Optical design of the ARAMIS-beamlines at SwissFEL

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Abstract. SwissFEL is a free electron laser facility for hard and soft X-rays at the Paul Scherrer Institut in Switzerland. The first hard X-ray FEL named ARAMIS will deliver photons in the wavelength range from 1 Å to 7 Å in up to three beamlines alternatively. The beamlines are equipped with crystal monochromators, cover the full wavelength range and offer a variety of operational modes.

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INTRODUCTION

The SwissFEL-facility at the Paul Scherrer Institut is planned as a multi FEL-facility with ARAMIS as its first hard X-ray FEL. Construction is well on the way and first lasing of ARAMIS is expected for the end of 2016. A first extension stage with the soft X-ray FEL ATHOS is already projected and will extend the wavelength range up to 70 Å. Two beamlines are under construction at ARAMIS serving two end stations. The ARAMIS-1 beamline with the end station ESA is dedicated to ultrafast photochemistry and serial femtosecond crystallography whereas the ARAMIS-2 beamline serves the end station ESB, specialized in pump probe crystallography on solid-state samples [1]. A third beamline, ARAMIS-3, is foreseen for phase 2 and will be dedicated to material science and nano-crystallography.

SOURCE

The source properties of ARAMIS were derived with the simulation code GENESIS [2] and later refined in start to end simulations [3]. They were obtained for optimized parameter sets and may not be achieved in all day operation. The values for long pulse operation with 200 pC bunch charge are summarized in Table 1 and serve as basis for the layout of the beamline components. The pulse length in this long pulse mode is 17 fs (rms) and independent of the photon energy. Wavefields at selected photon energies were provided for physical optics calculation of the beamline performance.

TABLE 1. Beam parameters for the ARAMIS undulator for 200 pC bunch charge.

Wavelength	(Å)	7	3.5	2.3	1.75	1.4	1.17	1
Source size*, σ_r	(µm)	44	31	29	28	27	26	25
Source divergence*, σ_θ	(µrad)	9.8	5.2	3.7	3.0	2.5	2.2	2.0
Pulse energy	(mJ)	1.65	1.6	1.55	1.50	1.45	1.4	1.39
Spectr. Bandw.*	(%)	0.45	0.31	0.26	0.24	0.23	0.22	0.21
Beam size* in 64 m	(µm)	630	330	240	190	160	140	130

*rms-values

The values for source size σ_r and divergence σ_θ given in Table 1 denote the rms-values of the two-dimensional intensity distributions. For a diffraction limited beam their product accounts to $\sigma_r \cdot \sigma_\theta = \lambda/2\pi$. The rms-values of the one-dimensional intensity distribution σ_x, when the beam is projected on the beam cross section, and the divergence σ'_x derived from that are smaller. For a Gaussian intensity distribution they are related by $\sigma_x = \sigma_r/\sqrt{2}$ and $\sigma'_x = \sigma_\theta/\sqrt{2}$, respectively. The values of the projected intensities were used for the layout of the beamline optics.

OPTICAL LAYOUT

The primary design goal for the beamline layout was the ability to operate three end stations alternatively with full access to the non operating stations. To achieve a reasonable beam separation, offset mirrors (OM) are used to steer the beam in three beamlines and separate the Bremsstrahlung from the FEL-beam. Two horizontally deflecting offset mirrors deflect the beam into the ARAMIS-1 beamline with a total deflection angle of 12 mrad. The central beamline stays in the direction of the FEL-beam and uses two vertically deflecting offset mirrors in a zigzag geometry. The requirements for the ARAMIS-3 beamline are not yet finalized. To keep all options open, horizontal offset mirrors with a total deflection angle of 8 mrad were considered as worst case with respect to the spatial restrictions along the beamlines and end stations.
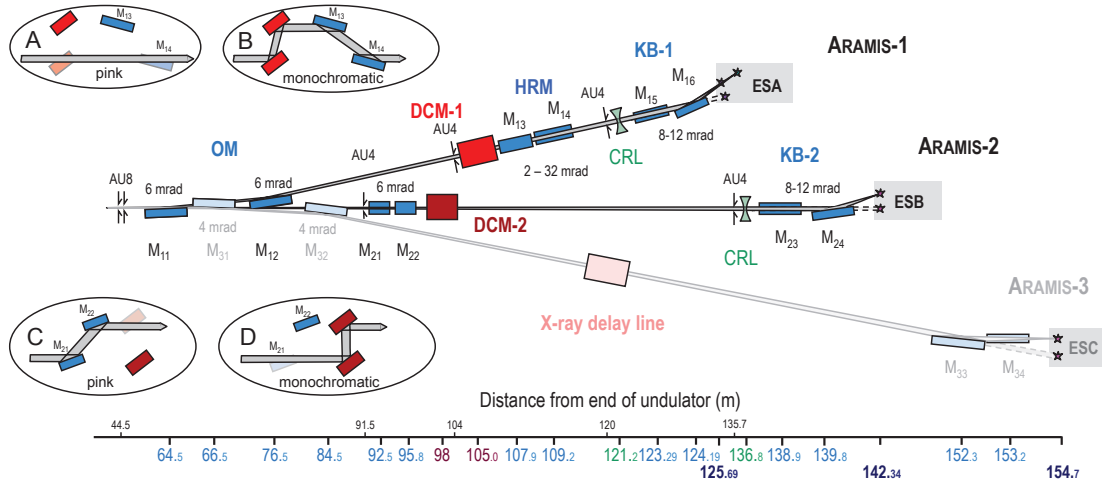

FIGURE 1. Top view of the ARAMIS beamlines. The FEL-beam is distributed by horizontally deflecting offset mirrors to the ARAMIS-1 and ARAMIS-3 beamlines. The ARAMIS-2 beamline utilizes vertically deflecting offset mirrors or alternatively the DCM-2. Insets A and B show the configurations for the pink and monochromatic mode of ARAMIS-1, insets C and D the corresponding settings for ARAMIS-2.

Many experiments will use the pink-beam mode where only the offset mirrors and eventually the focusing Kirkpatrick-Baez mirrors (KBM) are in the beam. Space for compound refractive lenses (CRL) is reserved for a future upgrade. On demand, double crystal monochromators can be activated in the beam paths without changing the focal positions in the end stations. In the ARAMIS-2 beamline this is accomplished by retracting the first offset mirror (M_{21}) and introducing the second crystal of the DCM-2 into the beam. In the ARAMIS-1 beamline the changeover is realized by introducing the first crystal of the DCM-1 and the mirror M_{14} into the beam. The four bounce scheme with two crystals and two mirrors became necessary, as the number of optical elements for the main pink beam mode ought to be minimized.

The offset mirrors are operated with an incident angle of 3 mrad giving a deflection angle of 6 mrad. They are bendable, made of single crystal 100-silicon and are coated with two different layer structures. A low-Z coating, 10 nm B_4C on 36 nm SiC, should withstand the FEL-beam and guarantee a high reflectance up to 12.4 keV, see Figure 2. The B_4C-layer is effective at lower photon energies and covers the drop in the reflectance due to the silicon K-edge of the SiC-layer. At higher photon energies it becomes transparent and the reflectance is driven by the SiC-layer with a critical energy of 12.4 keV. A mid-Z coating, 15 nm B_4C on 20 nm Mo, extends the operation range up to the Mo K-edge at 20 keV but has a higher damage risk and may operate at reduced fluence values only. In between both coatings a stripe of uncoated silicon serves as third reflecting area. It has the lowest critical energy of all coatings and may be used at low energies when high harmonic rejection becomes an issue. High harmonic contamination is a sensitive issue in many experiments and although the intensity of the third FEL-harmonic is only about 1% of the fundamental, its ratio is readily increased when absorbers or lenses are placed in the beam. Reflecting mirrors generally reflect the fundamental better than the higher harmonics and improve the spectral purity. Their specific rejection rate depends on the coating material, the layer structure and the deflection angle. These parameters provide an opportunity to tune the spectral response of reflection mirrors with respect to high spectral purity.

A harmonic rejection system with two mirrors is part of the four bounce monochromator scheme in the ARAMIS-1 beamline. The two mirrors are located behind the DCM-1 and became necessary to bring the beam back to its original height and direction when the beamline is operated in monochromatic mode. The beam offset between the DCM-1 and the mirror pair is a free parameter. It is set to 20 mm in the fix offset mode and allows for fixed deflection angles on the mirrors. In the harmonic rejection mode the beam offset can be chosen between 4 mm and 42 mm to operate the mirrors with optimum deflecting angles. This option came for free, but requires the operation of additional six motors in the HR-mirror chamber. Optionally, a similar system could be inserted behind the DCM-2 of the ARAMIS-2 beamline.
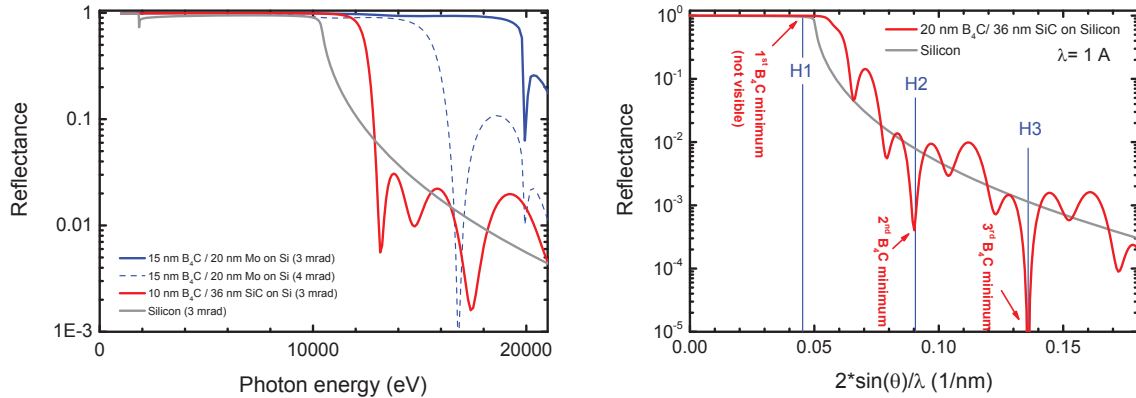
FIGURE 2. Reflectance of the beamline mirrors.
Left: Reflectance of the OM with an incident angle of 3 mrad and the KBM with 4 mrad, respectively.
Right: Reflectance of the HRM as function of the normalized incident angle for a wavelength of 1 Å. The incidence angle is selected to match the Kiessig-fringes of the B_4C-layer with the corresponding harmonics (H2, H3, ...) of the FEL. Note that the first Kiessig-fringe of the B_4C-layer would appear below the critical angle and is therefore not observed.

The harmonic rejection mirrors (HRM) have similar reflecting areas as the offset mirrors. They only differ in the thickness of the B_4C layer of the low-Z coating which acts as dedicated harmonic rejection (HR) coating. The right part of Figure 2 shows the reflectance of silicon and the HR-coating as function of the normalized incident angle. The values are calculated for a wavelength of 1 Å but show no significant variation within the wavelength range of the beamline. The bare silicon shows high reflectance up to the critical angle and then a smooth and continuous decrease. When this material is used for harmonic rejection, the incident angle θ is chosen such that the reflectance for the third harmonic (H3) is as low as possible while the reflectance of the fundamental (H1) is still on the plateau below the critical angle. By this a rejection rate around 10^{-3} for the third harmonic is achievable per reflection.
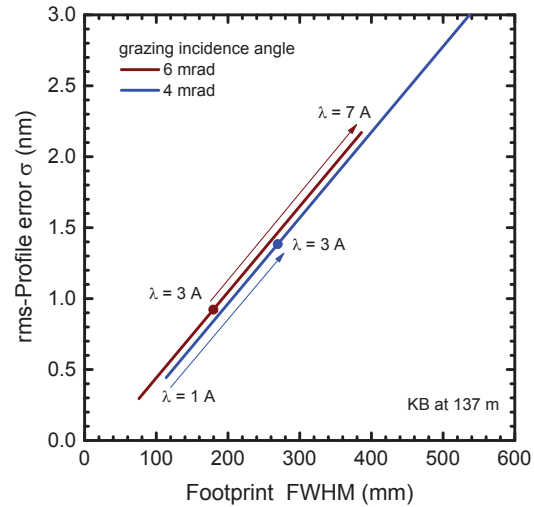
The HR-coating shows distinct Kiessig-fringes originating in the superposition of reflections from the two layers. A pronounced long period oscillation caused by the B_4C-layer and a weaker with shorter period caused by the SiC-layer. The thickness of the B_4C-layer is chosen to hide the first strong fringe below the critical angle while the higher fringes are still visible at larger angles. Afterwards the thickness of the SiC-layer is optimized for maximum visibility of the B_4C-fringes. For an efficient harmonic rejection at a given photon wavelength, the incident angle on the mirrors is selected to match the Kiessig-fringes of the B_4C-layer with the corresponding harmonics of the FEL. When scanning the photon energy, this matching condition results in a Bragg like condition for the incidence angle on the HRM, namely $\lambda = 2D\sin\theta$ with $D = 22$ nm for the specified HR-coating. By this an optimum rejection ratio below 10^{-4} for the third harmonic seems achievable over the full wavelength range of the beamline. A remaining small wavelength dependency is caused by the optical constants but does not alter the general picture. Ideally both HRMs are used with their respective HR-coatings. However, both mirrors must always operate with the same incident angle to guarantee a fixed beam direction. If both HR-coatings show substantial differences in their layer structure, i.e. thickness variation larger than 1 nm, and thus their fringe location, only one HR mirror can be used with its HR-coating while the other is operated with the bare silicon area. This facilitates the required fine tuning of the deflection angle without significantly influencing the rejection rate.

With incidence angles close to the critical angle, the coatings are operated nearby the maximum dose condition for the surface where the material is most susceptible to damage. This is acceptable, as the mirrors are located downstream of the DCM and see only a significantly reduced fluence with less risk of damage.

Both beamlines are equipped with double crystal monochromators with three crystal pairs. Two silicon crystal pairs, Si-111 and Si-311, are foreseen for standard and high resolution applications, respectively. An additional pair of InSb-111 crystals extends the wavelength range up to 7 Å (1.77 keV) in ARAMIS-1, whereas ARAMIS-2 may optionally insert a Si-511 crystal pair for highest energy resolution. The crystals are mounted on a common Bragg rotation axis that sets the Bragg angle for both crystals from 5°- 80°. The translation of the second crystal perpendicular to its surface allows for a constant beam offset of 20 mm as well as for a variable beam offset in the harmonic rejection mode. The second crystals are long enough to omit the translation parallel to their surface and therefore the beam spot moves along the second crystal while the photon energy is scanned. As the average heat load on the crystals is quite low, a side cooling or even intrinsic cooling scheme is not required. The first crystals are mounted on a copper block directly cooled with water, while the second ones are cooled via copper braids connected to this block.

A pair of KB-mirrors is foreseen as refocusing optics. The achromatic behavior and high throughput of the KB-mirrors was rated higher than the convenient in-line operation of the CRLs. The KB-mirrors with 500 mm optical length and B_4C/Mo-coating are bendable and operate with two sets of deflecting angles. Above 4 keV a deflection angle of 8 mrad improves reflectance and below 10 keV a deflection angle of 12 mrad increases the acceptance. By this an acceptance of more than 5-sigma can be maintained down to 2.5 keV decreasing to 3.5-sigma at 1.8 keV. The surface quality of the mirrors must be extremely good to reflect the FEL-beam without deteriorating the wavefront even at the shortest wavelengths. According to the Maréchal-criterium, the maximum allowed rms-profile error σ in a beamline with N mirrors and grazing incident angles θ must not be larger than $\lambda/(14\sqrt{N}2\sin\theta)$. This condition must be met over the length at which the mirror is illuminated at the respective wavelength. As the beam divergence is proportional to the photon wavelength, the central part of the mirrors must have the highest quality while its outer

FIGURE 3. Required mirror quality in terms of profile error over the length of the central mirror area. The Maréchal-criterium is applied for the KB-mirrors of the ARAMIS-1 beamline when 4 mirrors are in the beam.

parts are only illuminated at longer wavelengths when the Maréchal-criterium tolerates larger surface errors. This opens a way to ease the tight specifications of the mirror and simplify the task for the optics manufacturer. Figure 3 shows the maximum allowed profile error as a function of the beam footprint, i.e. the length of central mirror part, for a KB-mirror in the ARAMIS-2 beamline.

The beamline performance was evaluated with PHASE, a computer code for physical optics simulations. The results for the ARAMIS-1 beamline are summarized in [4]. Spot sizes below 1 µm and peak power densities of up to $10^{21}W/m^2$ can be expected. Due to the larger distance to the focal spot, the ARAMIS-2 has a slightly larger spot size with reduced power density.

SUMMARY

The design for the ARAMIS beamlines at SwissFEL is finalized and allows for the operation of three independent experimental stations with pink and monochromatic beam. Particular emphasis was put on harmonic rejection for high spectral purity. All major beamline components are under fabrication and installation will start at the end of the year.

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