be equipped with a flexible high precision diffractometer. However, there will also be enough space for special setups developed by users.

2.3.1.2 Coherence applications

A recent development at modern synchrotron radiation sources is the use of coherent undulator radiation for both, scattering and imaging applications. If coherent light is scattered from a disordered system it gives rise to a random diffraction or “speckle” pattern. Such a “speckle” pattern is an interference pattern and related to the exact spatial arrangement of the disorder although phase information is lost. Major progress has however been made in recent years (e.g. by the oversampling technique) to retrieve this phase information, thus allowing to reconstruct the pattern and to unravel real space information.

The improved coherence parameters at PETRA III (almost 100 μm spatial coherence length in the low-β configuration, see Tab. 2.2.3) will facilitate the reconstruction of complicated patterns and allow access to shorter (eventually atomic) length scales. One might anticipate that even disorder in magnetic systems will become accessible. This will only be possible due to the high brilliance B and the correspondingly increased coherent flux $F_c=(\lambda/2)^2 \cdot B$ provided by the PETRA III undulators.

The unprecedented coherence properties of the PETRA III source will also impact imaging techniques in the near field or Fresnel limit. Phase contrast imaging will benefit from an increased degree of coherence and the increased flux will allow not only to improve the resolution but might enable time series of phase contrast images limited only by the detector frame rate.

Of outmost importance is the possibility to study the dynamics of disordered systems with coherent light: If the spatial arrangement of a system changes as a function of time the corresponding speckle pattern will also change and fluctuate. Characterization of temporal intensity fluctuations is usually performed by correlation spectroscopy techniques and X-ray photon correlation spectroscopy (XPCS) gives access to the slow (>ns) dynamics on length scales ($Q > 10^{-3}$ Å^{-1}) not accessible to visible coherent light. Many applications lie in the soft condensed matter domain (dynamics of complex fluids, glass forming systems, or capillary wave dynamics) or in the area of critical fluctuations. Here it is in particular the increased coherent flux of the PETRA III facility that will allow to address questions of slow dynamics on even shorter length scales (<100 nm) than presently feasible. Furthermore, the improved beam parameters will permit the operation in heterodyne mixing mode (known from Dynamic Light Scattering) and to finally also address questions of non-equilibrium dynamics. The energy tunability, the polarization properties of the beam and the surface sensitivity of X-rays will allow XPCS to be applied to a multitude of surface/interface phenomena and to the dynamics of magnetic systems being barely possible or unachieved today.

2.3.1.3 High resolution diffraction

High resolution X-ray diffraction (HRXRD) using extremely collimated beams is widely used as a standard technique for structural investigations at a wide variety of length scales, from the atomic level to bulk behavior and to surfaces and interfaces. The technique is used for precise lattice parameter measurements to access very small changes in lattice spacing due to thermal expansion, strain, chemical composition, or due to the exposure to external fields, etc. At solid and liquid surfaces and buried interfaces HRXRD allows to determine parameters, such as layer thickness, chemical composition and interface roughness. By variation of the penetration depth in grazing incidence diffraction also depth-resolved studies are possible. Two-dimensional reciprocal space mapping methods are now standard for these applications. Lattice distortions and crystal quality can be examined by reflection profile analysis. Structural parameters of periodic and non-periodic nano- or mesoscopic structures can be investigated by high resolution reciprocal space maps.

The low emittance and high brilliance of PETRA III provides ideal beam conditions to generate a photon beam of ultra-high collimation and high monochromatization over a wide energy range. The high coherence length of the beam will provide access to length scales ranging up to tens of micrometers. The brilliance available also at higher photon energies (25–45 keV) will enable experiments at internal solid/solid and liquid/solid interfaces. This is of special importance, as interface processes are so far mostly studied in model surface experiments. The high brilliance will also allow in situ studies of process dynamics which determine diffusion, growth and phase transitions. Research on very small sample volumes and highly diluted materials will become feasible. The beamline will be equipped with an UHV chamber connected via a transfer tunnel to a UHV preparation chamber for surface research.

2.3.1.4 Micro- and nano-tomography

In recent years micro-tomography using synchrotron radiation became a valuable tool for the non-destructive three-dimensional investigation of specimens in fields such as medicine, biology and materials science. At DORIS III absorption- and phase-contrast techniques were developed and applied at photon energies in the range of 8 to 150 keV. At the wiggler-beamlines BW2, W2, and BW5, a public user instrument for microtomography makes use of the large, intense, and incoherent X-ray source. Experiments at DORIS III are optimized for performing absorption-contrast microtomography on large samples. Due to the divergence of the source the spatial resolution of a tomogram is limited to about 2 μm.

PETRA III will allow for new absorption- and phase-contrast techniques which make use of the coherence of the X-ray beam. Different features of the specimens can be mapped simultaneously. By using a standard setup the spatial resolution can easily be increased to resolve about 0.7 μm structures. For resolving smaller structures in the 100 nm regime new techniques have to be developed. Recently first results were obtained performing cone-beam tomography by creating a nanometer divergent X-ray source using a KB multilayer arrangement and magnifying the sample onto a two dimensional X-ray detector.
The standard user experiments for microtomography at PETRA III will require a large monochromatic, parallel and intense beam. The photon energies will range from 8 to 150 keV and the required beam size is about $5\times1\,\mathrm{mm}^2$. To achieve a smooth beam profile the beamline will have as few optical elements as possible. The experimental hutch will allow for a variable sample detector distance from almost 0 to 10 m. For cone-beam geometry, optical elements will be added to the beamline to achieve a divergent X-ray source in the nm regime. The high brilliance of PETRA III and the development of faster detectors will also enable time resolved tomographic studies.

2.3.2 High-energy resolution spectroscopy

2.3.2.1 Inelastic scattering

Inelastic X-ray scattering (IXS) with meV energy resolution allows one to study elementary excitations in condensed matter, providing detailed insight into the mechanisms of phase transitions and dynamic processes. These properties play a crucial role in nanoscale materials because the modification of the dynamic properties due to the reduced dimensionality very often forms the basis for a new functionality. In this field, inelastic X-ray scattering at PETRA III will open new research areas that are hardly accessible at existing facilities. Particularly exciting are the study of low-energy excitations in disordered metallic alloys and the study of lattice dynamics in high-T_c superconductors and correlated electron systems, for example. A unique feature of IXS at PETRA III will be the combination of inelastic scattering with microfocusing techniques. Experiments on smallest amounts of material like thin films, single crystallites within a polycrystalline material and tiny grains of material in diamond-anvil cells under extreme conditions of pressure and temperature will be possible. Metastable and non-equilibrium phases become accessible that can only be produced in small quantities like tiny crystals or thin films.

The small beam sizes available at PETRA III allow for a very efficient implementation of spectrometers with sub-meV resolution. This will help to clearly identify low-energy collective excitations that are often observed in disordered materials and in the vicinity of phase transformations. KB mirror optics will be used for the generation of sub-μm focal spots for the investigation of extremely small amounts of material. The instrument proposed here consists of a vertical spectrometer for the investigation of excitations in single crystals with 2–3 meV energy resolution and a horizontal spectrometer for the study of dynamical properties of disordered materials with sub-meV energy resolution. In general, the properties of the radiation delivered at PETRA III will stimulate the development of innovative experimental techniques in this field that are hardly possible at existing sources. The utmost performance of these techniques is achieved if the experimental stations are installed at the 20 m long undulator, because many of these experiments are strongly flux-limited. This will put this beamline significantly ahead of those that are currently in operation.

2.3.2.2 Nuclear resonant scattering

Nuclear resonant scattering (NRS) using synchrotron radiation has a long standing history in Hamburg since the first experiments almost 20 years ago at the DORIS storage ring. The advent of high-energy 3^{rd} generation synchrotron sources has turned this method into a routine experimental technique. With increasing brilliance of the radiation, this method became sensitive to smallest amounts of material like single monolayers, nanoparticles and samples in high-pressure cells. This trend will continue at PETRA III, so that magnetic ordering and vibrational dynamics in reduced dimensions can be revealed. The narrow energy bandpass makes NRS an ideal tool to study dynamical properties on very short time scales. Examples are diffusive and relaxational processes that can be studied on time scales ranging from ps to μs. The much faster dynamics of phonons becomes accessible in an energy resolved mode with resolutions in the sub-meV range. Moreover, the high brilliance at PETRA III will allow for the application of ultrathin isotopic probe layers to study magnetic and dynamic properties with atomic resolution.

Due to the narrow linewidth of the nuclear resonances involved (typically some neV to μeV) NRS experiments are extremely flux hungry. For this reason such experiments have to be performed at the 20 m insertion device at PETRA III. An experimental station at this insertion device will provide $1.6 \cdot 10^7$ ph/s in an energy bandpass of $0.1\,\mu$eV. This is four times higher than on other NRS beamlines at present 3^{rd} generation synchrotron radiation sources. Besides the established and widely used techniques where a resonant isotope is needed as part of the sample, the increased spectral flux available at PETRA III could make time-domain interferometry a more widespread technique. This offers the option to study dynamical properties of samples that do not contain resonant isotopes.

2.3.3 Materials science

2.3.3.1 High energy X-rays for materials science

The activities on the new high energy materials science beamline will be concentrating on three intersecting topics: Industrial research, applied research, and fundamental research. The industrial user community will be provided with fast, robust, and standardized experimental techniques and online data analysis routines. Applied research will focus on the in-situ investigation of real manufacturing processes, the optimization of systems of high interest (e.g. fuel cells, battery electrodes), ”classic” as well as cutting edge materials (e.g. Mg-base alloys, TiAl, trip-steel, bulk metallic glasses, composites, ceramics, ”smart materials”), and materials processing. Fundamental research will yield new insight in the field of metallurgy (e.g. micro structure, grain boundary engineering or the understanding of complex phenomena such as plastic deformation), rapidly emerging fields like biomimetics (e.g. biomineralization) and nanoscience. The length scales at which the different experiments are aiming at will range from the macroscopic over the mesoscopic scale down to the investigation of nano structures, atoms, and their displacements down to the range of 10^{-15} m. All applied techniques will be non-destructive, allowing bulk investigations of several centimeters thick samples.

The beamline will have an insertion device with a main energy of 120 keV, tunable in the range from 50–300 keV and optimized for sub-micron focusing. Positioning units for samples up to 1 t will be available. A 150 m long flight tube will be installed for small angle scattering experiments at high energies. The beamline will stand out by the combination of three unique main features: Firstly, the high flux, ultra fast data acquisition systems, and the beamline infrastructure will be the basis for complex in-situ experiments for the observation of highly dynamic processes. Secondly, an exceptional flexibility in beam shaping and focusing down to spot sizes below 1 μm will be available for the high energy X-rays. Thirdly, the beamline will provide the possibilities to merge different analytical techniques such as diffraction, tomography, small angle scattering, and spectroscopy. By exploiting these techniques simultaneously it will be the first beamline, where the boundaries between the different analytical techniques are gradually disappearing, being one of the prerequisites for a leap in materials science and engineering research.

2.3.3.2 Powder diffraction

Powder diffraction is the method of choice for crystal structure determinations if no single crystals can be obtained or if samples have to be investigated under conditions where single crystals are not stable, for example during a phase transition. New experimental techniques as well as new data evaluation methods developed recently provide means to solve crystal structures from powder diffraction data with increasing complexity.
Other important applications of powder diffraction are in-situ studies such as formation of new phases in chemical reactions. Further examples are reactions of solids with gases or liquids as they are common in catalysis research like the adsorption of molecules into zeolites or ion exchange reactions between solids and liquids.

Undulator photon beams from a low emittance high energy storage ring like PETRA III have several advantages for powder diffraction experiments: (i) the high brilliance provides intrinsically very parallel photon beams that are needed to resolve neighboring diffraction profiles, (ii) even at energies as high as the foreseen 50–60 keV a very high photon flux is available, (iii) very small focal spot sizes can easily be achieved by suitable optics for experiments on small sample volumes as they are needed for example in high pressure investigations. The high photon energy of the proposed station has the advantage of a reduced radiation damage mainly for organic materials that contain mostly light atoms, less absorption and therefore the possibility to collect more accurate data for heavily absorbing samples, and the option to penetrate through sample or reaction containers in case of in-situ studies.

2.3.3.3 Unfocused small angle scattering

Classical Small-Angle X-ray Scattering (SAXS) experiments average over a large sample volume and give structural and quantitative information of high statistical significance on a mesoscopic length scale between 1 and several 100 nm, which can be correlated with macroscopic physical and chemical parameters of the analyzed materials (alloys, semiconductors, glasses, macromolecules in solution, metal nano particles, composites). In addition to the normal SAXS signal, the anomalous signal close to absorption edges of suitable atoms can be exploited for contrast variation. This so-called ASAXS method has gained quite some importance in materials science, catalysis and polyelectrolytes.

Due to the low emittance of PETRA III, the beam parameters at a high-β section are best suited for the design of an unfocused SAXS beamline with high Q-resolution. Additionally the energy spectrum covered by a PETRA III standard undulator will allow to make use of the element-selective ASAXS technique and to extend the classical energy range of this technique (5–35 keV) up to energies of about 90 keV. The extension to higher energies will give access to the K-absorption edges of the heavier elements ($Z > 53$). The energy range in combination with the high flux of a 3^{rd} generation source offers the opportunity to address numerous challenging scientific objectives in solid state physics, catalyst research, chemistry and biology, which are not accessible by the existing state of the art (A)SAXS-experiments.

2.3.3.4 Microfocus applications

A scattering beamline with micro- or nano-focus capabilities will enable static and time resolved measurements in the WAXS[5] to the USAXS[6] regime for the investigation of phase formations and transformations in a vast variety of isotropic and anisotropic materials like polymer systems, colloids or nanostructured samples. Using an extremely small focus allows the spatially resolved investigation of hierarchically organized samples in the field of life science like bones or wood and synthetic systems like polymer composites. WAXS, SAXS and USAXS under grazing incidence conditions allow one to study short and long range ordered

---

[5] Wide Angle X-ray Scattering

[6] Ultra Small Angle X-ray Scattering

systems on substrate surfaces like dewetting polymer films on metals, adhesives during detaching from a surface or self organization of quantum dots on semiconductor surfaces. To a certain extent all these techniques can be combined with a micro focus in order to investigate a sample by 2D-scanning techniques.

Due to the extremely low divergence of the undulator located at a high-β section of PETRA III, a focus of 7 μm vertical and 40 μm horizontal width (FWHM) with 13 μrad vertical and 120 μrad horizontal divergence (FWHM) can be achieved. A Kirkpatrick-Baez (KB) mirror arrangement with a first mirror at 57 m behind the source and a second one at 75 m will reach such a focus which is then at 85 m distance from the source and has a total flux of $3{\cdot}10^{13}$ photons/s using a Si(1 1 1) double crystal monochromator at 10 keV. The low divergence still maintained in this focus allows to resolve correlation distances of up to 1000 nm in the vertical direction and about 200 nm horizontally, the latter can be increased by accepting a corresponding flux reduction. This high brilliance beam will surpass all others available for comparable scattering applications at existing 3^{rd} generation synchrotron radiation facilities worldwide.

2.3.4 X-ray absorption and resonant scattering

2.3.4.1 Absorption spectroscopy

In general, X-ray absorption fine structure (XAFS) and X-ray absorption near edge structure (XANES) are no typical high-brilliance applications. However, if very small sample regions have to be investigated as it is the case in high pressure experiments, for example, a highly brilliant source is mandatory. This applies as well for XAFS tomography or for μ-XAFS if a very high spatial resolution is desired. Furthermore, the considerable brilliance of a PETRA III undulator at higher photon energies allows to measure XAFS at the K-edges of heavy elements with reasonable flux. Despite the life time broadening these spectra yield more precise spectral information than measurements at the L_3-edges, because the scan range can be larger and the matrix effects are negligible. Higher energies offer the possibility to study these elements, for example during in situ experiments in catalysts.

The design of the beamline has a monochromatic beam (ΔE/E $\sim 10^{-4}$) tunable over an energy range of up to 2000 eV while covering an energy range between 2.4 and 80 keV using different crystals. It will be followed by an optional pair of mirrors for the suppression of higher harmonics radiation. The final focusing device for spot sizes < 1 μm will be close to the sample. Depending on the photon energy, KB-mirrors and different kinds of lenses will be used. A low-β section will be of advantage to achieve a very small focus. The experimental hutch will be equipped with all necessary installations to perform in-situ experiments with toxic and/or flammable gases and liquids.

2.3.4.2 High-energy photoelectron spectroscopy

Photoelectron spectroscopy is a key method to study electronic properties of matter in solid state physics and materials science, providing unique information on chemical bonding and composition, on electronic correlations and other atomic many-body effects. In conventional applications using UV and soft X-ray excitation, the information is obtained from the topmost atomic layers due to the short electron mean free path. This is a serious limitation since electronic properties near the surface often differ from those of the bulk material. Buried interfaces and structures cannot be reached at all. The high surface sensitivity can be overcome with hard X-rays emitting energetic photoelectrons with a correspondingly larger escape depth up to about 10 nm around 10 keV kinetic energy. At the same time, the short photon wavelength can be utilized to excite X-ray standing waves in crystalline materials thus allowing to correlate structural and electronic information on an atomic scale.

Hard X-ray photoelectron spectroscopy with high-energy resolution down $\approx$ 10 meV is extremely challenging and requires an intense and brilliant source as well as highly sophisticated and efficient electron detection. At present, strong attempts are being made to implement this promising new technique at 3^{rd} generation X-ray sources. The experimental station proposed for PETRA III specifically utilizes the low emittance properties. The low divergence beam from a high-β undulator is ideally suited for high-resolution monochromatization ($\approx$ 10 meV at 10 keV) preserving the high monochromatic flux ($\approx 10^{11}$ photons/s) needed to cope with low photoelectric cross sections and electron analyzer transmission. Furthermore, the achievable resolving power of the analyzer is directly linked to the focus size on the sample which can be easily brought down to 10 μm with suitable optics such as KB-mirrors. If sub-micron focussing of the beam is accomplished, lateral spatial resolution for studies of inhomogeneous materials is achieved in a scanning mode of operation. In combination with the high bulk-sensitivity, this will make the instrument a unique tool for studies of the electronic and chemical properties directly of bulk material and, in particular, buried nano-structures.

2.3.4.3 Hard X-ray microprobe

Hard X-ray microprobe beamlines combine the non-destructive elemental micro-analysis capability of μ-XRF (microscopic X-ray fluorescence analysis) with the ability of performing complementary μ-XAS (X-ray absorption spectroscopy) and/or μ-XRD (X-ray diffraction) measurements. These instruments provide simultaneously correlated information on the local elemental composition, chemical state, the local structural environment of specific elements and/or the local crystallographic structure of the examined materials. Hard X-ray microprobe techniques are mostly applied in materials, geological, biological, biomedical, and environmental sciences, as well as archeology and arts.

The hard X-ray microprobe beamline will enable different complementary X-ray microbeam methods to be performed simultaneously or sequentially during one experiment. Scanning X-ray fluorescence microscopy measurements in combination with broad beam radiography imaging will be the most straightforward technique to characterize heterogeneous samples in terms of local elemental composition and density. Microscopic X-ray absorption spectroscopy (μ-XANES, also μ-EXAFS) and microscopic X-ray diffraction will provide information on the local speciation and structure. Tomographic methods (fluorescence mi-

crotomography, XANES microtomography) and confocal arrangements of X-ray optics for the primary beam and fluorescence photons give access to quantitative three-dimensional measurements.
The beamline will provide beam sizes down to the 100 nm range utilizing the outstanding small source size and high brilliance of PETRA III, but also larger beam sizes of 1–10 μm and an unfocused beam for flat field imaging will be available. The accessible energy range covers the K-edge energies from sulfur to uranium (E = 2.4–116 keV) and the flux is maximized by the use of KB mirrors. For broad band excitations a pink beam option is foreseen.

2.3.4.4 Resonant scattering

Correlated electron materials provide one of the biggest challenges of condensed matter research today. Complex magnetic ordering phenomena occurring in nano structured multicomponent materials are an example of the consequences of electronic correlations. Of particular interest are materials with exceptionally strong electronic correlations. The complex interplay of spin, charge, orbital and lattice degrees of freedom gives rise to a variety of different phases having insulating, metallic or superconducting properties, being anti-ferro, ferro- or paramagnetic and possessing different structures. The most prominent examples are transition metal oxides, which exhibit high-T_c superconductivity or the colossal magnetoresistance effect. The competition between the different phases can result in an electronic or structural phase separation from the Å to the μm scale.
Resonant X-ray scattering is an ideal tool to characterize the ground state of these new materials. It probes correlations of spin, charge, orbital and lattice degrees of freedom. The resonance technique provides element sensitivity and even band selectivity, giving detailed information on the electronic structure.

The resonant scattering experiments will take advantage of the excellent beam properties of the PETRA III source in the following aspects: (i) The high brilliance of more than 10^{21} photons/(s mm^2 mrad^2 0.1% BW) at 12 keV allows the design of X-ray optics that enable a high Q-resolution of about 10^{-5} Å^{-1} with considerable flux. (ii) A highly polarized beam, essential for the resonant scattering technique, can only be obtained on a small emittance source. At PETRA III a very high degree of linear polarization (close to 99.99 %) should be achievable. The high degree of linear polarization combined with small divergence provides the possibility also for a highly circular polarized beam using a phase retarder. (iii) Spatial resolutions ranging from micro- to nanometers can be acquired using a microfocus device which is important when studying nano-devices or phase separated materials. (iv) The high degree of coherence enables speckle experiments to resolve domain shapes and probe dynamic properties utilizing the time correlation function.

2.3.4.5 Variable polarization XUV beamline

Soft X-rays are ideal for spectroscopic investigations ranging from magnetism in nano structures to biological systems. Many absorption edges of practically all important elements lie in the soft X-ray range (100 eV to 3 keV) which opens up the possibility to uniquely determine the element-specific local electronic structure in complex materials by exploiting atomic resonances. Until recently really high brilliance light sources were not available for such investigations. Experiments at the latest 3^{rd} generation synchrotron light sources are now beginning to demonstrate the enormous scientific potential of this spectral region. Currently, investigations are still limited by the light source and improved sources will immediately produce new science. In the future, polarization-dependent studies with soft X-rays will play a key role in enhancing our knowledge of the structure of matter.

Suitable insertion devices at high-energy storage rings can provide very high brilliance of circularly polarized light in the energy range of 500–2000 eV as has been demonstrated at both the ESRF and SPring-8. Helical undulators operating in the first harmonic provide the highest flux and complete polarization, but require machine energies greater than 3 GeV. Insertion devices on lower energy machines like BESSY II, ELETTRA, and ALS only produce circularly polarized light up to about 500 eV in the first harmonic and newer machines like SLS and SOLEIL will extend this limit to 700–900 eV. The variable-polarization soft X-ray beamline at PETRA III will be unique and will open up completely new scientific opportunities by providing the highest brilliance and flux in the important spectral region from 500 eV to 2.5 keV . With current technology it is possible to achieve a spectral resolution of 10000 at 1 keV with an extremely high flux (more than 10^{12} ph/s) focused on the sample. Compared to the best present day sources the PETRA III soft X-ray beamline will provide up to two orders of magnitude higher flux at photon energies above 1 keV. This beamline will promote significant progress in fields ranging from surface science to molecular and cluster physics, magnetic studies, condensed matter physics and nanotechnology.

2.3.5 Structural biology

2.3.5.1 Macromolecular crystallography

Over the last fifty years biological X-ray crystallography has evolved into an advanced field of life sciences and has provided unprecedented three dimensional structural information on the molecular level of a large number of complicated biological processes. Knowledge of spatial structures has allowed to delineate the molecular origins for diseases such as cancer, autoimmune diseases and microbial infections. The performance and contribution of biological X-ray crystallography can be readily assessed by the huge number of new structures being deposited in the Protein Data Base (PDB), which is increasing at a nearly exponential rate. As a result, the growth in demand for synchrotron radiation beamlines for macromolecular crystallographic experiments has risen substantially both in absolute numbers and in overall proportion. New challenges for the future are the understanding of the function of large macromolecular assemblies. At present, the largest structures determined, though bearing internal symmetry, are from viral assemblies. Some of these structures have imposed unprecedented challenges in terms of the size of available crystals, which may be as low as a few microns, and unit cell dimensions, in a few cases even exceeding 1000 Å. Many of these projects have only become feasible with the recent availability of the highest brilliance beamlines at 3^{rd} generation synchrotron sources providing both a small focal spot size and a beam divergence small enough to resolve individual reflections even for the largest unit cells.

A number of beamlines for structural biology at PETRA III are proposed by the EMBL and MPG outstations at DESY. Due to the high brilliance of PETRA III about 10^{13} ph/s will be available in the monochromatic beam. Minimal focal spot sizes in the 10 μm range are envisaged. At the same time, the maximal divergence will not exceed 0.5 mrad even for the smallest focus. The different stations will be optimized for different applications such as wide range energy tunability, high-throughput structure determination, microfocus and special applications like investigation of large macromolecular complexes. All of them will be highly automated for optimum use of the beamtime.

2.3.5.2 Biological absorption spectroscopy

X-ray absorption spectroscopy determines the electronic structure of probe atoms and their structural vicinity. In biology typical probe atoms are metals or other elements of limited occurrence. In proteins metals fulfill a variety of essential functions: They stabilize the secondary protein structure, they serve as a binding partner in transport processes, they define the pathway for electron transfer, and they act as the key element in catalytic reactions. In at least 30% of the gene products, metals are believed to play a key role; these are classified as metallo-proteins. Cutting edge applications are (i) Time-resolved BioXAS experiments to facilitate insights in reaction dynamics/kinetics and structural characterization of intermediate states, (ii) spatially resolved XANES (tomography) facilitating spatially resolved speciation with respect to oxidation state and ligand environment and (iii) high-resolution fluorescence for site-specific measurements, these experiments have the added advantage that they provide greatly improved spectral resolution for XANES studies.

A BioXAS station at PETRA III with an energy range from 5 keV to 35 keV will cover K- and L- edges of most important probe elements in biological materials. A 2 m long standard $K_{\max} = 2.2$ undulator will provide sufficient flux for this station. The main advantage of PETRA III for BioXAS will be the small focal spot sizes. For tomography experiments at a low-β section a demagnification below 100 nm is possible with parabolic refractive Be-lenses. With KB mirrors similar spot sizes can be achieved. The high brilliance of PETRA III will also provide sufficient intensity for resonant inelastic X-ray scattering (RIXS) which is looking at the decay of excited states and is a powerful tool in determining site sensitive information on probe atoms as well as in understanding electronic structure of probe atoms and their ligands.

2.3.5.3 Biological small angle scattering

During the last decade, small-angle X-ray scattering (SAXS) has become an increasingly important tool for the study of biological macromolecules. The method enables studies of native particles in solution, from individual proteins to large macromolecular complexes, under nearly physiological conditions. SAXS not only provides low resolution models of particle shapes but in many cases answers important functional questions. In particular, kinetic SAXS experiments allow one to analyze structural changes in response to variations in external conditions. Fundamental biological processes such as cell-cycle control, signalling, DNA duplication, gene expression and regulation, some metabolic pathways, depend on supra-molecular assemblies, and their configurational changes over time can be studies by SAXS techniques. There are well recognized basic problems for studying such complex systems, especially their dynamic changes by other structural techniques like spectroscopy, NMR and macromolecular X-ray crystallography.

The recent resurgence of biological SAXS is due to the synergy of software and hardware development. New powerful data analysis methods have become available, which have tremendously improved resolution and reliability of models deduced from SAXS data leading to an enlargement of the user community.

A SAXS station for biological applications is proposed by the EMBL outstation. As the SAXS pattern is collected in the vicinity of the primary beam, the data quality depends critically on the beam size and divergence. SAXS is therefore among the techniques, which profit most from the low emittance undulator radiation on a 3^{rd} generation sources. Furthermore, the high flux of these sources is extremely important for the analysis of weakly scattering biological samples. Currently, high quality scattering patterns can be collected in less than a second using sub-mm beam sizes on the undulator SAXS beamlines at 3^{rd} generation sources. The biological SAXS beamline at PETRA III will provide a resolution range from about 2000 nm to 0.1 nm and will be tunable in an energy range of 4 to 20 keV in order to enable ASAXS studies using all relevant biological ions from Ca to Mo.

2.4 Future Upgrade Prospects

After the conversion of PETRA described in this report there will still be several future upgrade options for more beamlines. They all have the advantage that they do not need any significant change of the magnetic lattice of the storage ring.

- In the beginning one experimental station per undulator will be built. The efficiency of each beamline can be increased by constructing additional experimental stations with reproducibly positionable roll-in/roll-out equipment.
- In case of sufficient user demands, bending magnet stations can be build where the available space permits.
- The damping wigglers are designed to be cost effective and adapted to their main function to reduce the emittance. They generate a wide fan of extremely hard radiation. This radiation could be used for materials science experiments where a large beam is needed. However, the possibility to install additional wigglers that are better suited for hard X-ray experiments than the present damping wiggler design also exists.
- A number of positions around the PETRA storage ring exist where additional insertion devices can be placed without major changes of the magnetic lattice. There are two other positions at PETRA (buildings 43 and 45, see map in Fig. 2.2.1) where long

undulators could be placed as well as three positions (in or close to buildings 44, 46a/b and 48) for 5 m long IDs. Thus in total about 18 insertion device positions are available at the converted storage ring. The position of the additional insertion device positions are summarized in Tab. 2.4.1.

- On the long term it is envisaged to increase the storage ring current up to 200 mA.

in building	max. ID length [m]	max. BL length [m]
43	20	360
44	5	180
45	20	320
46	5	220
48	5	170

Table 2.4.1: Positions at the PETRA III storage ring where further IDs could be installed. The building number can be looked up in Fig. 2.2.1. The ID position labeled with ’46’ is actually not in building 46 but in the straight section closest to these buildings.

About half of the PETRA storage ring is underground. What seems to be a disadvantage at first sight might be a significant advantage for some of the future upgrade possibilities. Experience with ID’s for extremely high photon energies (more than several 100 keV) at ESRF, APS and SPring-8 has shown severe problems with radiation shielding which will be significantly relaxed at underground experimental stations.

2.5 Summary of Project Costs and Timetable

2.5.1 Project costs

The project cost estimates include all costs related to (i) the refurbishment of 7/8, and the reconstruction of 1/8 of the PETRA storage ring, (ii) the refurbishment of the pre-accelerators and accelerator infrastructure, (iii) all construction work necessary for the new experimental hall including radiation protection, offices and laboratories, (iv) the beamlines and experimental stations to be built and operated by DESY, and all costs for manpower.

The PETRA III upgrade project comprises about 13 beamlines at independent undulators. About seven of these beamlines will be built and operated by DESY. All other beamlines will be built or financed by external institutions like EMBL, GKSS and the Max Planck Society (MPG). The cost estimates given in this report do not include the beamlines and experimental stations built by external institutions.

On the basis of year 2003 prices the PETRA III project amounts to about **192 M€** of which 71 M€ are needed for the storage ring, 64 M€ for the new experimental hall including the DESY beamlines, and 57 M€ for personnel.

2.5.2 Time table

In Fig. 2.5.1 an overall time table of the most important milestones for the PETRA III project is given. The preparation and R&D for the PETRA III project has already been started (as of begin of 2004). The construction work will start in **July 2007**. First photons for user experiments are expected in **2009**.

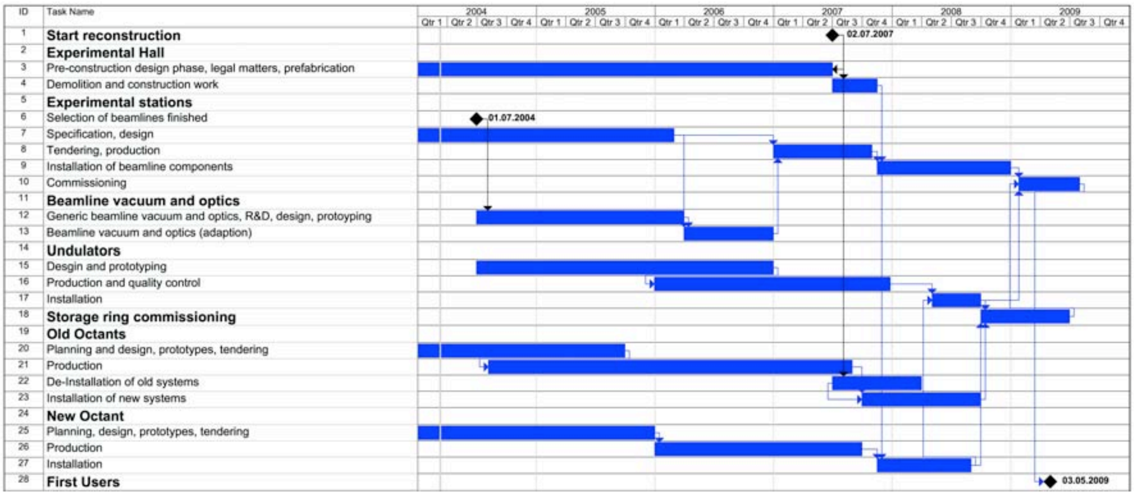

Figure 2.5.1: Summary of the time table and milestones of the PETRA III project. (Please use your readers zoom function for a more detailed view.)

Bibliography

Bernstein, F., Koetzle, T., Williams, G., Meyer Jr., E., Brice, M., Rodgers, J., Kennard, O., Shimanouchi, T. & Tasumi, T. (1977). *J. Mol. Biol.* **112**, 535–542.

Kim, K.-J. (1995). *Optical Engineering* **34**, 342–352. 1

Ropert, A., Filhol, J., Elleaume, P., Farvacque, L., Hardy, L., Jacob, J. & Weinrich, U. (2000). Towards the ultimate storage ring-based light source. *Proceedings of the 7th European Particle Accelerator Conference (EPAC 2000)*, pages 83–87. 2.2.1

Shenoy, G., Lewellen, J., Shu, D. & Vinokurov, N. (2003a). Variable-Period Undulators-A Potential Source for Storage Ring, ERL and FEL Applications. *Proceedings of the 8th International Conference on Synchrotron Radiation Instrumentation (SRI'03)*, San Francisco, USA. 2.2.3

Shenoy, G. K., Lewellen, J. W., Shu, D. & Vinokurov, N. A. (2003b). *J. Synchrotron Rad.* **10**, 205–213. 2.2.3

Tanaka, T. & Kitamura, H. (2003). *Program: SPECTRA*. RIKEN, Institute of Physical and Chemical Research. 2.2.2