International Workshop on the Science with and the Instrumentation for Small Quantum Systems at the European XFEL

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Report of Working Group II on

Dilute Ion Targets

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I. Introduction

The first International Workshop on the Science with and the Instrumentation for Small Quantum Systems at the European XFEL was held at the University of Aarhus on October 29th-31st 2008. As an integral part of the workshop two working groups were arranged with the goal of discussing specific aspects of experiments on Small Quantum Systems (SQS) with the XFEL light source. The Working Group II on dilute ion targets (WGII) was organized during Thursday, October 30th (14:00-17:30) and on Friday, October 31st (9:00-10:30). The working group program was formulated by Henrik B. Pedersen (University of Aarhus, Denmark) and Stefan Schippers (Giessen University, Germany). It was structured into three sessions on i) ion-target preparation, ii) ion-XFEL interaction, and iii) XFEL beam and additional laser sources. Each session included short (10 min) presentations followed by 10 min discussions (see Appendix I). The WGII sessions were attended by about 40 % of the workshop participants (see Appendix II). The present report summarized the discussions and conclusion from the WGII.

Experiments with targets consisting of charged particles are challenging because the target number density is usually limited by space charge effects to less than 10^5 - 10^6 cm^{-3}. These densities are several orders of magnitude lower than what can be realized for, e.g., neutral atomic or molecular beams, and consequently the experimental approaches for studying light – charged-matter interactions are distinctly different from experiments with gaseous targets. These techniques, however, combined with the ultra intense XFEL light sources open for investigations into several unexplored territories of fundamental science as will be reviewed shortly in Section II. The properties of the XFEL light source and the requirements to the XFEL beam delivery are briefly discussed in Section III.

From the WG II discussions two specific experimental approaches emerged that should be pursued for studying the interaction of radiation from the European XFEL with dilute ion targets. The first approach makes use of a fast beam that is circulating in a compact electrostatic storage ring and the

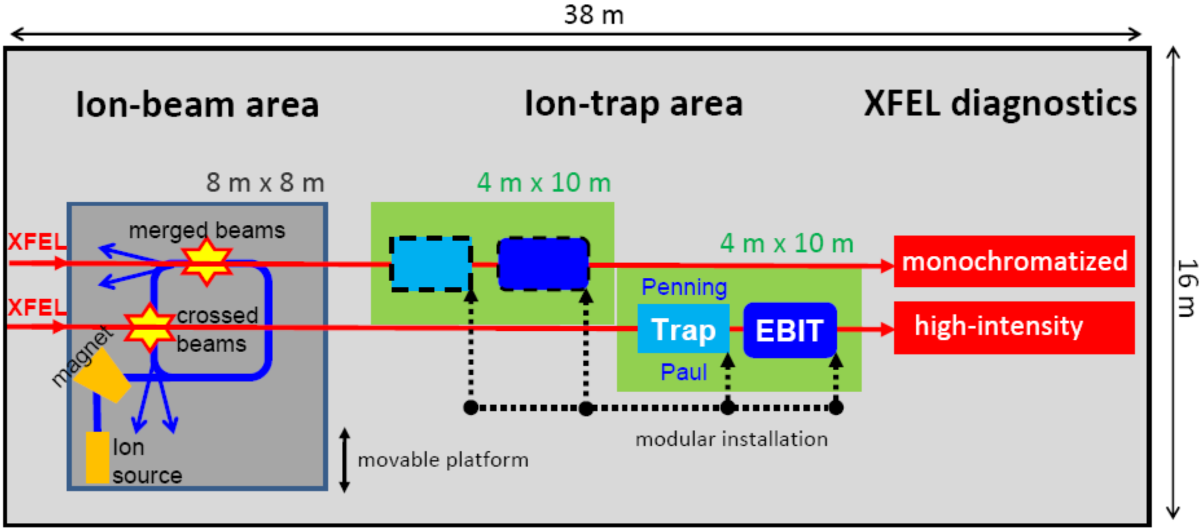

Figure 1: Layout of the SQS ion-beam and ion-trap installations in the designated SASE-3 area of the experimental hall with approximate space requirement estimates. The two photon beams from the SASE-3 undulator enter from the right. Dimensions are only approximate. The ion beam facility will be permanently installed. The ion traps are small-scale devices that do not require a perment installation. They can be flexibly moved into the high intensity beam and the monochromatized beam, alike, as indicated by the dashed arrows.

second approach employs trapped ions. Figure 1 presents an overview over the proposed experimental installations. Details will be described and discussed in the later sections IV of the present report.

II. Science with dilute ion targets at the European XFEL

The workshop in general and the WGII in particular demonstrated that there is a multi-faceted scientific case for experiments with ionic targets at the XFEL to study fundamental interactions and dynamical processes of SQS ranging from atomic ions to complex molecules in a wide range of charge states and mass-to-charge ratios. The scientific case for SQS at the European XFEL has been laid out comprehensively in the XFEL technical design report (TDR, see http://xfel.desy.de/tdr/tdr/). The following topics were found to constitute large interest with dilute ion targets in TDR and have been confirmed in the WG II discussions:

- *Inner shell ionization in atomic ions in both low and high charge states*.
- *Molecular dynamics following x-ray photoionization revealed by kinematically complete momentum imaging.*
- *Multiphoton studies in the x-ray spectral region.*
- *X-ray photons scattered at trapped ion crystals in Penning or Paul Traps.*

These have been complemented in the WGII discussions by the following further topics based on recent research developments:

- *Photoelectron spectroscopy and photoelectron-photoion coincidences in photoionization of atomic ions:* Only three pilot experiments on x-ray photoelectron spectroscopy of atomic ions have been reported. The results were discouraging so far, because of too low signal rates and too adverse signal/background ratios. With the exceptionally high photon flux from the European XFEL this situation will change. Photoelectron spectroscopy of atomic ions would allow to study phenomena along isoelectronic sequences and to follow trends as a function of nuclear charge yielding more fundamental insight into atomic ionization dynamics.

- *Photofragmentation of large biomolecular ions:* In living cells many biomolecules are protonated, deprotonated, or otherwise charged, and moreover active ionic biomolecular spieces (e.g. chromophores), are often embedded in larger molecular structures where solvation effects are limited. Therefore, it is of large interest to investigate ionized biomolecules in dilute ion targets. Size and conformation selected biomolecular ions will form extremely dilute beams, and photoionization, coincidence photofragmentation and electron spectroscopic experiments require highest photon fluxes. Structural information on biomolecular ions is usually obtained by breaking them by one of several "slow-heating" methods, such as infrared multiphoton dissociation, collision-induced dissociation or blackbody infrared radiative dissociation. Core-hole ionization will open a completely new window to biomolecular fragmentation, which will most likely involve the breaking of bonds not accessible to the "slow-heating" methods.

- *Inner shell photodetachment and photofragmentation of atomic and molecular anions:* The photofragmentation dynamics of negative ions display fundamental aspects of electron correlation in atomic and molecular systems, and x-ray two-electron detachment has indeed been studied with intense ion beams at synchrotrons using merged beams setups. The extreme photon pulse intensity at the XFEL opens the possibility to extend these studies to crossed beams where photoelectron and photofragments momentum imaging becomes feasible. For instance, by measuring the energy and angular correlation of the emitted electrons in x-ray two-electron detachment details on postcollision interactions will be illuminated.

- *Photoionization and photofragmentation of (endohedral) fullerene ions, mass selected cluster ions, and complex molecular ions:* Endohedral fullerene ions are prototype systems of high scientific interest that are only available in extremely dilute targets. Merged-beams experiments with sub-picoampére beams have been successfully carried out at a 3rd generation synchrotron light source. It is desirable both to work with better characterized, i.e, cooled ions in the merged-beam geometry, and to extend the studies to the crossed beams geometry opening for photoelectron and photofragment momentum imaging. Both the cooling process and the crossed beams geometry will effectively dilute the target even more, thus strongly emphasizing the benefit from the extreme photon fluxes available from XFEL.

- *Investigations of Highly Charged Ions with an EBIT.* Pioneering results carried out with an EBIT at the Free Electron Laser at Hamburg, FLASH on the resonant excitation of Fe^{23+} ions by 49 eV photons (and in the year 2008 at 65 eV photon energy) have recently demonstrated for the first time resonant fluorescence laser spectroscopy in the soft x-ray region, and the enormous potential of this method. Also in the year 2008, experiments at the BESSY-II synchrotron investigating ions not typically associated with EBITs, namely N^{3+} being photoionized to N^{4+} have also shown the capabilities of modern EBITs to operate at energies of the ionizing electron beam as low as 50 eV but going up when needed to tens of keV, and thus accessing a range of charge states from the only multiply ionized to the genuinely highly charged ions. Free electron lasers (FELs) have opened a new avenue for investigating the interaction of VUV to x-ray radiation with HCIs, which are perhaps the most abundant form of visible matter in the Universe. Newest x-ray observations of intergalactic gas clouds containing highly ionized matter in the temperature range from 300,000 K to 5,000,000 K have strengthened this hypothesis. The proposed HCI target would therefore enable many different experiments related to their photoionization, photoexcitation, and precision spectroscopy. The areas of investigation would include relativistic atomic structure theory in the regime of nonperturbative quantum electrodynamics (QED), multiphoton ionization, and radiative lifetime measurements in the femtosecond region. Moreover, the high target area density would grant access to nuclear structure investigations. Such experiments have been already carried out using standalone EBITs, but in combination with the brilliant photon beams of the future XFEL, far reaching precision tests of the Bohr-Weisskopf effect and other finite nuclear size effects, as well as studies of parity violation, photo-nuclear interactions, or the excitation of isomeric levels are conceivable. Another very interesting possibility arises from instantaneously ionizing cold and dense trapped ion ensembles with XFEL photon bunches. The strongly correlated plasmas produced in this way would have novel properties, which can be diagnosed through various spectroscopic methods. Due to their relevance for astrophysics, initial experiments with the EBIT would address most likely the absorption spectra of the highly ionized matter surrounding active galactic nuclei (AGN). The observational data cannot be modeled with existing atomic models because of wavelength uncertainties and lack of laboratory benchmarks. Later, pump-probe experiments at XFEL will aim at determining radiative lifetimes in the femtosecond regime, essential for astrophysics and plasma physics.

- *Photoionization of single trapped atomic and molecular ions:* Through sympathetic cooling through the Coulomb interaction with a laser cooled atomic ion, a single trapped target ion can be spatially localized to about 1 μm in all dimensions. Combined with the very tightly focus of the XFEL photon beam (1 μm focus), one can hence obtain really high photoionization yields even for a spectral filtered photon beam, or in studies of low cross section processes. Techniques are available for essential 100% efficiency *in situ* analysis of mass and charge state of the target ion before and after photoionization. This feature opens up the possibility of investigating consecutive photoionization of a particular target ion. Furthermore, repeated photoionization from a specific charge state can be achieved by momentarily introducing a gas in the trapping region for realizing a charge exchange collision after photoionization has been detected. This "recycling" principle may reduce the number of times a new ion will have to be loaded, and hence in particular be of interest when experimenting with rare or difficult producible ion species.

- *X-ray spectroscopy of single Highly Charged Ions (HCIs)*: As in the case discussed above, through sympathetic cooling, a single trapped HCI ion can be spatially localized to about 1 μm in all dimensions. Combined with the very tight focus of a spectral filtered XFEL beam (1 μm focus), one can do absorption spectroscopy on HCIs by detecting the recoil kick that a HCI will receive through the absorption of a single X-ray photon. The recoil energy can for X-ray photons be much larger than the initial temperature of the HCI when sympathetically cooled, and hence the absorption can be detected simply by observing a sudden chance in the temperature of the combined system of the HCI and the laser cooled ion.

III. XFEL beam parameters and features

As a branch of the upcoming XFEL facility, the SASE 3 undulator will be a dedicated extremely intense high spectral brightness source in the soft X-ray region. This branch will deliver short (< 30 fs) pulses of 10^{12}-10^{14} photons in the energy range 250-3000 eV (5.0 - 0.41 nm) with an effective repetition rate of up to 30000 pulses per second. The time-averaged photon flux will be 10^{17}-10^{16} /s /0.01% bandwidth, 3-5 orders of magnitude larger than at any other synchrotron radiation facility (figure 2).

Two photon beam lines are planned in the user area behind the SASE3 undulator delivering monochromatized (1-2 x 10^{-4} bandwidth) and direct light (10^{-2}-10^{-3} bandwidth) from the free electron laser. At the XFEL facility, the user area behind these two beam lines will have a footprint of 16 x 38 m^2. In the startup scenario for the XFEL this area is foreseen to hold experimental stations for Small Quantum Systems (SQS) and Soft x-ray Coherent Scattering (SCS).

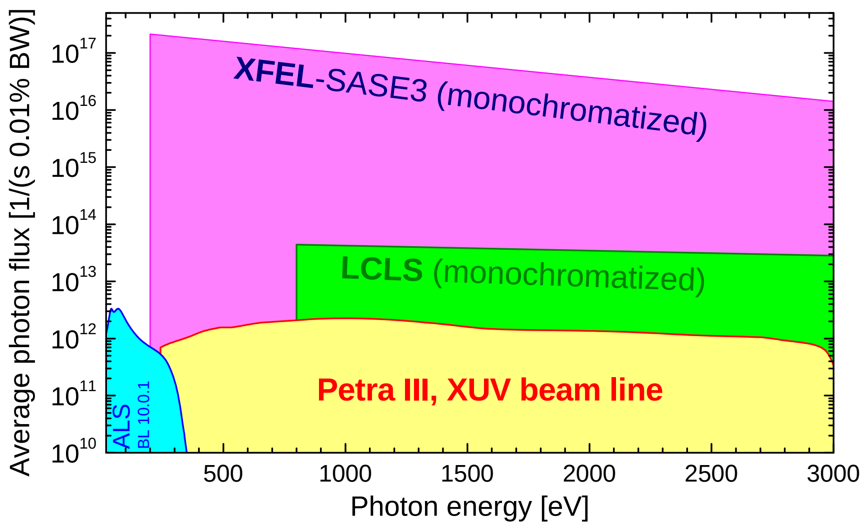

Figure 2: Comparison of the average photon flux per 10^{-4} bandwidth at different VUV and XUV beam lines. The XFEL and LCLS curves are rough estimates based on the respective undulator output parameters.

The XFEL radiation from the SASE3 undulator is excellently suited for experiments with dilute ion targets. All experiments listed above depend on and efficient use of the superior parameters of XFEL.The general requirement of experiments with dilute ion targets is that the photon beam intensity should be as high as possible both per pulse and time-averaged. Besides intensity, the following further radiation parameters and features have been discussed in WG II:

Photon energy range: The envisaged photon energy range 250-3100 eV is compatible with the requirements for experiments with dilute ion targets. For spectroscopic studies of biomolecular and e.g. (endohedral) fullerene ions photon energies down to below the carbon K-edge at about 284 eV should be available.

Pulse repetition rate and time structure: Time of flight detection methods are compatible with the envisaged repetition rate of up to 30 kHz. A repetition rate as high as technically feasible is very much welcomed because of the increased average photon flux. To enable multiple use of the same XFEL beam it would often be advantageous to control the specific time structure of portions of XFEL pulse train or different pulses trains, i.e. for instance by variation of the pulse spacing during a single pulse train.

Polarization: The SASE3 startup scenario foresees only linear polarized radiation. Most experiments are not constrained by this choice. In the farther future, however, circularly polarized radiation should be available for studies of orientation phenomena as well as circular dichroism effects.

Focus: A typical diameter of an ion beam in a storage ring is 1 mm. Therefore, the photon beam diameter may be rather large at any interaction point within the storage ring. In fact, for merged-beams interactions a parallel photon beam with a diameter of up to a few hundred micrometers would be optimal. A tighter focus of below 100 μm is needed for the EBIT and Penning trap experiments where the target ion cloud has spatial extensions of this size. Studies with single ions in a Paul trap require a focus size of 1 μm.

Monochromaticity: Photon-hungry experiments (e.g. crossed beams) prefer beam intensity above resolving power. These experiments are content with the SASE3 undulator's 0.1-1% bandwidth at the high intensity branch. Some spectroscopy experiments (EBIT, Penning trap, merged-beams) require higher resolving powers in the 1×10^4 to 2×10^4 range and efficient suppression of higher harmonics. The monochromatized photon beam branch should be accessible for these experiments.

Tunability: Spectroscopy experiments (merged-beams, traps) need to tune the photon energy across resonances. At synchrotron light sources users can tune the photon energy by simultaneous control of undulator gap and monochromator settings. Ideally, such a scheme should be made available at the monochromatized SASE3 photon beam as well. For maximum flexibility the tunability range should be as large as possible.

Diagnostics: Experiments aiming at the determination of absolute reaction cross sections need to know the absolute average photon flux. Many experiments will make use of the time structure of the FEL radiation and therefore require pulse-to-pulse diagnostics of the absolute intensity, the degree of polarization, the energy spectrum as well as the spatial and temporal intensity distributions.

IV. Instrumentation for dilute ion targets at the European XFEL

It is a challenge to the user communities around XFEL to help defining in detail the most efficient use of the complete area available for user experiments. From the large diversity of experimental approaches discussed in the WGII to study ion-XFEL interactions it seemed evident that the experimental stations must be made *modular* so they can either be completely removed from the XFEL beam lines or be made transparent for the XFEL photons. Since most experiments on dilute ion targets absorb only a few photons from the total XFEL beam a *serial* arrangement of experiments with dilute ion targets seems reasonable. Indeed, the XFEL time structure could be adapted to service dilute target experiments in series with different needs on the same beam line, e.g. with different portions of XFEL train or different pulse trains matched to particular experiments.

While the specific scientific questions under study in general demand a specialized interaction and detection setup in particular the experiments with fast moving ions beams showed remarkably similar demands in terms of ion target preparation and manipulation.

IV.1 Ion-beam instrumentation

The discussions in the WGII emphasized a great potential for studies involving XFEL interactions with an ionic target in the form of a fast moving beam. For accelerated particles, powerful methods exist to prepare single-component, often even quantum state specific, ion samples and to precision control their kinematics before the photon interaction. Beams with well-defined energy and mass-to-charge ratio can be readily obtained using electric and magnetic separation. Even methods for conformer selection, in particular relevant for large complex molecules, have been developed based on separation by ion mobility. Advanced technologies for transport and manipulation of ion beams are available and in strong further development to the benefit of preparing temporally and spatially localized targets for the XFEL-ion interaction in geometries for both crossed and merged beams arrangements.

The preparation of the internal state of excitation or the alignment of the target ions can be foreseen, among others, through methods based on laser irradiation. Two universal methods for preparing ion targets at low internal temperature were particularly discussed. First, by storage of the ion beam for extended times scales (milliseconds to seconds) the ion ensemble will equilibrate thermally with the surrounding blackbody radiation. If the ion storage device is cooled to cryogenic temperatures a target containing essentially pure electronic, vibrational, and rotational ground states ions can be obtained. This method is for instance being explored with the CSR-project in at the Max Planck Institute for Nuclear Physics (MPIK) in Heidelberg and with the DESIREE project at the University of Stockholm. Second, an ionic ensemble can be cooled (equilibrate) efficiently through collisions with cold He buffer gas in a smaller scale Radio-Frequency (RF) trap. This method is for instance used at the MPI-K and at the University of Aarhus.

A central issue for all experiments involving the interaction of a target ion beam with the XFEL is the achievable density of the ionic target that translates directly to the feasibility of the experiments through the strength of observable signal above the background. Although the XFEL will be sufficiently intense to allow several experiments with ionic targets, technologies for increasing the target intensity are very important especially for larger complex molecules and cluster ions where the initial yield from known ion sources is low (picoampères and below).

Two schemes for increasing the ion target density were discussed, both of which involve an electrostatic ion storage ring as a central device. In the first scheme, ions of a few hundred keV kinetic energy is stored in a cryogenically cooled storage ring under phase-space cooling through the interaction with a cold electron target. By continuous electron cooling, ions can be injected (stacked) up to the space charge limit of the storage ring. In the second scheme, ions are first accumulated in an RF trap under He-buffer gas cooling, then the time integrated ion cloud is extracted and send into a small electrostatic storage ring at few keV energy. After storage the ion beam can be bunched to match the XFEL time structure. It should be noted, that the ion bunching will happen over several revolutions of the ion beam in the storage ring so the added energy dispersion of the ion target is relatively low. Estimates showed that both these ion accumulation schemes would make experiments with initially low current beams feasible.

The detection of photofragments after an XFEL-ion interaction benefits in general from the concept of a fast moving target, since the fragments have unique mass, charge, and energy and are therefore universally separable from the original ion beam as well as from particles which are produced by interactions of the XFEL beam with the residual gas. Present techniques (and techniques under development) allow kinematically complete measurements of photofragments in the crossed beams geometry. The photon-ion merged-beams technique is well established with installations operating or being under construction at the synchrotron light sources ALS, ASTRID, PETRA III and SOLEIL. As implemented presently, it is most well suited for detection of heavy charge fragments, however, various developments towards both light fragment and photoelectron detection were discussed and seem technologically feasible. With the high intensities of the XFEL light source, reactions with cross sections below 10^{-22} cm^2 would be accessible.

IV.1.1 Ion storage-ring

The central device of the envisaged ion-beam facility is an electrostatic storage ring (figure 1). As compared with a single-pass experiment a storage ring offers several decisive advantages in terms of target accumulation and preparation as discussed above. The participants of WG II agreed that an electrostatic storage ring is to be preferred over a magnetic ring because a non-cryogenic prototype version can be built cheaper and more compact. Moreover an upgrade to a cryogenic version would still be possible at a later stage. Since electric fields deflect ions independently of their mass an electrostatic storage ring can store light atomic and small molecular ions as well as heavy cluster and biomolecular ions.

The crossed-beams and merged-beams interaction sections will be integrated in the storage ring (figure1). In the crossed-beams scenario ions and photons interact in a relatively small (of the order of 1 mm x 1mm x 1 mm) volume which is easily accessible by detectors for the reaction products and which is ideal for coincidence time-of-flight and imaging detection schemes. A larger reaction-volume and thereby higher signal count rates are realized in the merged-beam scenario where the ion beam moves collinearly with the photon beam in one of the straight sections of the storage ring. A typical interaction length is of the order of 1 m. Correspondingly, signal rates will be enhanced by factors of up to 1000 as compared with the crossed-beams arrangement. As a trade-off the collection of reaction products, especially of photoelectrons and fluorescence radiation, becomes more difficult because of the elongated interaction volume.

One arm of the storage ring should hold a dedicated device for ion bunching for matching of the time structure of the ion target to the XFEL time structure. Further, the storage ring concept must still allow modular replacement of the interaction regions and detector setups for crossed- and merged-beams experiments for specialized user installations.

The storage ring should be located at the beginning of the photon beam lines so that other users can use the photon beams simultaneously further downstream. There are several ways for realizing an overlap between the stored ion beam and both SASE3 photon beams. A fixed installation could span both photon beam lines with the high-intensity and the high-resolution beam used for crossed-beams and merged-beams interactions, respectively. In this scenario which is indicated in figure 1 the dimensions of the storage ring are related to the distance between the two photon beam lines. An even more flexible concept is the installation of the storage ring on a movable platform. This would open up the possibility to move either the crossed-beams or merged-beams sections into any of the two photon beam lines. Additionally, the size of the storage ring can be chosen more flexibly.

IV.1.2 Ion-beam line

The ions will be injected into the ring via a separate ion-beam line which comprises an interchangeable ion source, a charge/mass analyzing magnet, slits with adjustable sizes for mass/charge selection and beam collimation, a radio frequency trap for accumulation and buffer gas cooling of ions, ion optical devices for beam forming and steering as well ion beam diagnostics.

A floor space of approximately 1.5 m x 2 m should be reserved for the ion source. A flexible mounting of ion sources to the ion beam line is required. Users will want to bring their own ion source since different ions sources are required for the production of the various types of ions such as highly charged atomic ions (e.g. ECR ion source, EBIT), negative ions (e.g. rf charge-exchange ion source), cold small molecular ions (e.g. hollow-cathode ion source), biomolecular ions (e.g. electrospray ion source), cluster ions (e.g. sputter ion source), solvate ions (e.g. flowing afterglow ion source) etc.

A tunable conventional double focusing magnet is needed for the mass/charge (A/q) selection of the desired ion species from the primary ion beam. Ions with A/q =2000 (approximate upper limit for the envisaged studies) accelerated to an energy of 4 keV have a magnetic rigidity of $B\rho = 0.4$ T m. The maximum B field strength that can be achieved is around 1.5 T so that a bending radius of 30 cm will be sufficient. At a deflection angle of 90° the focal length for double focusing will then amount to 60 cm on both sides of the magnet. The mass/charge analyzing magnet and the associated sections of the beam line will thus be rather compact. A floor space of about 1 m x 1 m will be required.

The detailed scheme for implementing an RF trap is still under consideration, however, in the presently envisioned scenario, a compact multi-pole RF trap will be placed on a separate high-voltage platform to which the mass-selected ion beam can optionally be decelerated, accumulated, and cooled to low temperature (< 50 K) through He-buffergas collisions in a cryogenic environment before extraction and injection into the storage ring. With this scenario, a floor space of 1 m x 2 m will be required.

The ion optical devices will be based on quadrupole electric fields that give a large beam forming and steering flexibility and requires only moderate electrode potentials.

IV.1.3 Space and infrastructure requirements, costs

In summary, the proposed ion-beam facility will cover an area of about 8 x 8 m^2 including space for the storage ring and the ion beam line. Additional space will be needed for placing power supplies, data acquisition etc.

Usual laboratory supplies are requested such as cooling water, electric power, liquid nitrogen, liquid helium (for the cooling of the RF trap), internet connections etc.

A rough estimate for the costs of the ion-beam facility's hardware amounts to about 2 M€.

IV.2 Ion trap instrumentation

The discussions at the WGII regarding trapped ions led to the conclusion, that the optimal use of the XFEL for ion trap research would require a versatile setup incorporating an EBIT as well as a Penning and a Paul trap. With respect to the latter, the envisioned research will be based on sympathetic cooling of a single target ion through the Coulomb interaction with a laser cooled atomic ion. In addition to the Paul trap, there will be the need for laser systems for providing laser cooling. Depending on the desired flexibility of the use of laser cooled ions with different charge-to-mass ratios, the number of lasers available may be varied.

Trapped highly charged ions (HCIs) can be produced in an electron beam ion trap (EBIT) and used as a high density ion target for photon-ion interaction experiments. The main advantage of this approach is the (by comparison with merged beam methods) huge increase of the target area density. With ion densities on the order of 10^9 to 10^{10} ions per cm^3, and interaction lengths of 4 to 25 cm, the target are density can be pushed easily to 10^{11} per cm^2, a value four orders of magnitude higher than those achieved in state-of-the-art ion-photon merged beam apparatuses. Existing advanced experiments in this field (ALS, Aarhus) using merged ion beams from ECR sources have not reached any charge states higher than 7+ due to their very low target density. Due to the long trapping times (many seconds and higher) attainable with EBITs in both their normal (with the electron beam on) and in the magnetic trapping mode (with the electron beam turned off, becoming a Penning trap) of operation, the photon-ion interaction can be of extended duration. Besides of constituting an experiment per se as ion target, an EBIT can provide pulsed or continuous beams of HCIs to the other instruments.

A cryogenic Penning trap provides an environment that is characterized by very low residual gas pressures of below 10^{-12} mbar. Consequently, storage times in a Penning trap can be extremely long (day or even weeks). Moreover, a harmonic trapping potential can be best realized in Penning traps which, therefore, offer highest mass resolution. The harmonic potential and trapping fields have further advantages that ions can be manipulated in a highly controlled way. Clouds can be rotated and compressed by quadrupole excitation or by rotating walls. By cooling of the trap inventory ion crystals can be achieved. When illuminating the rotating crystals by the XFEL x-ray pulses in a stroboscopic manner, the geometry of the trapped rotating crystals can be followed in real time. Experiments with trapped and cooled highly charged ions will yield spectroscopic information of highest precision.

IV.2.1 EBIT

The proposed EBIT will use an electron beam of up to 500 mA and maximum energy of about 40 keV. The beam is guided through various drift tubes to the center of the ion trap and compressed by an 6 T magnetic field to a diameter of less than 60 μm. Ions produced by this intense beam are trapped in the radial direction by the negative space charge of the electron beam itself and axially by applying appropriate potentials at the drift tubes. Typical ion densities in the trap range from 10^6 to 10^{11} ions/cm^3 depending on the ion charge state. Several ports allow injection of the FEL beam into the trap, observation of fluorescence emission after photoexcitation of the trapped ions and ion extraction. The interaction volume for the collinearly merged FEL beam and ion trap cloud is $2{\cdot}10^{-5}$

cm^3, resulting from estimated diameter of 0.1 mm for the respective overlap region (see Fig. 3). A typical figure for the number of ions N_{ion} in the working volume is $N_{ion} = 5\cdot10^9$ ions·cm^{-3} × 2⍰10^{-5} cm^3 = 10^5 ions. Photoionized ions generated within the trap volume after a suitable interaction time are extracted by lowering the potential wall produced by the downstream drift tubes. Behind the

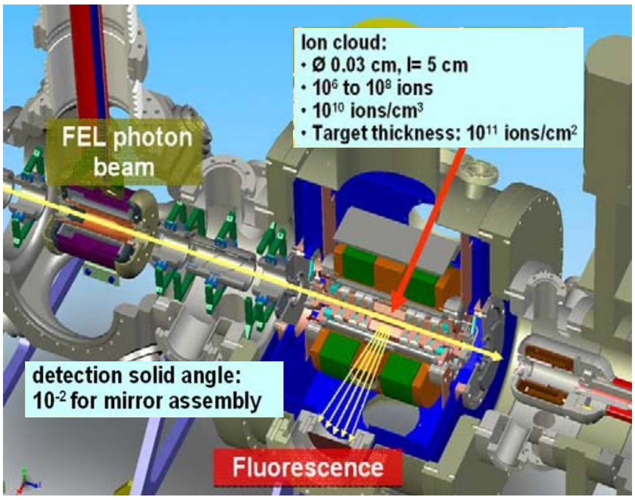

Figure 3: FLASH-EBIT. The photon beam entering from the left excites or ionizes the trapped HCI. Fluorescence is detected through the side ports. The ions can be dumped towards a q/m analyzer to detect changes in their ionization state.

collector, an electrostatic 90° deflector guides the ions towards a Wien-type velocity filter. A position-sensitive microchannel plate (MCP-PSD) detector is used to register the extracted ions with high efficiency; a single ion can be discriminated by this setup. This ion counting capability secures a very wide dynamic range and, in combination with the spatial separation of the individual charge states at the MCP-PSD, excellent background rejection. In comparison with solid angle achievable for fluorescence photon detection (typically 1%), the extracted ions can be guided to the MCP-PSD with nearly 100% efficiency.

IV.2.2 Paul trap

The heart of this part of the trapping facility will be a linear Paul Trap situated in a vacuum chamber evacuated by an ion pump to a base pressure of a few times 10^{-11} torr, to avoid unwanted loading of impurity ions from the background by the XFEL beam. The target ions in the experiments will have to be delivered from various ion sources (ICR, EBIT, ...) while the ions for laser cooling will be produced locally by electron ionization of neutral atoms originating from a oven. The vacuum chamber will have to incorporate a series of view ports for accessing the ions by laser beams and for photo detection. Besides the electrode structure of the linear Paul trap, the vacuum chamber will have to include some electrodes to guide the target ions from the ion sources. RF fields for driving the Paul trap, oscillating fields for ion identification as well as DC fields for gating ions into the trap will be needed. These fields will have to be computer controlable.

IV.2.3 Penning trap

The Penning trap consists of a set of electrodes in a UHV vacuum system which is mounted inside a superconducting magnet. The latter is required for the generation of a strong and homogeneous magnetic trapping field (typically 6-7 T). The footprint of the trap is about 2 m x 3 m. The inventory of the trap can be investigated either inside the trap or after extraction from the trap. Methods for observation of reactions with the trapped ions in situ are non-destructive FT-ICR (Fast Fourier transform Ion Cyclotron Resonsnce) and optical and X-ray fluosescence spectroscopy. The Penning trap has to be moved into one of the XFEL beams. Electrodes and magnet of the Penning trap need to designed appropriately. For imaging the ion cloud and further use of the ions, a short ion extraction beam line is required. For injection into the Penning trap from a separate cooler trap the cold ions are decelerated to 0 V potential.

IV.2.4 Space and infrastructure requirements, costs

Based on the experience of building several EBITs, the investments and purchases necessary are (2008 prices) on the order of 550 k€. The device would use a cryogen-free superconducting magnet and reach electron beam energies up to 40 keV at currents of 500 mA.

A footprint of 4 m length along the FEL beam, 2 m on the right hand side with respect to the beam propagation and 2 m on the left-hand side would be needed, although a more compact setups is possible. Additional 10 square meters in a close location for electronic racks and experiment control are necessary. The EBIT operation requires about 15 kW of electrical power for cryocoolers and electronics, as well as 8 kW cooling water power (15 l/min at less than 30° C). A compressed air supply, gas lines for laboratory gases and the exhaust of vacuum pumps are needed. Ideally, a temperature-stabilized (less than 2°C variation) environment would improve the experimental accuracy and optimize the long term operational stability.

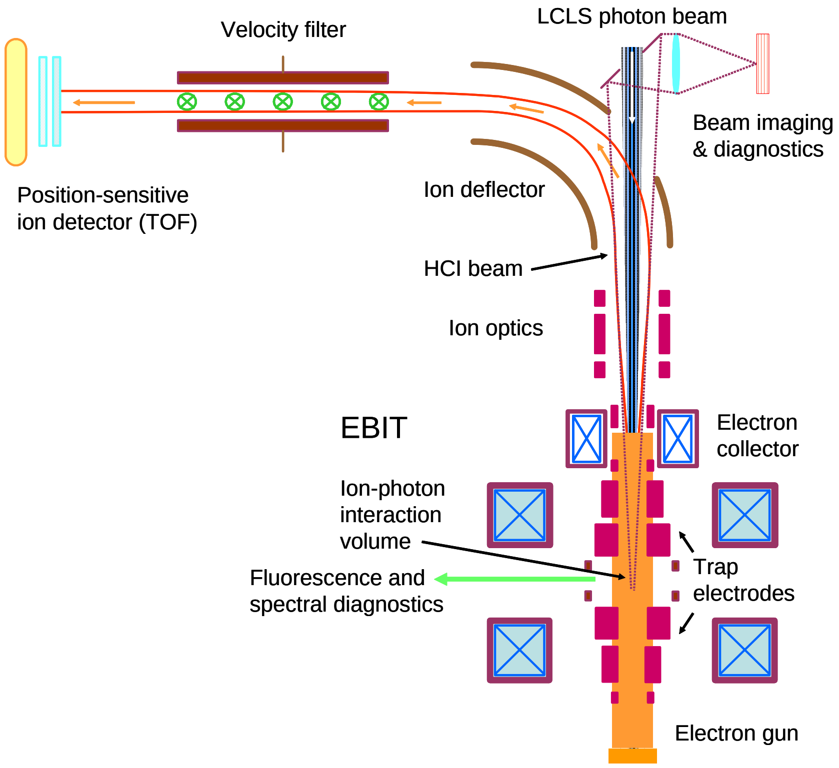

Figure 4. Scheme of the EBIT setup for photoionization studies.

For setting up lasers and optic for laser cooling in a Paul trap, an optical table of the dimension 1.5 m x 2.5 m will at least be needed. The estimated cost for being able to cool a single ion species will be 250 k€. This cost includes the lasers, optics, laser diagnostics, optical table, photon detectors and other basic electronics. The expenses for constructing the Paul trap setup (excluding guiding of ions from ICR, EBIT or other ions sources) will in total among to 150 k€ including the basic electronics and control system. The costs for installing a Penning trap at one of the XFEL user ports is 230 k€. A rough estimate of the costs for the ion extraction beam line and the cooler trap is 100 k€.

IV.3 Detectors for particles and photons

The importance of dedicated particle and photon detectors was emphasized in the WGII in connection with all experiments. For several experiments with ionic targets, particle detectors of unit efficiency, high speed, and multi-hit capability are ideal with the detected signal containing maximal and high resolution information on the properties of the registered particle, such as arrival time, spatial position (imaging), mass, charge, and energy.

Particle detectors based on the Multi Channel Plate (MCP) technology are commonly used in experiments with fast or trapped ions. Exciting developments have happened in the last two decades through the development of specialized anodes and specialized front end electronics which have dramatically improved the performance of MCP detectors in terms of simultaneous time and position resolution as well as multi-hit capabilities. MCP based detectors will beyond doubt play an important role for experiments with ion targets at the XFEL. One drawback of these devices is the absence of event-by-event particle mass identification which should be addressed by forefront developments in semi-conductor and cryogenic calorimetric detectors.

Particle and especially photon detectors based on semi-conductor technology were also discussed and reviewed in the working group. Especially for high energy (X-ray) photon detection, novel and ongoing developments of detectors that meet many criteria for an ideal detector can be foreseen to emerge in the coming years among others from XFEL related projects. Experiments on ion targets could benefit from following these developments closely, for instance in view of the potential for diffractive XFEL scattering from stationary or moving ionic targets.

IV.4 Additional laser facilities.

Several experiments with ionic targets require further laser equipment together with XFEL. Discussed in WGII were CW lasers used to laser cool Mg-ions in a linear Paul Trap, intense pulsed lasers used for controlling the spatial alignment of individual ions and molecular state preparation, as well as femtosecond lasers precisely synchronized to the XFEL for pump-probe studies. The experience from FLASH shows that users increasingly request optical lasers in synchrony with the FEL pulse and the availability of precise synchronization schemes. Similarly, additional laser facilities around the XFEL in a broad spectrum of parameters will beyond doubt be beneficial for several experiments on ionic targets.

V. Working group evaluations and conclusions

V.1 Scientific cases and user communities.

At the workshop, the scientific case for studies of SQS in dilute ion targets at the XFEL as described in the TDR was reviewed and majorly expanded. As outlined in this report, a multitude of novel unique scientific possibilities arises from the combination of the specialized technologies for preparation, manipulation and detection with dilute ion targets and the extreme flux and particular time structure of the XFEL light source.

The participation in the WGII showed a wide community around experiments with dilute ion targets: In the field of experiments with dilute ion beams representatives of seven different European groups were present, and three groups were represented in the field of trapped ions. This large participation demonstrated the existence of a strong community around experiments with dilute ion targets that may indeed be expected to expand in the coming years as the XFEL user facility comes closer to completion.

The discussions in the WGII demonstrated a common benefit within the community using fast moving ion targets of having a multi-purpose facility for ion beam production, transport, accumulation, cooling, and storage permanently present at the XFEL facility. For specific experiments users would bring specialized ion sources, interaction zones, and detectors. Several specific research groups expressed interest in forming a multi-national structure for developing an ion beam facility adapted to the XFEL opportunities, presently including the groups of Jean-Marc Bizau (Orsay), Mats Larsson (Stockholm), Henrik B. Pedersen (Aarhus), Alfred Müller, Stefan Schippers, (both Giessen), and Andreas Wolf (Heidelberg). It can be anticipated that in the future more groups, e.g., from the European ITSLEIF network (http://www.its-leif.org) will join this initiative.

With respect to setting up an ion trap facility, the three ion trapping groups represented at the meeting by Michael Drewsen (Aarhus), Jose R. Crespo Lopez-Urrutia (Heidelberg) and Reinhard Schuch (Stockholm) are very willing to combine forces to establish a flexible setup that can encompasses the research activity outlined Sec. II. The vision will furthermore be to build a versatile trap facility that will clearly be of interest for the broader ion trapping community in Europe and abroad. Based on a stationary infrastructure centered about an EBIT, a Penning trap and a linear Paul trap, various users should supply specific photo- and electronics-detectors.

V.2 Recommendations and suggestions.

The requirements for the XFEL delivery and diagnostics to experiments with dilute ion targets was summarized in Section III, and the WGII suggest that the XFEL and beamlines behind the SASE3 undulator will be developed to meet these requirements.

With respect to the use of the experimental area behind the SASE3 undulator, the WGII recommends a general beamline organization based on

- Modular (replaceable) experimental stations
- Serial arrangements of experiments with dilute targets

In the WGII the benefit from certain experimental infrastructures for experiments with dilute ion targets was reviewed. In this respect the WGII recommends:

- Promotion of a development project for an ion beam facility, preferably on a movable platform, to be permanently installed in the beginning of the photon beam lines. For the initial experimental phase in the scope of the present report, the facility will provide a compact electrostatic room-temperature storage ring for ion beam energies up to about 10 keV and include additionally a separator magnet, ion beam optics and diagnostics, an RF-trap for accumulation and cooling, and an integrated device for ion beam bunching. The storage ring should accommodate modular (replaceable) interaction regions for crossed and merged beams experiments.

- Promotion of the development of a versatile ion trap facility, which incorporates an EBIT, a Penning trap and a linear Paul trap. For carrying out single ion experiments there will furthermore be the need for a permanent optical setup including lasers for laser cooling of atomic ions and detection of the induced fluorescence by a CCD-camera. The facility should be flexible designed such the three types of traps can either be used individually or applied in “tandem”.

Appendix I: Program of Working Group II on dilute ion targets

Working Group II: Dilute Ion Targets

Chair: Henrik B. Pedersen/Stefan Schippers
Location: 1525-323

THURSDAY, OCTOBER 30		
	SESSION I: Ion Target preparation	
14.00-14.10	**Henrik B. Pedersen/Stefan Schippers** Introduction	
14.10-14.30	**Lutz Lammich** Fast Ion Beams	
14.30-14.50	**Andreas Wolf** High energy ion beams and chrogenic storage rings	
14.50-15.10	**José R. Crespo López-Urrutia** Electron Beam Ion Traps (EBITs)	
15.10-15.30	**Reinhold Schuch** Penning Ion Traps	
15.30-16.00	Coffee/Tea (Physics canteen)	
	SESSION II: Ion-XFEL interaction	
16.00-16.20	**Michael Drewsen** Trapped ion-XFEL interactions	
16.20-16.40	**Jean-Marc Bizau** Ion beam-XFEL interactions	
16.40-17.00	**Ottmar Jagutzki** Detection of electrons and heavy fragments	
17.00-17.20	**Andreas Schwarz** Dectection of Photons	
17.20-17.30	**Discussion and conclusion**	
FRIDAY, OCTOBER 31		
	SESSION III: XFEL-beam and additional laser sources	
09.00-09.30	**Stefan Düsterer** Experience from FLASH	
09.30-10.30	Discussions and drafting of report	
10.30-11.00	Coffee/Tea (Physics canteen)	

Appendix II: Participants of Working Group II on dilute ion targets

Jean-Marc Bizau	*LIXAM, CNRS, Université Paris-Sud, Orsay, France*
Michael Drewsen	*University of Aarhus, Denmark*
Stefan Düsterer	*HASYLAB, DESY, Germany*
Marko Förstel	*Max-Planck-Institute for Plasma Physics, c/o BESSY, Berlin, Germany*
Jan Grünert	*European XFEL, DESY, Hamburg, Germany*
Ottmar Jagutzki	*ROENTDEK, University of Frankfurt, Germany*
Lutz Lammich	*University of Aarhus, Denmark*
Mats Larsson	*Stockholm University, Sweden*
Jose R. Crespo Lopez-Urrutia	*Max-Planck-Institute for Nuclear Physics, Heidelberg, Germany*
Serguei Molodtsov	*European XFEL, Hamburg, Germany*
Henrik B. Pedersen	*University of Aarhus, Denmark*
Stefan Schippers	*Giessen University, Germany*
Reinhold Schuch	*Stockholm University, Sweden*
Andreas Schwarz	*European XFEL,DESY, Hamburg, Germany*
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Thomas Tschentscher	*European XFEL, DESY, Hamburg, Germany*
Andreas Wolf	*Max-Planck-Institute for Nuclear Physics, Heidelberg, Germany*