

TECHNICAL REPORT

# Diffraction Orders of the SASE3 Monochromator

Feasibility of simultaneous usage  
for two-colour X-ray pump –  
X-ray probe experiments and  
requirements to protect the  
beamline from damage

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# Introduction

The SASE3 beamline will be equipped with a soft X-ray grating monochromator (for details, see Ref. [1]). The grating disperses the beam and diffracts it in different directions, while only one diffraction order is usually used by the experiment. Other diffraction orders can induce damage to the beamline or, alternatively, can be used in parallel with the main diffraction order for experiments or diagnostics. To avoid damage to the beamline, beam dumps for diffraction orders not in use need to be installed. The simultaneous usage of 1<sup>st</sup> and 0<sup>th</sup> diffraction orders was proposed as one of the schemes for X-ray pump – X-ray probe experiments [2]. The purpose of this report is to provide information necessary to the design of (i) the beam splitting instrument for two-colour X-ray pump – X-ray probe experiments and (ii) the beam dumps for dispersed beam and the exit slit along with diagnostics.

The data presented in this work comprises a detailed analysis on the interplay between diffraction orders of the SASE3 monochromator, which includes transmission by optics (due to both efficiency and geometrical transmission), constraints on the operational range, and details on the spatial separation of the orders. The possible harmful orders to be dumped and their geometry are identified and described; the dispersed beam at the exit slit plane is discussed. In addition to simultaneous usage of different diffraction orders, a feasibility of simultaneous usage of the free-electron laser (FEL) fundamental and the third harmonic in a scheme of spatial separation by the grating is analysed.

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# 1 Methods

Details on the optical design of the SASE3 monochromator can be found in Ref. [1]. In short, the monochromator consists of a system that includes a face-up pre-mirror followed by a face-down grating, which is located 300 m after the source and provides meridional focusing onto the exit slit located 100 m downstream. There are two pre-mirrors foreseen, each operating at a fixed grazing incidence angle, which is 9 mrad for the high-energy pre-mirror and 20 mrad for the low-energy pre-mirror. To follow the notation introduced in Ref. [1], the grazing angle between the beam and optical surface of the pre-mirror is referred to as “incidence angle  $\theta$ ”; similarly, for gratings, the grazing angle between the incoming beam and optical surface is referred to as “incidence angle  $\alpha$ ”, and the angle between the diffracted beam and the optical surface is referred to as “diffraction angle  $\beta$ ”. In this notation, the fix-focus constant is  $\text{cff} = \sin\beta / \sin\alpha$ . The length of the optical surface of the pre-mirrors is  $L_{\text{mirr}} = 580$  mm, of the gratings  $L_{\text{gra}} = 500$  mm. There are two gratings foreseen: the low-resolution grating with a groove density of 50 l/mm and the high-resolution grating with a groove density of 150 l/mm. The gratings are to be blazed; the data presented here assumes a design value of the blaze angle of  $0.1^\circ$  for the 50 l/mm grating; the blaze angle of the 150 l/mm grating was tuned to  $0.4^\circ$  (from the original design value of  $0.3^\circ$ ) to allow operation in the 2<sup>nd</sup> diffraction order in a wider energy range. The optical elements will be coated with  $\text{B}_4\text{C}$ .

In this work, as a monochromator we consider a system of two optical elements: a pre-mirror and grating, and an exit slit. Calculations of monochromator transmission presented here include (i) reflectivity of the pre-mirror, (ii) efficiency of the grating, (iii) geometrical transmission by both optical elements, and (iv) for the 1<sup>st</sup> and 2<sup>nd</sup> diffraction orders, transmission through the exit slit. Grating efficiencies have been calculated<sup>1</sup> using

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<sup>1</sup> The optical elements have not been fabricated yet, and such parameters as surface roughness, coating thickness, and coating density, as well as exact blaze angles are still

“Reflec” code [3], which is part of the “Ray” package [4] developed at BESSY. The same code has been used for the reflectivity estimations for the mirrors. The thickness of the B<sub>4</sub>C coating on the Si substrate has been assumed to be 50 nm, the roughness 0.2 nm, and the density 2.25 g/cm<sup>3</sup>. The geometrical transmission is defined by geometry (length of optical elements, angles, and distances) and by photon beam properties determining beam size at the optics location. The geometry is briefly mentioned above and in detail in Ref. [1]. The beam size of the fundamental has been estimated from expected divergence assuming far field conditions. Details on expected photon beam properties can be found in Ref. [5]. Although the divergence is expected to be dependent not only on photon energy but on electron beam charge as well, we have used an analytical approximation from Ref. [6] related to the upper boundary (Eq. 1 and Fig. 6 in Ref. [6]). For the third harmonic, we assumed a beam size equal to that of the fundamental.

To assure safe operation of optics under ultimately intense X-ray FEL fluxes, as one of limitation we consider operation in total external reflection geometry. Here, the high-energy cut-off of the working range has been set by the condition of keeping the angle of incidence of the fundamental both on the pre-mirror and on the groove surface below the value of the critical angle<sup>2</sup>. The low-energy cut-off is not so strictly set here and mostly corresponds to substantially dropping transmission (both by efficiency and geometrical cut).

All geometrical considerations relate to dispersion direction, which is vertical. Thus, the beam size in the dispersion direction is referred to as the “beam size”, the open aperture in the dispersion direction as the “open aperture”, and the vertical transversal coordinate with respect to the beam axis as the “transversal coordinate”; geometrical cut is considered only in the dispersion direction.

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unknown. If the first three parameters could affect efficiency only slightly (provided they are within the specification range), the value of the blaze angle (even within the specification range) could noticeably shift the efficient range; however, the general picture would not change drastically.

<sup>2</sup> This means not only that the angle of incidence on the pre-mirror (which is, in the present design of inside diffraction orders and inline geometry, less shallow than those of grating), but also that the grating blazing angle affects the high-energy cut-off.

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## 2 Lower diffraction orders

This chapter discusses lower diffraction orders: the 0<sup>th</sup> order in case of 1<sup>st</sup> order operation and both the 0<sup>th</sup> and 1<sup>st</sup> orders in case of 2<sup>nd</sup> order operation. The efficiency calculations have been performed in order to estimate the monochromator capabilities for 0<sup>th</sup> order – 1<sup>st</sup> order (Section 2.1, “1<sup>st</sup> order operation”) and 0<sup>th</sup> order – 2<sup>nd</sup> order or 1<sup>st</sup> order – 2<sup>nd</sup> order (Section 2.2, “2<sup>nd</sup> order operation”) beam splitting geometry for X-ray pump – X-ray probe experiments. The geometrical considerations for these schemes, such as angular and spatial separation between the orders, are presented in Section 2.3, “Geometrical considerations”. The constraints on beam-dump geometry are discussed in Section 2.4, “0<sup>th</sup> order (lower-order) dumps”, and the dispersed beam at the exit slit is described in Section 2.5, “Dispersed beam on exit slit”.

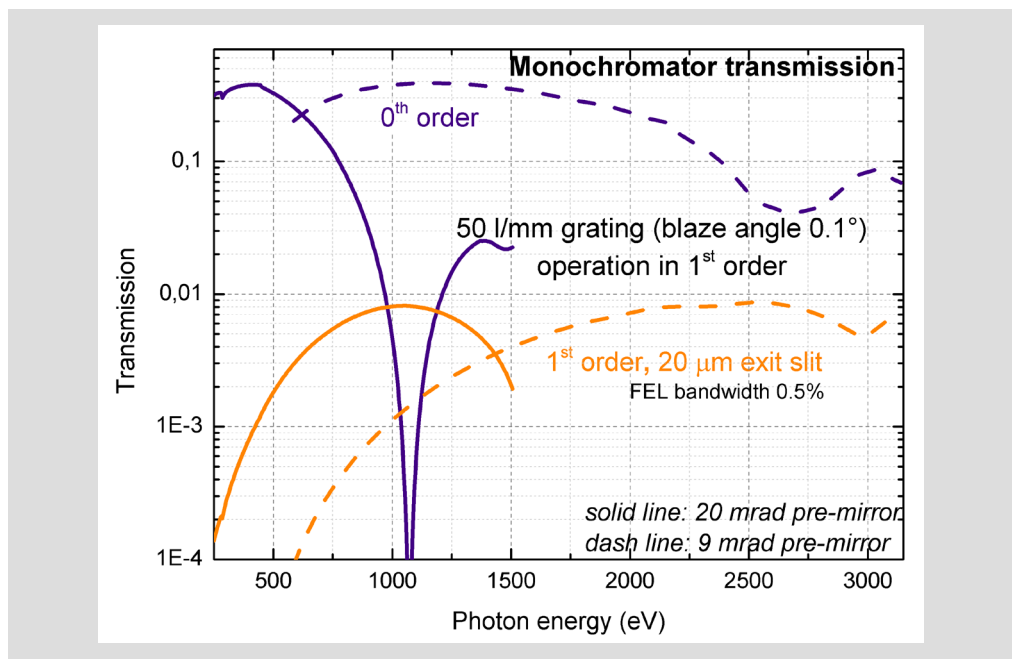
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### 2.1 1<sup>st</sup> order operation

It has been proposed to use 0<sup>th</sup> diffraction order, while the monochromator operates in 1<sup>st</sup> order, for the X-ray pump – X-ray probe experiments [2]. To investigate the capability of the SASE3 monochromator in such a scheme, the monochromator transmission has been calculated comprising efficiencies and geometrical transmission, as discussed in Chapter 1, “Methods”. Since the pump–probe scheme requires spatial overlap, the size of the 1<sup>st</sup> order beam in the dispersion direction should be commensurate to the size of the 0<sup>th</sup> order beam in the focal plane. The latter is expected to be equal to the source size demagnified by optics; the demagnification factor for the 0<sup>th</sup> order is equal to 3 ( $M = d / f$ , where  $d = 300$  m is the source pre-mirror distance and  $f = 100$  m is the focal distance). Thus, the size of the 0<sup>th</sup> order beam in the focal plane is slightly dependent on the photon energy and electron beam charge. For

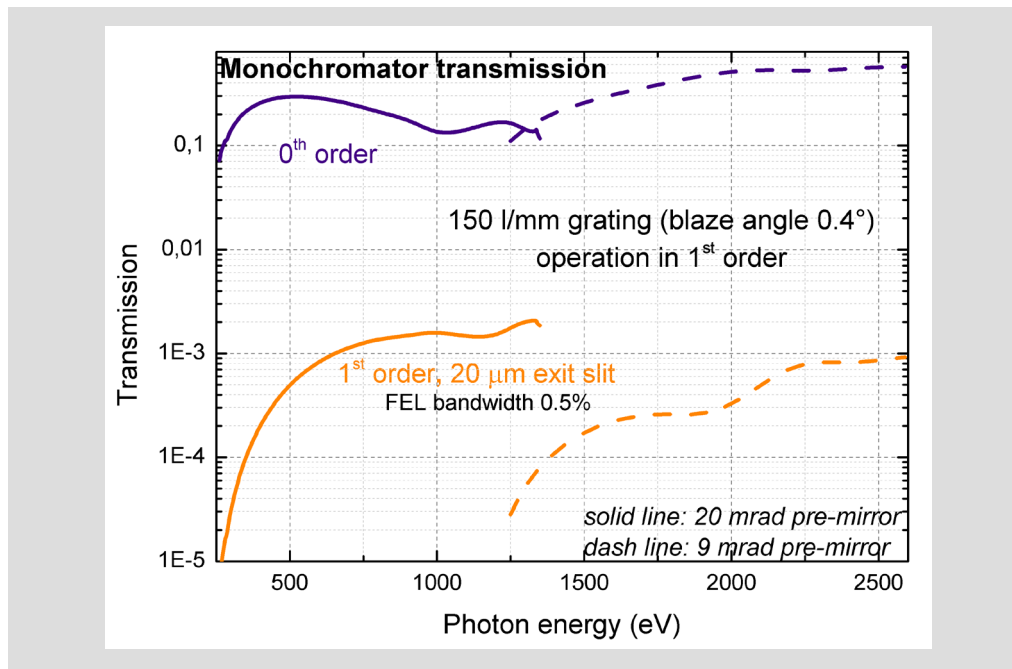
simplicity, the exit slit has been set to the constant value of 20  $\mu\text{m}$  to confine the 1<sup>st</sup> order beam<sup>3</sup>; the FEL bandwidth was assumed to be 0.5%.

The resulted monochromator transmission for 50 l/mm and 150 l/mm gratings is presented in Figure 1 and Figure 2, respectively. One can see that the 0<sup>th</sup> order beam surpasses that of the 1<sup>st</sup> order in most parts of the operation range by about two orders or magnitude. This tendency is due to the closed exit slit for the 1<sup>st</sup> order beam: though the full beam in both 0<sup>th</sup> and 1<sup>st</sup> orders for the blazed grating could reach few to several tens of percent (for the 1<sup>st</sup> order, see Figure 16 on page 20), the 20  $\mu\text{m}$  width of the slit allows to transmit 0.5–2% of the 1<sup>st</sup> order beam, depending on photon energy in case of the 50 l/mm grating and 0.2–0.75% in case of the 150 l/mm grating. Thus, in addition to the lower efficiency of the 150 l/mm grating, its higher dispersion leads to more substantial difference between 1<sup>st</sup> and 0<sup>th</sup> orders compared to low-resolution grating.



**Figure 1:** Monochromator transmission for the 50 l/mm grating (blaze angle 0.1°) operating in the 1<sup>st</sup> diffraction order. The exit slit is set to 20  $\mu\text{m}$  for the 1<sup>st</sup> diffraction order.

<sup>3</sup> 0<sup>th</sup> order beam in the focal plane is expected to be slightly smaller in the high-energy range and could be slightly larger at low energies.



**Figure 2:** Monochromator transmission for the 150 l/mm grating (blaze angle 0.4°) operating in the 1<sup>st</sup> diffraction order. The exit slit is set to 20 μm for the 1<sup>st</sup> diffraction order.

Though incommensurate pump and probe intensities could be desirable for some experiments, the focused 0<sup>th</sup> order beam could produce damage to the exit slit (e.g. by ablation) if not attenuated.

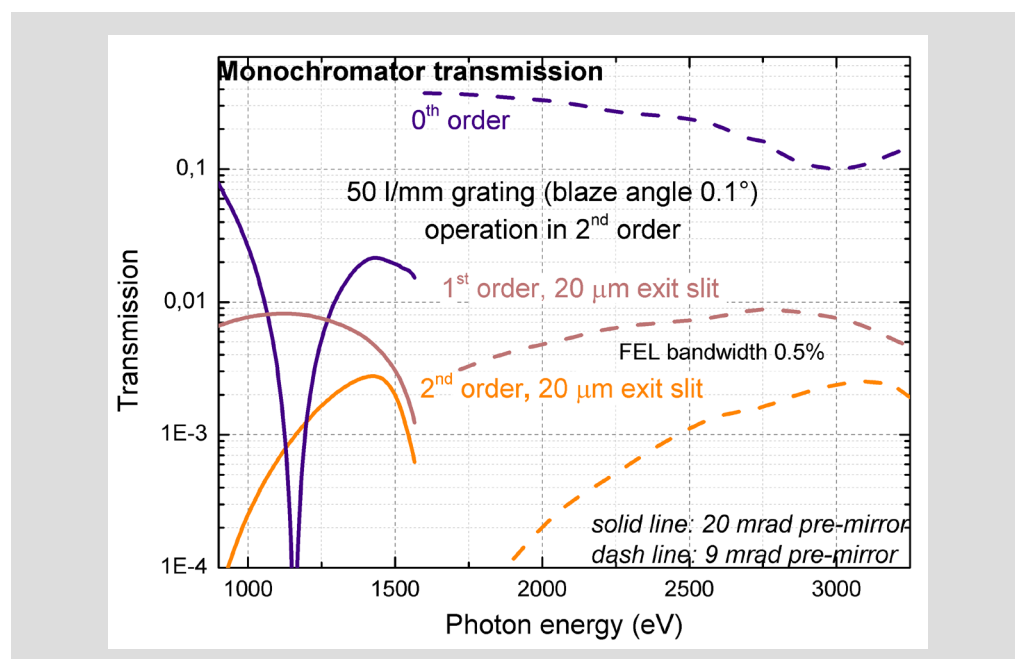
## 2.2 2<sup>nd</sup> order operation

We have exploited the idea of using two diffraction orders and have investigated case of 2<sup>nd</sup> order operation. The results of our calculations are similar to those in the previous section. The case of 2<sup>nd</sup> order operation is presented in Figure 3 and Figure 4 for 50 l/mm and 150 l/mm gratings, respectively. Compared to 1<sup>st</sup> order operation, the case of 2<sup>nd</sup> order operation follows the same tendency: the 0<sup>th</sup> order efficiency is very similar (just slightly different due to different angle of incidence on the grating), and transmission of 2<sup>nd</sup> order is lower than that of 1<sup>st</sup> order due both to the lower efficiency of 2<sup>nd</sup> order (see Figure 16 on page 20) and to higher dispersion. An operational

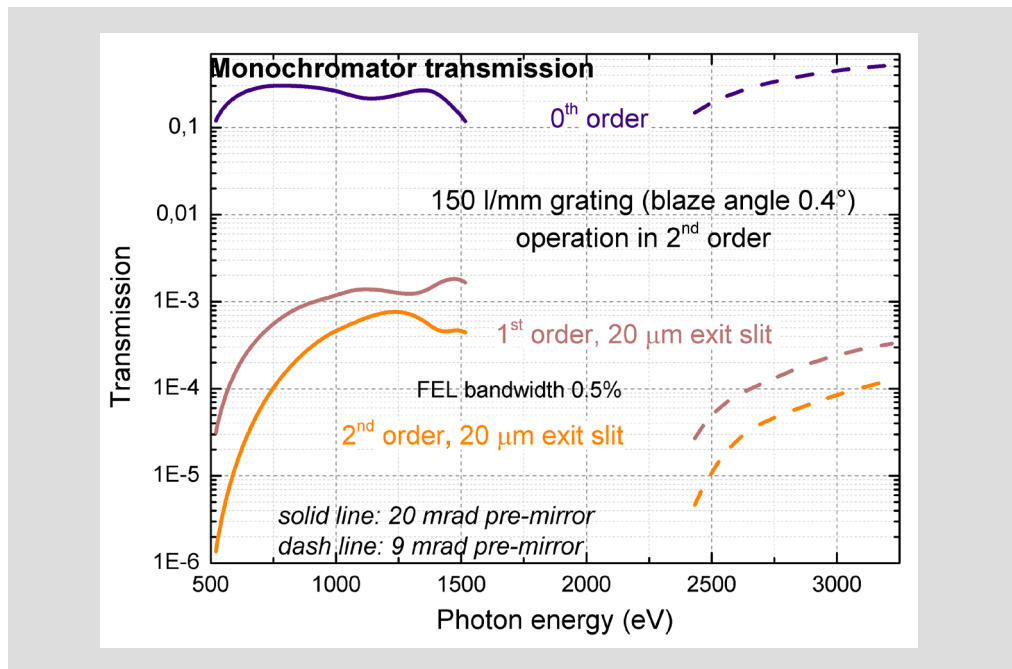


range can be extended to slightly higher photon energies compared to 1<sup>st</sup> order operation.

However, in addition to the 2<sup>nd</sup> order – 0<sup>th</sup> order splitting scheme, one can use 2<sup>nd</sup> order – 1<sup>st</sup> order splitting. The latter scheme provides the following advantages: (i) both beams are monochromatic and (ii) in the case of 2<sup>nd</sup> order – 1<sup>st</sup> order splitting, the sizes of both beams are governed by the exit slit; thus, provided that the experiment accepts a larger spot size on the sample and a larger bandpass, the exit slit could be opened much wider (since transmission through the 20  $\mu\text{m}$  slit is 0.2–2%, depending on photon energy, grating, and diffraction order), thus increasing the flux by possibly more than an order of magnitude.



**Figure 3:** Monochromator transmission for the 50 l/mm grating (blaze angle 0.1°) operating in the 2<sup>nd</sup> diffraction order. The exit slit is set to 20  $\mu\text{m}$  for the 1<sup>st</sup> and 2<sup>nd</sup> diffraction orders.

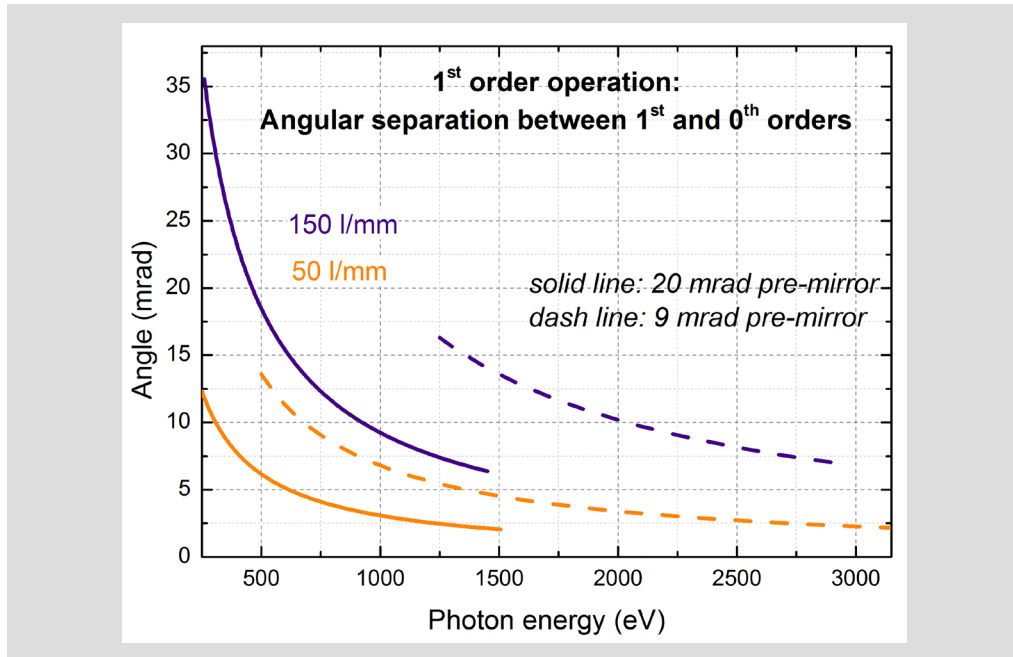


**Figure 4:** Monochromator transmission for the 150 l/mm grating (blaze angle  $0.4^\circ$ ) operating in the  $2^{\text{nd}}$  diffraction order. The exit slit is set to  $20\ \mu\text{m}$  for the  $1^{\text{st}}$  and  $2^{\text{nd}}$  diffraction orders

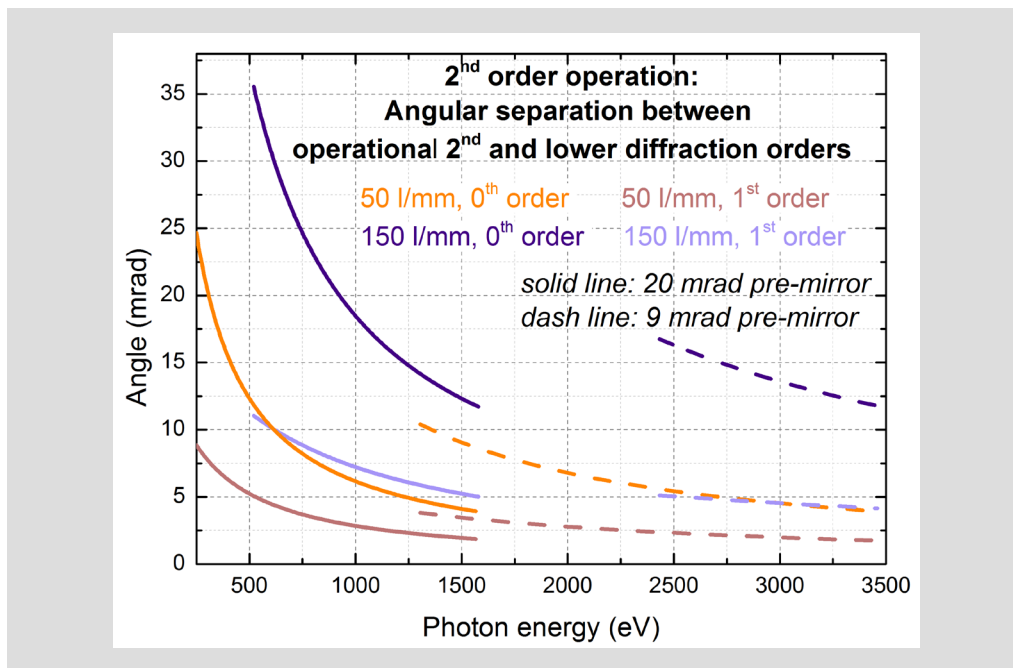
## 2.3 Geometrical considerations

Information on angular and spatial separation between diffraction orders can be useful for designing beam splitting optics, for diagnostics, and for the design of beam dumps discussed below.

Figure 5 (Figure 6) represents angular separation between the operational  $1^{\text{st}}$  ( $2^{\text{nd}}$ ) order and the lower diffraction orders.



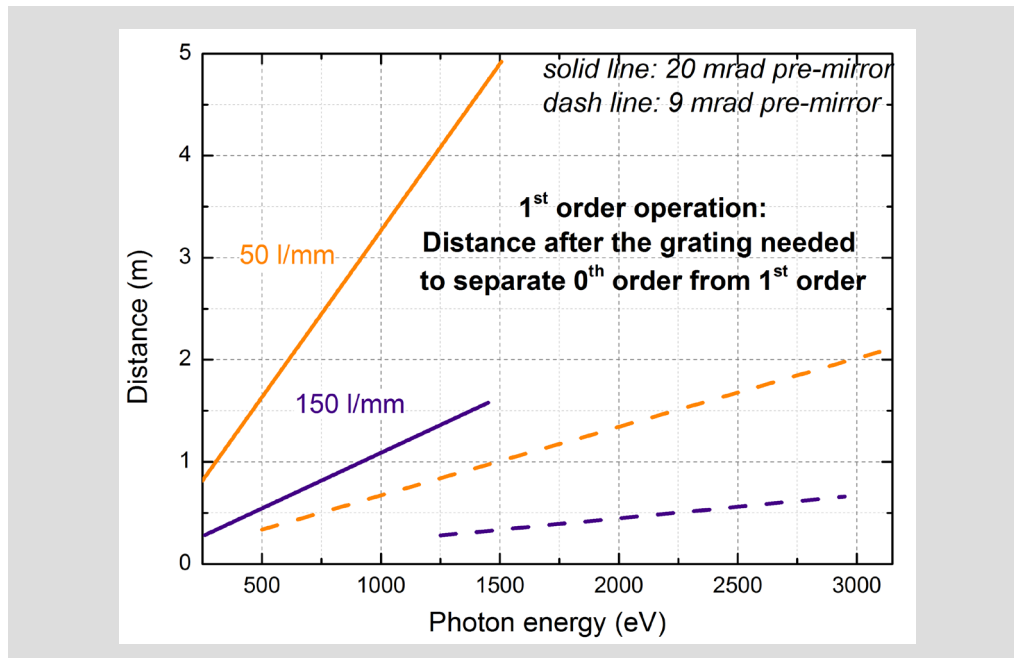
**Figure 5:** Angular separation between the operational 1<sup>st</sup> order and the 0<sup>th</sup> order



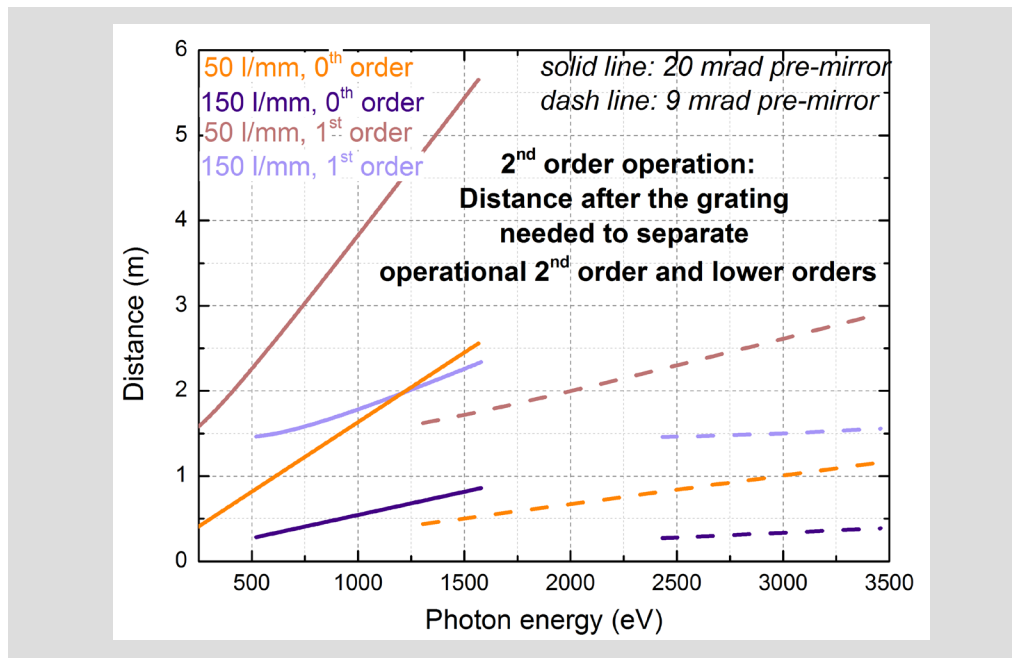
**Figure 6:** Angular separation between the operational 2<sup>nd</sup> order and the lower (0<sup>th</sup>, 1<sup>st</sup>) orders

Figure 7 (Figure 8) shows distance of separation between the operational 1<sup>st</sup> (2<sup>nd</sup>) order and the lower diffraction orders. The full separation occurs at distances < 5m (< 6m) for the whole working range in case of operation in

1<sup>st</sup> (2<sup>nd</sup>) order. To estimate distance of full separation, the maximal beam sizes in dispersion direction of relevant orders behind the grating have been estimated as given by the open aperture of the optics. Just behind the grating, the open aperture of the 1<sup>st</sup> (2<sup>nd</sup>) order was estimated as  $s_{\max} = L_{\text{grat}} \cdot \sin(\beta)$ , and  $s_{\max} = L_{\text{grat}} \cdot \sin(\alpha)$  for the 0<sup>th</sup> order. For the inside orders, the operation scheme used at the SASE3 monochromator, the former is larger.



**Figure 7:** Distance after the grating needed to separate the 0<sup>th</sup> order from the operational 1<sup>st</sup> diffraction order

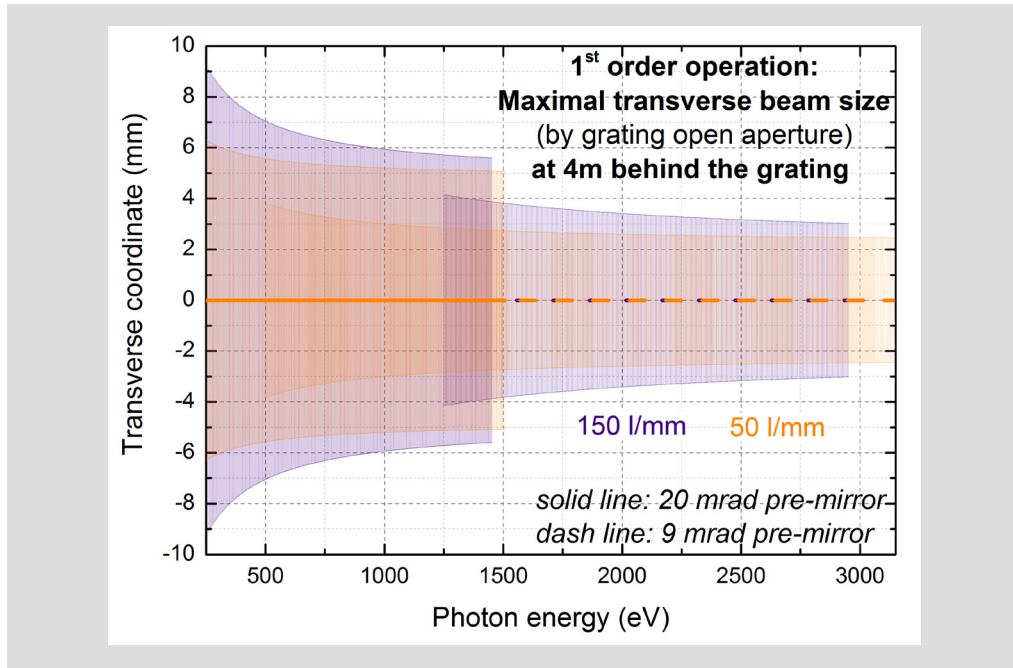


**Figure 8:** Distance after the grating needed to separate the lower (0<sup>th</sup>, 1<sup>st</sup>) orders from the operational 2<sup>nd</sup> diffraction order

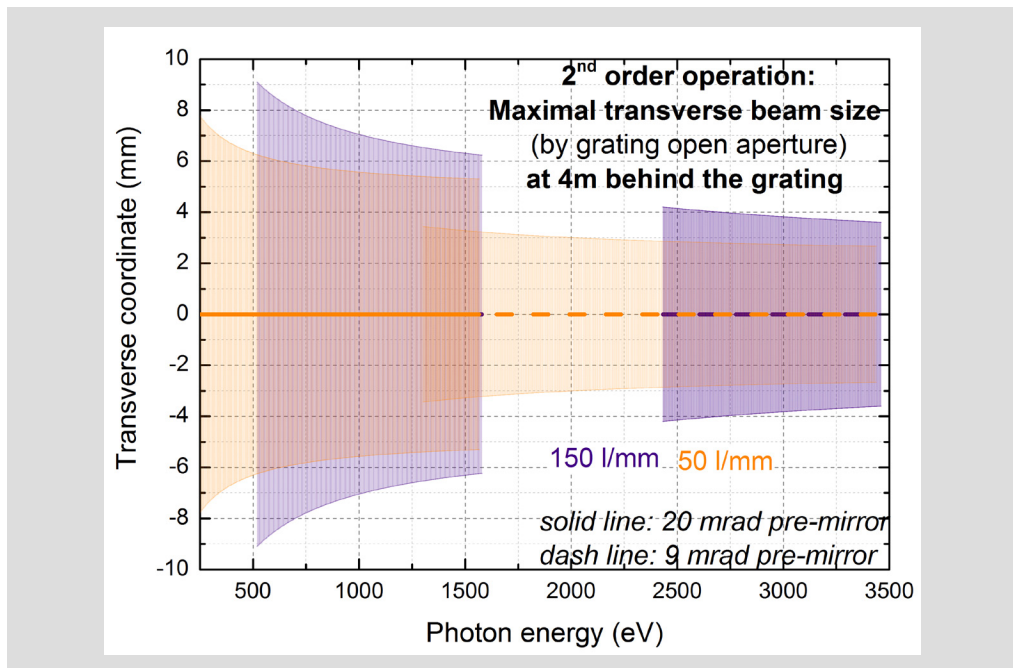
The maximal beam size of the operational 1<sup>st</sup> (2<sup>nd</sup>) order at 4 m behind the grating<sup>4</sup> is presented in Figure 9 (Figure 10). Since for the constant included angle operation of a grating this size depends on photon energy for the same grating, the transversal coordinate (from the beam axis) of separation varies with photon energy. One can see that maximal beam size stays below  $L_{\text{grat}} \cdot \sin(2\theta)$ <sup>5</sup>: the beam cross-section is < 20 mm for the low-energy pre-mirror and < 9 mm for the high-energy pre-mirror.

<sup>4</sup> Estimated as  $s_{\text{max}} \cdot (f - d)/f$ , where  $d$  is distance after the grating; dispersion of 1<sup>st</sup> (2<sup>nd</sup>) is not taken into account as it is negligible at such distances and small FEL bandwidth.

<sup>5</sup> Since  $\beta < 2\theta$ , where  $2\theta$  is deflection angle, and  $\beta \rightarrow 2\theta$  at low-energy tail.



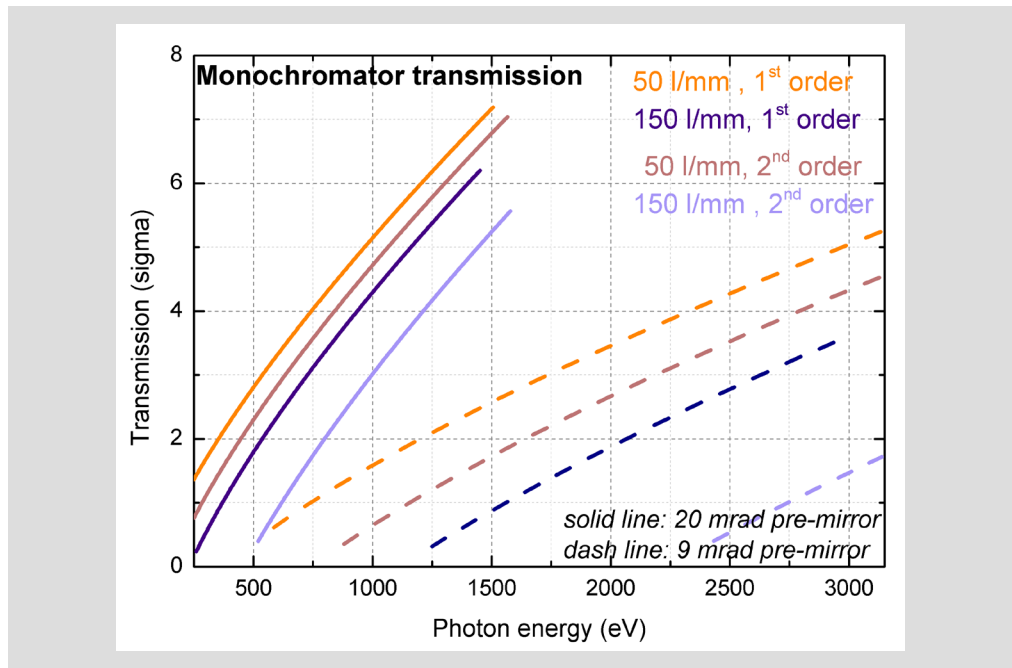
**Figure 9:** Maximal vertical beam size (shaded area, given by the open aperture of the grating) of the operational 1<sup>st</sup> diffraction order at 4 m behind the grating



**Figure 10:** Maximal vertical beam size (shaded area, given by the open aperture of the grating) of the operational 2<sup>nd</sup> diffraction order at 4 m behind the grating

The distances of full separations of the orders presented here relate to the open aperture, while the illumination of the open aperture is expected to vary

strongly with photon energy and other monochromator settings. Expected geometrical transmission of the monochromator in dispersion direction in terms of  $\sigma$  beam size is presented in Figure 11. One can see that, in the low-energy tail of operational ranges, the grating is over-illuminated (the beam is cut by the grating, and beam size corresponds to the open aperture), and, in the high-energy range, the grating is under-illuminated (the beam size is smaller than the open aperture).



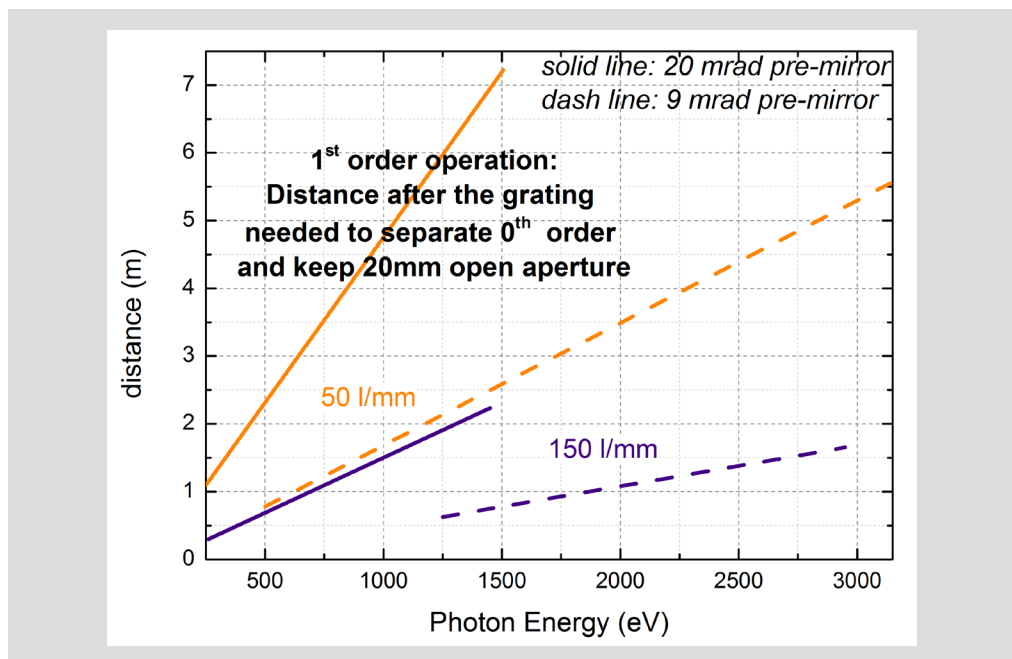
**Figure 11:** Geometrical monochromator transmission in terms of expected beam size in dispersion direction

## 2.4 0<sup>th</sup> order (lower-order) dumps

In the standard configuration, only one diffraction order goes through the beamline to the experiment. However, the efficiency of the other diffraction orders can be substantial and often even higher than that of an operational order. Thus, transmission of 0<sup>th</sup> diffraction order in case of 1<sup>st</sup> or 2<sup>nd</sup> order operation (Figures 1–4) is 10–50% for the most part of the working range. Transmission of the 1<sup>st</sup> order in case of 2<sup>nd</sup> order operation reaches a similar

level.<sup>6</sup> Such intense beam can induce damage in the beamline if not dumped properly. To avoid damage to equipment, beam dumps for intense diffraction orders that are not in use are to be designed and installed.

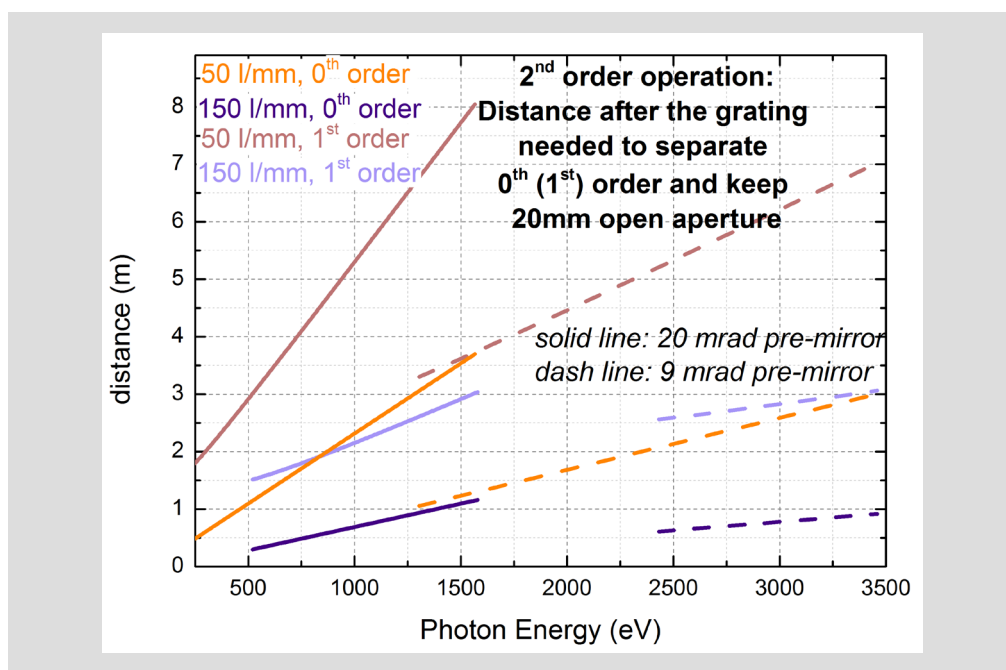
As one of the necessary conditions for the beam dump, we consider a full spatial separation of operational and non-operational orders. The distances of such separation (for non-operational lower diffraction orders) have been discussed in Section 2.3, “Geometrical considerations” (Figure 7 and Figure 8). Practically, it would be desirable to avoid realignment of the beam dump along with change of photon energy (or grating and diffraction order). To fulfil this condition, one could fix the maximal open aperture to 20 mm. As shown in Figure 12 and Figure 13, this condition results in slightly longer distances needed for separation of the 0<sup>th</sup> diffraction order, namely up to 7.2 m for the case of 1<sup>st</sup> order operation and 8.1 m for the case of 2<sup>nd</sup> order operation.



**Figure 12:** Distance after the grating needed to separate the 0<sup>th</sup> order and keep a 20 mm open aperture for the operational 1<sup>st</sup> diffraction order

<sup>6</sup> In Figure 3 and Figure 4, the exit slit is closed. Opening of the slit would add about two orders of magnitude.

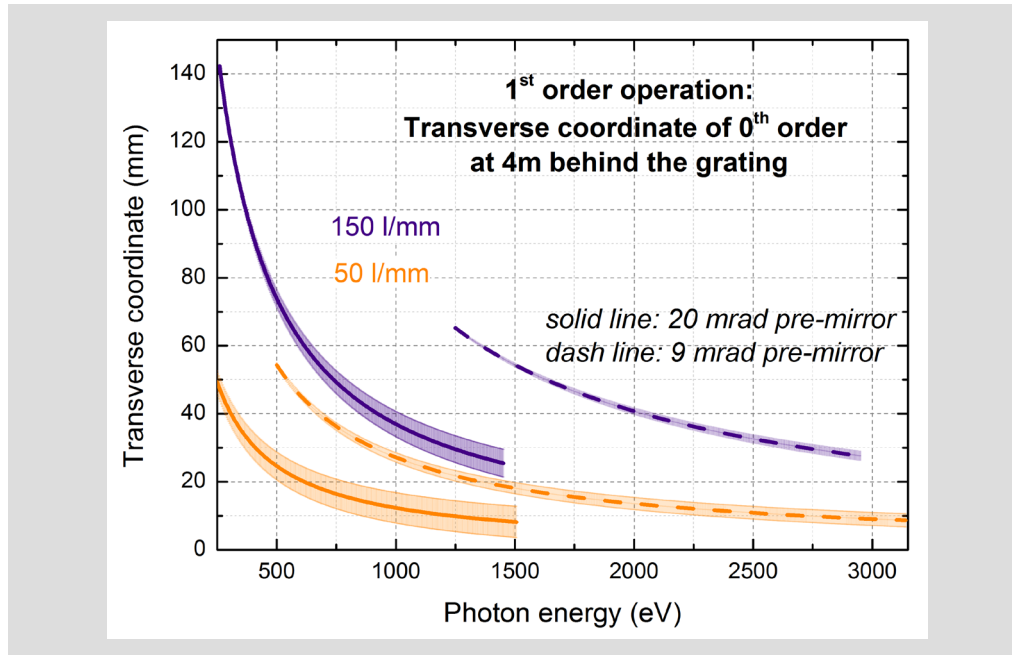




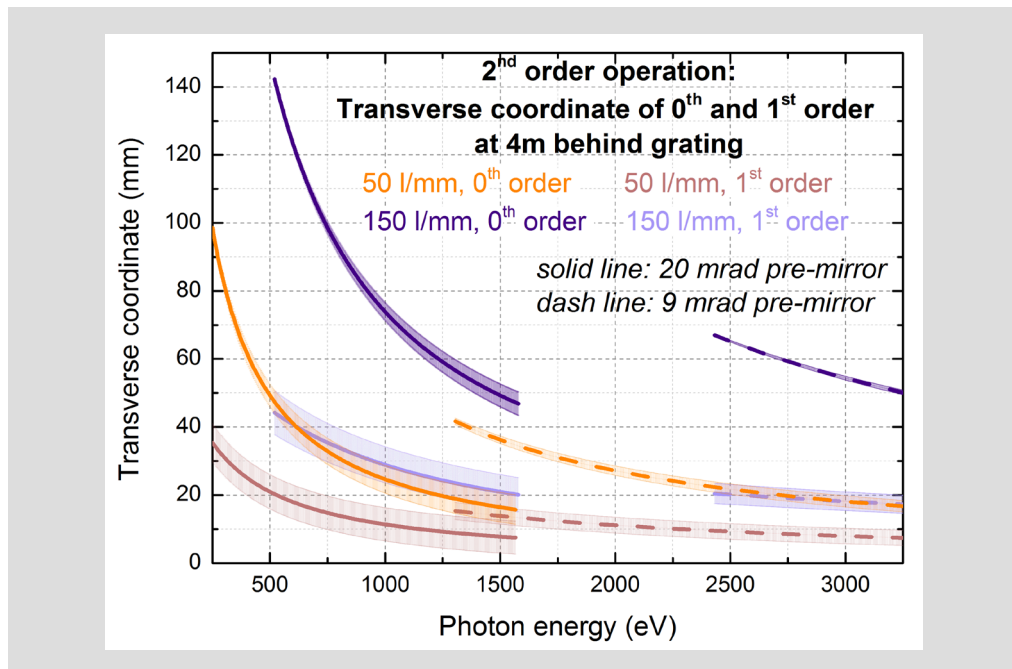
**Figure 13:** Distance after the grating needed to separate the 0<sup>th</sup> order and keep a 20 mm open aperture for the operational 2<sup>nd</sup> diffraction order

On the other hand, moving the beam dump far from the grating would result in larger offsets from the beam axis, in particular for high-resolution cases. Already at 4 m behind the grating, the transversal offset from the beam axis reaches 140 mm (Figure 14 and Figure 15). Such an offset (i) exceeds the dimension of the DN150 beam pipe and (ii) requires a transverse vertical dump dimension of ~ 150 mm to catch the 0<sup>th</sup> (lower) order beam for all possible operational points already separated from the main beam. This makes construction of a single dump complicated, taking into account the grazing incidence geometry of the dump most likely to be chosen. Based on this observation, a possible solution would be to install second beam dump at ~ 2 m behind the grating. In addition, as shown in Figure 14, at 4 m behind the grating, no full separation of the 0<sup>th</sup> order from the 20 mm open aperture (10 mm half-size corresponding to upwards direction in Figure 14 and Figure 15) occurs for the 50 l/mm grating above 800 eV (low-energy pre-mirror) and above 2250 eV (high-energy pre-mirror). The situation is similar for the case of 2<sup>nd</sup> order operation (Figure 15). To assure proper dumping of lower orders at high-energy regions of the working range of the 50 l/mm

grating, a third dump at a longer distance of about 8 m can be installed. In summary, three dumps located approximately at 2 m, 4 m, and 8 m behind the grating could be a solution (Figure 26(a)). The transverse size of each dump in this case could be < 40 mm. The detailed design of the dumps is to be developed.



**Figure 14:** Transverse vertical coordinate (from the beam axis of the operational 1<sup>st</sup> order) of the 0<sup>th</sup> order beam (maximal beam size given by the open aperture of the grating is shaded) at 4 m behind the grating

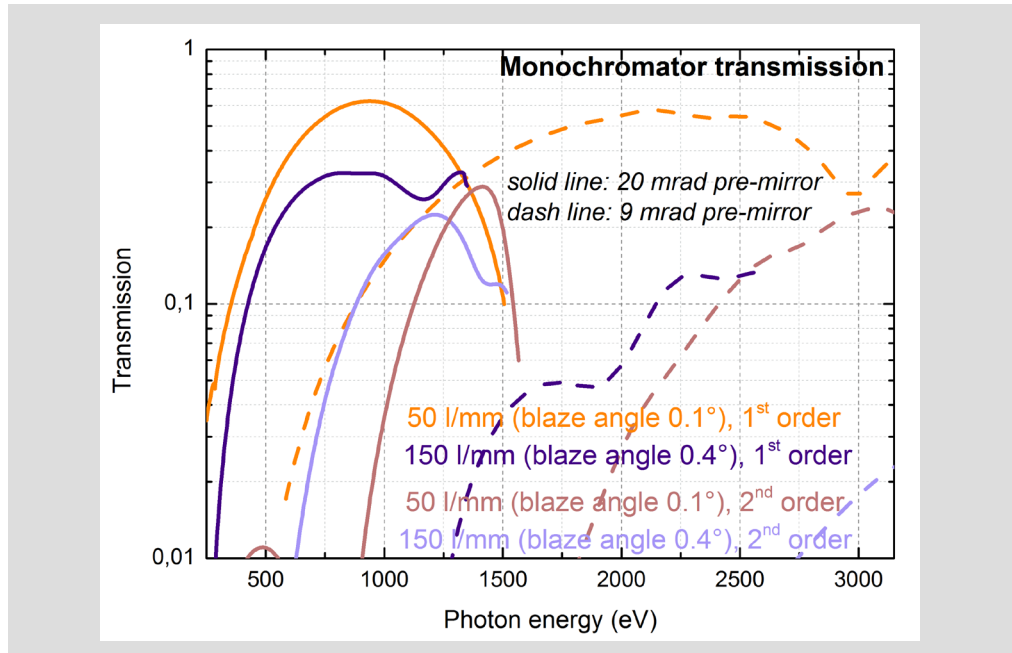


**Figure 15:** Transverse vertical coordinate (from the beam axis of the operational 2<sup>nd</sup> order) to the lower- (0<sup>th</sup>, 1<sup>st</sup>) order beam (maximal beam size given by the open aperture of the grating is shaded) at 4 m behind the grating

## 2.5 Dispersed beam on exit slit

Extremely intense X-ray FEL beam puts demand to sustain ultrahigh fluxes not only on beam dumps but on the exit slit as well. To estimate the load on the exit slit, the monochromator transmission before the slit and the expected size of the dispersed beam are presented in Figure 16 and Figure 17, respectively. One can see that in case of the low-energy pre-mirror, one of the worse situations is operation with a 50 l/mm grating in 1<sup>st</sup> diffraction order at 800 eV, which corresponds to a transmission of ~ 60% and a beam size of 1.8 mm FWHM. Using these values, the load on exit slit could be estimated and compared to the load on beam dumps. For instance, operation with the same pre-mirror and grating at 400 eV leads to a transmission of the 0<sup>th</sup> order beam of ~ 40% (Figure 1) and to a beam size of ~ 8 mm at 4 m behind the grating (Figure 14). Another grating leads to lower loads on the slit (due to higher dispersion and lower efficiency) but to a higher load on dumps: for instance, the 150 l/mm grating at 400 eV has ~ 30% transmission of the

0<sup>th</sup> order (Figure 2) and ~ 4 mm beam size (Figure 14). In the case of high-energy pre-mirror, the sizes of beam on dump in general become smaller (Figure 14–15). To look into the details of load on dumps and the exit slit, horizontal beam sizes should be taken into account as well.



**Figure 16:** Monochromator transmission after the grating (before the exit slit) operating in 1<sup>st</sup> or 2<sup>nd</sup> diffraction order

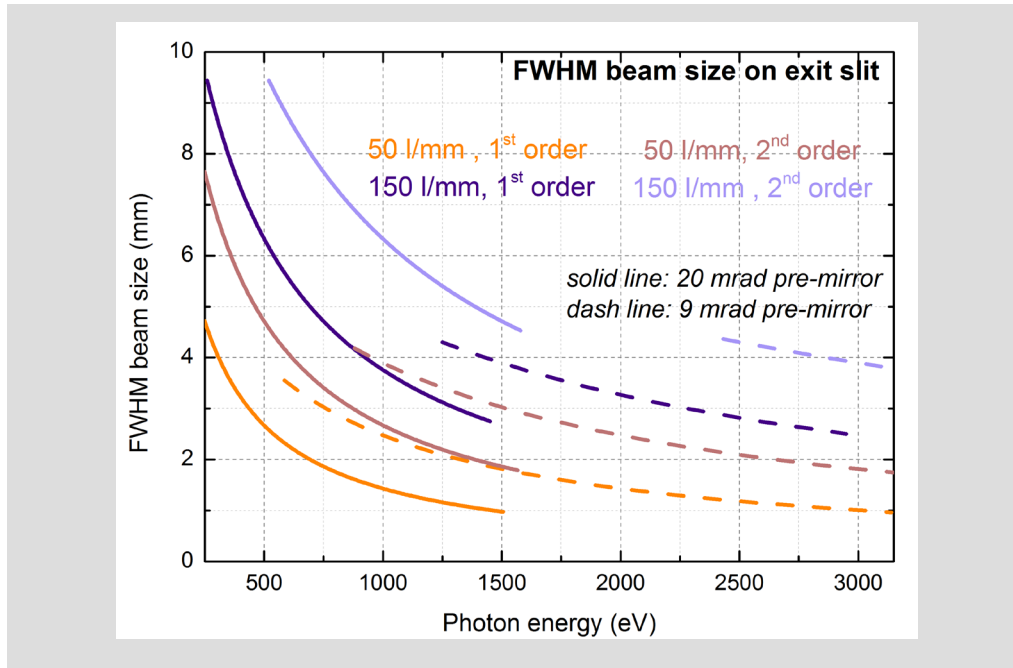


Figure 17: FWHM beam size at the exit slit assuming a 0.5% FWHM FEL bandwidth

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## 3 Higher diffraction orders

In this section, the need for dumps to catch higher diffraction orders, directed down with respect to operational order, is discussed.

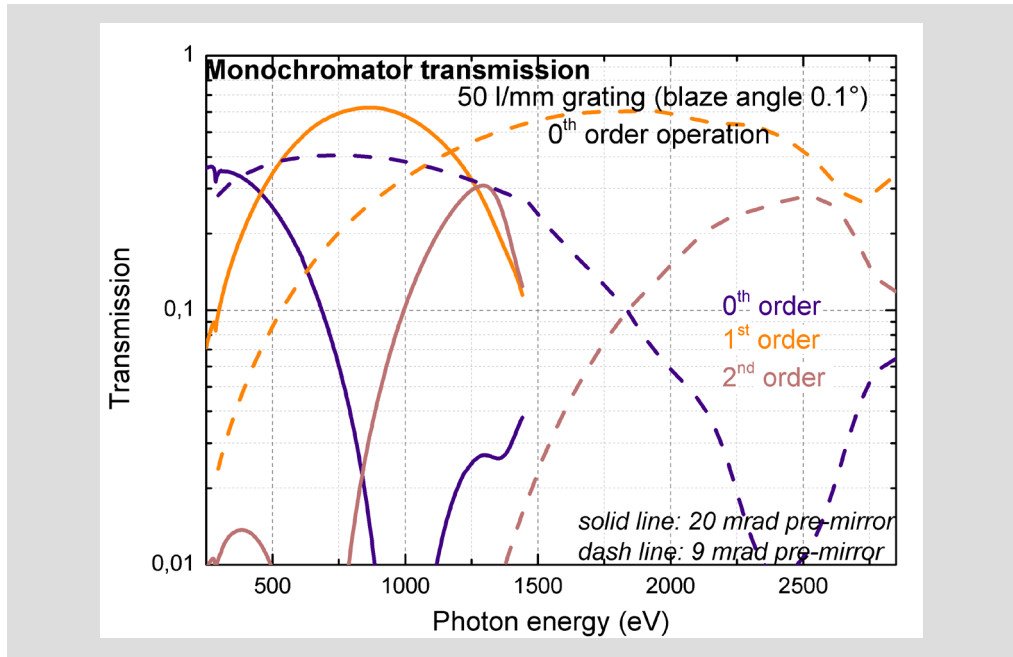
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### 3.1 0<sup>th</sup> order operation

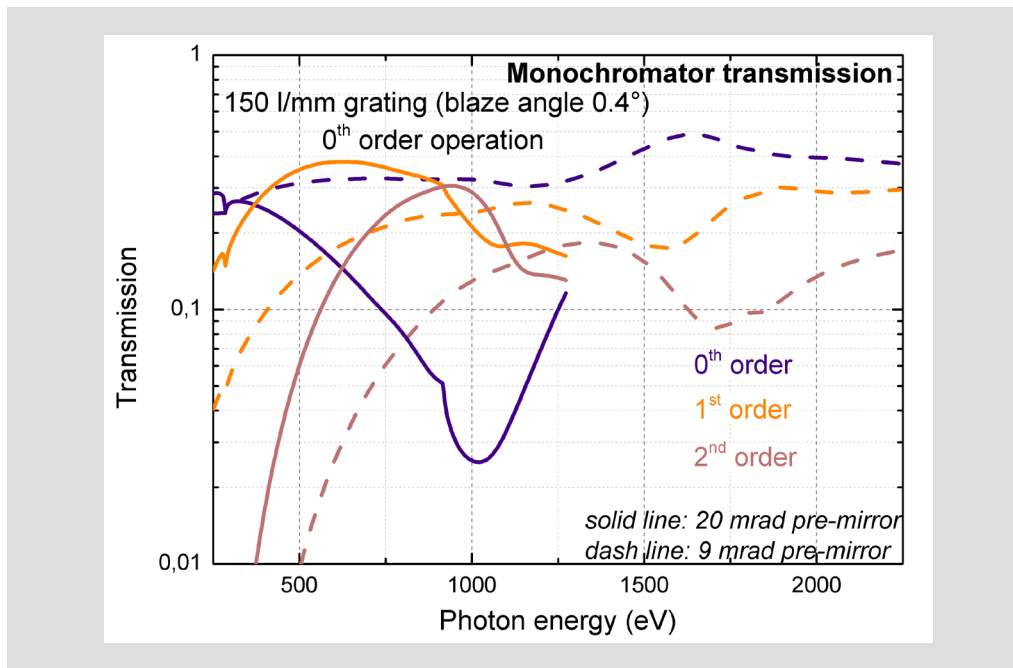
In addition to dumps coming from above to catch 0<sup>th</sup> (lower) diffraction orders, there could be a need for dump(s) to catch higher diffraction orders in case of 0<sup>th</sup> order operation. A demand to work in 0<sup>th</sup> order could come from experimentalists (e.g. in order to have more intense or short pulses for temporal overlap with the pump–probe laser) because operation in the 0<sup>th</sup> order does not require grating or mirror change and thus could help in changing beam conditions while keeping the beam path and position of the spot on sample unchanged. If such a demand arises<sup>7</sup>, dumps for higher diffraction orders should be installed from below because, for blazed grating, 1<sup>st</sup> order and even 2<sup>nd</sup> order efficiency is extremely high under certain conditions. The monochromator transmission after the grating (before passing the exit slit) has been estimated for 0<sup>th</sup>, 1<sup>st</sup>, and 2<sup>nd</sup> diffraction orders in case of 0<sup>th</sup> order operation (Figure 18 and Figure 19). The transmission of 1<sup>st</sup> and 2<sup>nd</sup> diffraction orders is seen to be above 10% over most of the operation range. Thus, to allow 0<sup>th</sup> order operation, the higher order dumps are to be installed from below to the beam axis.

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<sup>7</sup> Note that operation in the 0<sup>th</sup> order is not allowed for the whole range of operation in higher diffraction orders due to the demand to stay below the critical angle for the beam incident to the groove surface of blazed grating (to avoid damage). Operation in the 0<sup>th</sup> order implies an increase of angle of incidence to the groove surface and thus a cut-off of the high-energy tail starts at lower photon energies. More sensitive is the 150 l/mm grating with a higher blaze angle.



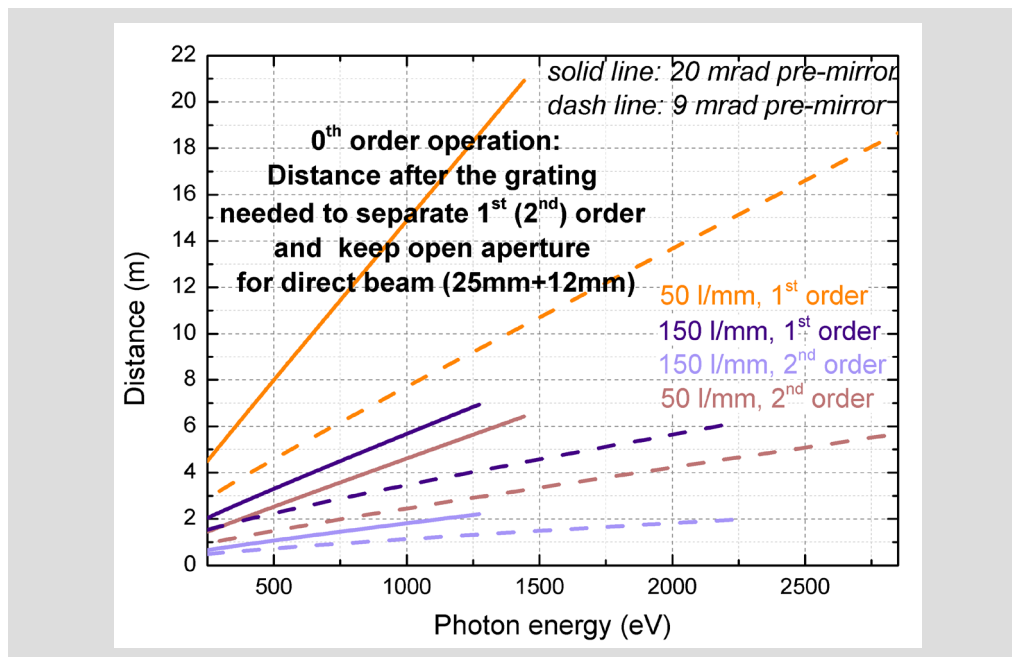
**Figure 18:** Monochromator transmission after the grating (before passing the exit slit) operating in the 0<sup>th</sup> diffraction order; case of the 50 l/mm grating (blaze angle 0.1°)



**Figure 19:** Monochromator transmission after the grating (before passing the exit slit) operating in the 0<sup>th</sup> diffraction order; case of the 150 l/mm grating (blaze angle 0.4°)

The full beam separation happens at similar distances to the case of 1<sup>st</sup> and 2<sup>nd</sup> order operation discussed above (just at slightly longer distances due to

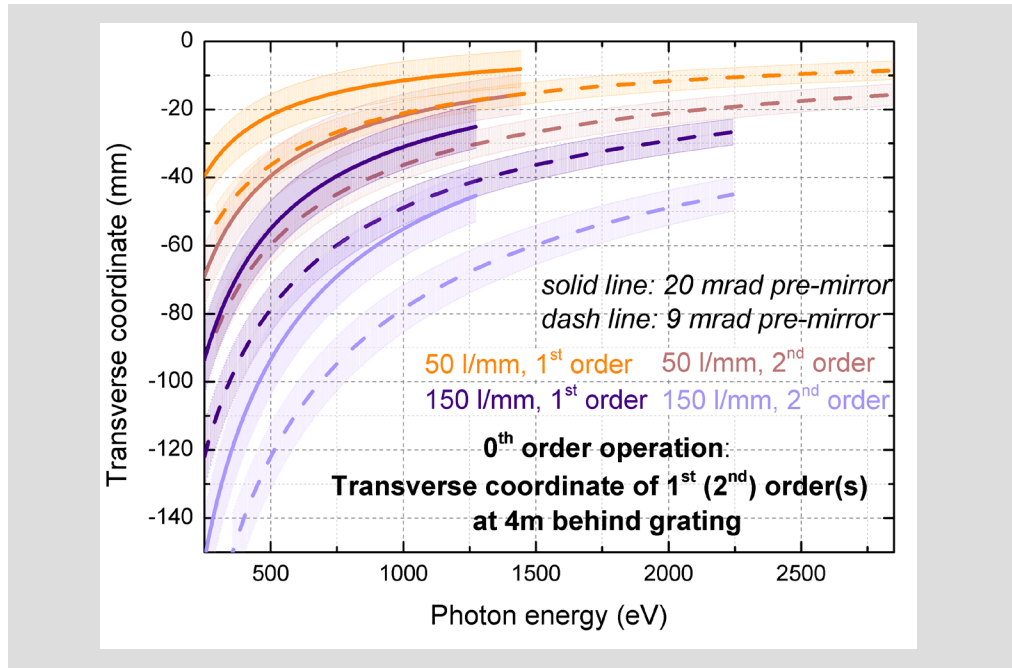
slightly smaller angular separation). Thus, it is possible to install dumps symmetrically to those for 0<sup>th</sup> (lower) orders (the same longitudinal position but below beam axis); however, in this case, the dumps should be retractable to open the path for the direct (pink) beam with an axis at 25 mm below the monochromatic beam axis. To estimate the feasibility of fixed (non-retractable) beam dumps for higher orders, the distances for separation of higher orders along with keeping the beam path for direct beam open has been estimated (Figure 20). The full separation of higher orders happens at 21 m in this case.



**Figure 20:** Distance after the grating needed to separate operational 1<sup>st</sup> or 2<sup>nd</sup> diffraction orders and keep the aperture open for the direct beam (25 + 12 mm)

The maximal beam size of the 0<sup>th</sup> order in the dispersive direction (given by an open aperture) is constant over the photon energy range: ~ 10 mm for the 20 mrad pre-mirror and ~ 4.5 mm for 9 mrad pre-mirror. Maximal beam sizes in the dispersion direction of higher orders to be dumped are larger than in the case of lower orders to be dumped (Figure 21 compared to Figure 14 and Figure 15). The transverse offset of higher orders from the beam axis is presented in Figure 21. The offset is negative to show the reverse direction (to the offsets in case of 1<sup>st</sup> and 2<sup>nd</sup> order operation).



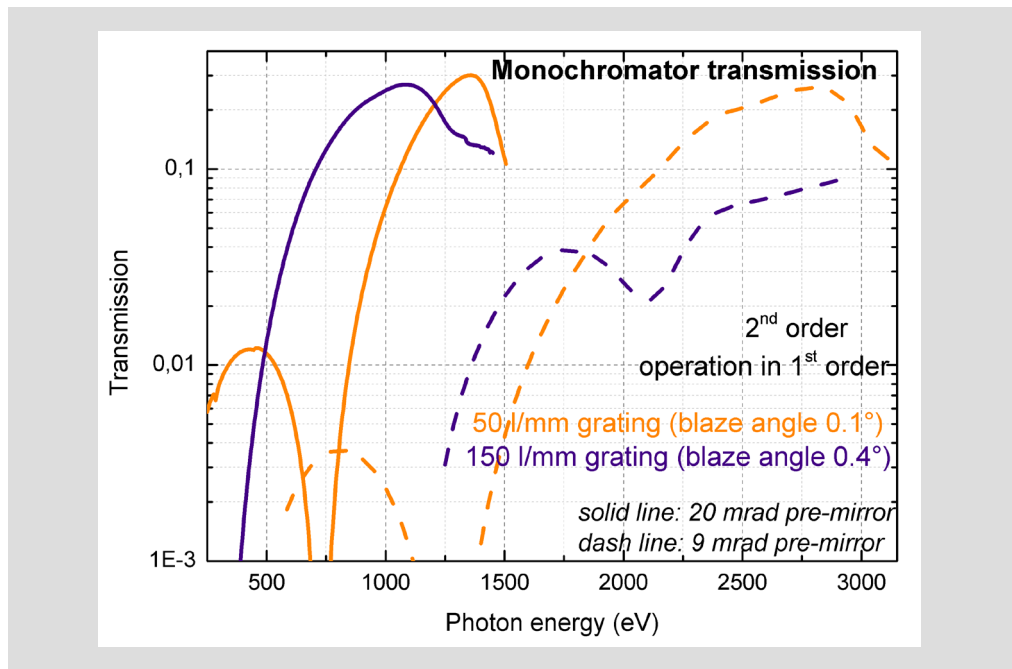


**Figure 21:** Transverse vertical coordinate (from the beam axis of the operational 0<sup>th</sup> order) of the 1<sup>st</sup> or 2<sup>nd</sup> diffraction order beam (maximal beam size given by the open aperture of grating is shaded) at 4 m behind the grating

The geometrical arrangement of higher-order dumps is to be developed taking into account the information presented in this and the following section.

## 3.2 2<sup>nd</sup> order in case of 1<sup>st</sup> order operation

If 0<sup>th</sup> order operation in the absence of proper dumps could be forbidden, the standard 1<sup>st</sup> order operation would lead unavoidably to the 2<sup>nd</sup> order pointing in the same downward direction. The monochromator transmission of the 2<sup>nd</sup> order in case of 1<sup>st</sup> order operation is presented in Figure 22. It is not negligible and, for certain ranges, surpasses 10–20%, indicating a need for the dumps to be installed from below to catch the 2<sup>nd</sup> order.



**Figure 22:** Monochromator transmission of 2<sup>nd</sup> order (before passing the exit slit) in case of 1<sup>st</sup> order operation

The situation is considerably different compared to those previously discussed. The angle between the 2<sup>nd</sup> order and the operational 1<sup>st</sup> order is very shallow (Figure 23). This leads to long distances of full spatial separation reaching 16 m in case of expected to be frequent operation with a 50 l/mm grating in the range 0.8–1.5 keV (Figure 24). The full separation happens at different longitudinal positions, as discussed in Section 2.3, “Geometrical considerations”, on page 10. The fixed open aperture for the 1<sup>st</sup> order beam would result in longer distances of separation. Thus, to fulfil the condition of keeping an open aperture of 20 mm, allowing full beam to pass through in full operational range, the dump should be located 21 m behind the grating (Figure 25). As discussed in Section 3.1, “0<sup>th</sup> order operation”, on page 22, the dump should be retractable, allowing for the pink beam at 25 mm below the monochromatized beam axis. And as discussed in Section 2.4, “0<sup>th</sup> order (lower-order) dumps”, on page 15, due to the substantial angular spread of beams to be dumped at different monochromator settings, along with the possible demand for grazing incidence geometry of dumps, additional dumps are to be installed at distances closer to the grating.

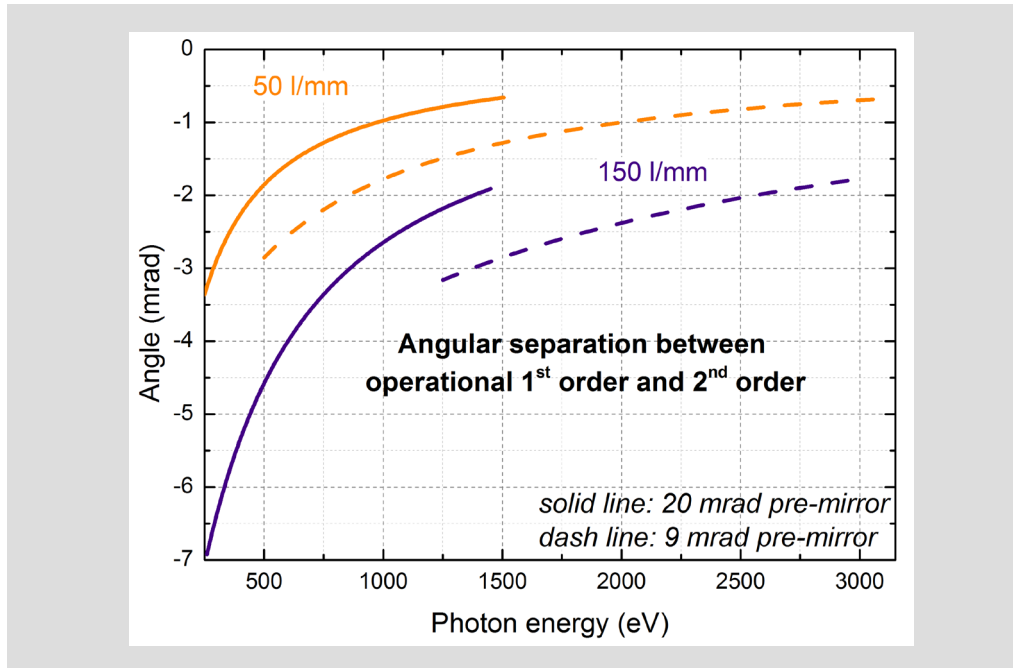


Figure 23: Angular separation between the operational 1<sup>st</sup> and the 2<sup>nd</sup> orders

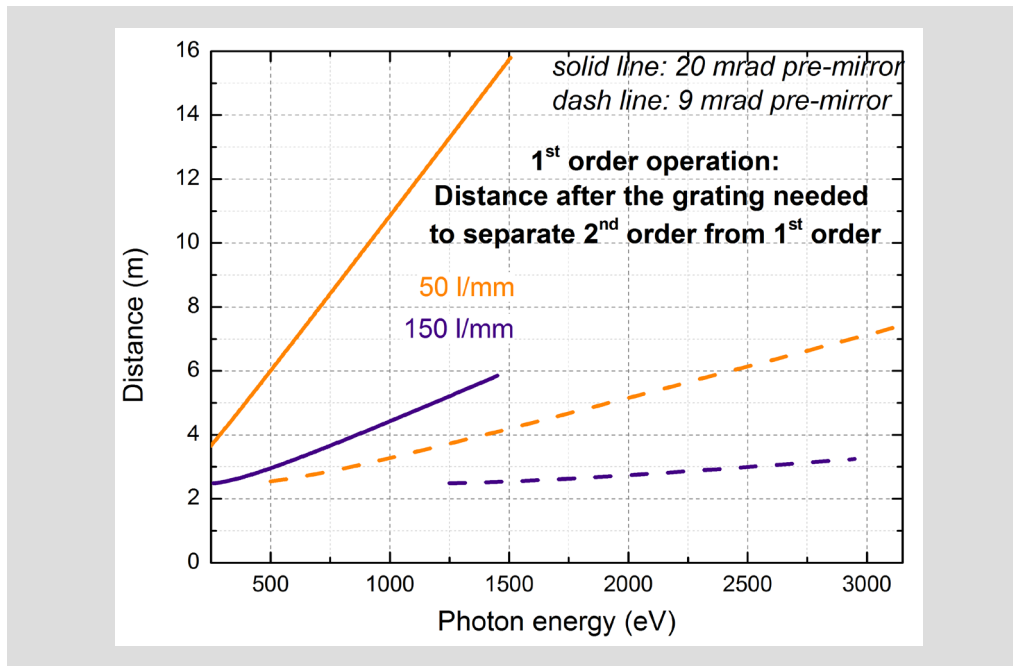
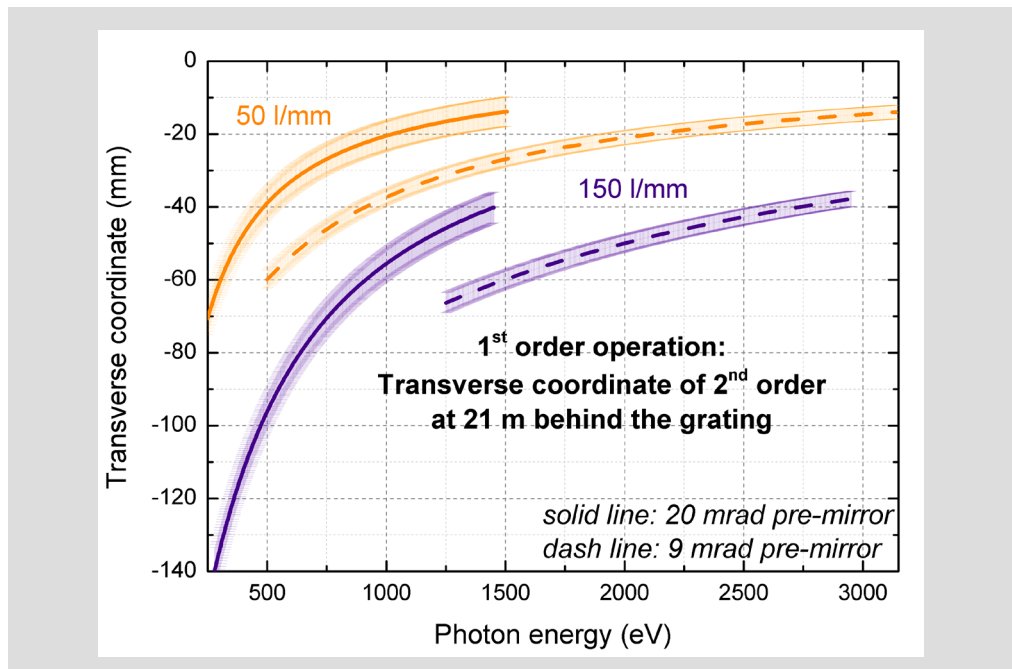
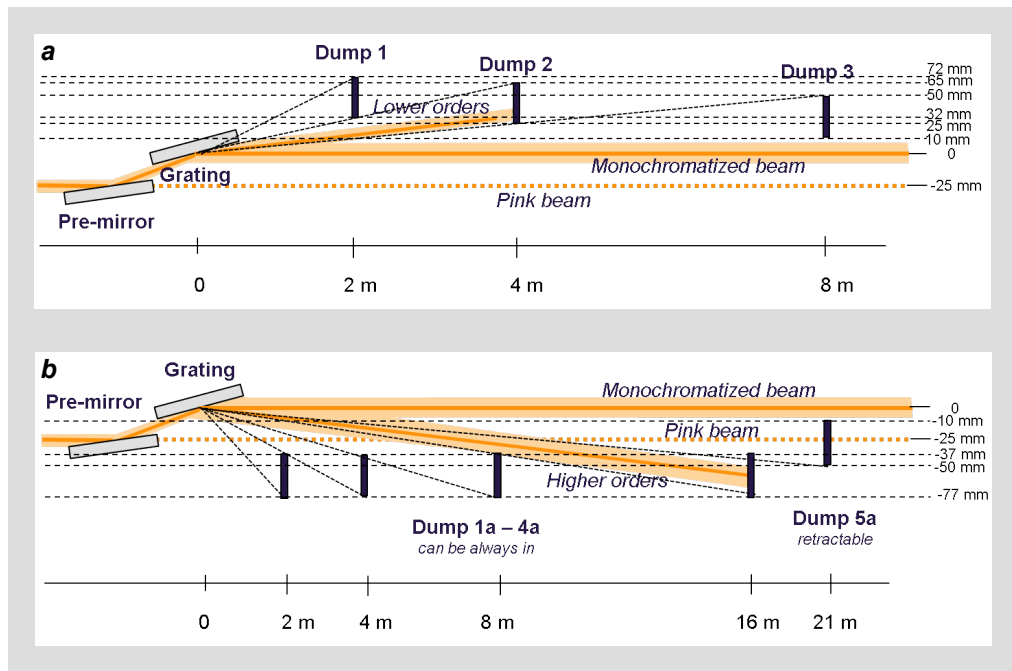


Figure 24: Distance needed to separate the 2<sup>nd</sup> order from the operational 1<sup>st</sup> order



**Figure 25:** Transverse coordinate (from the beam axis of the operational 1<sup>st</sup> order) of the 2<sup>nd</sup> order beam (maximal beam size given by the open aperture of the grating is shaded) at 21 m behind the grating

Summing up the geometrical considerations from this section and Section 2.4, “0<sup>th</sup> order (lower-order) dumps”, on page 15, the possible scheme for the beam dumps is presented in Figure 26. The final design and arrangement of the dumps is to be developed.



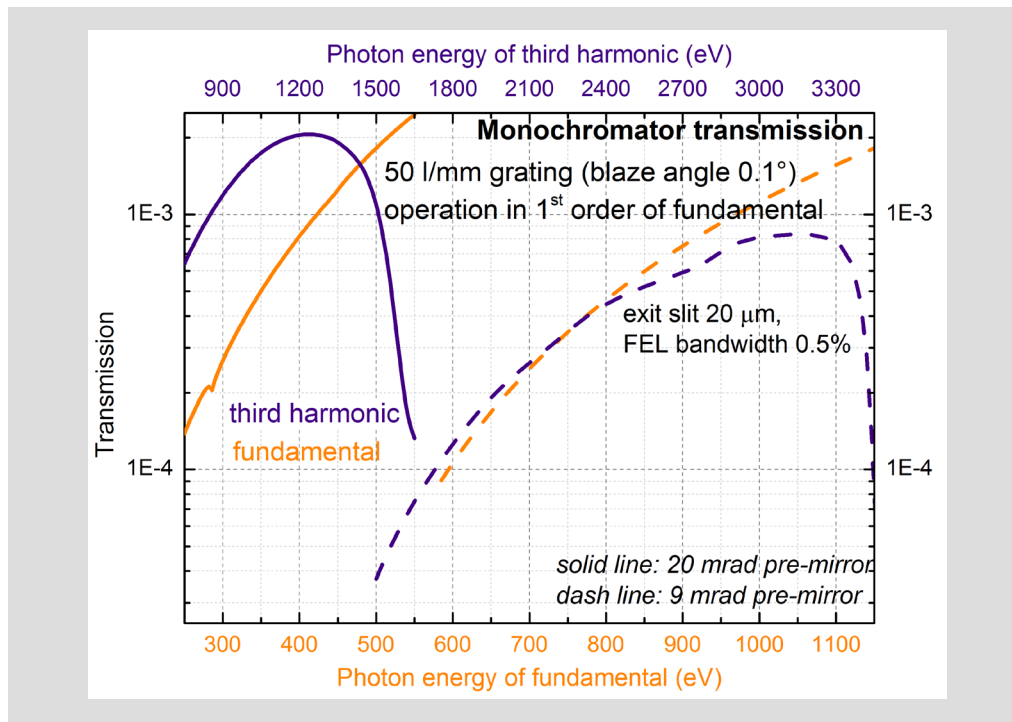
**Figure 26:** Possible geometry of the beam dumps for (a) lower and (b) higher diffraction orders after the monochromator

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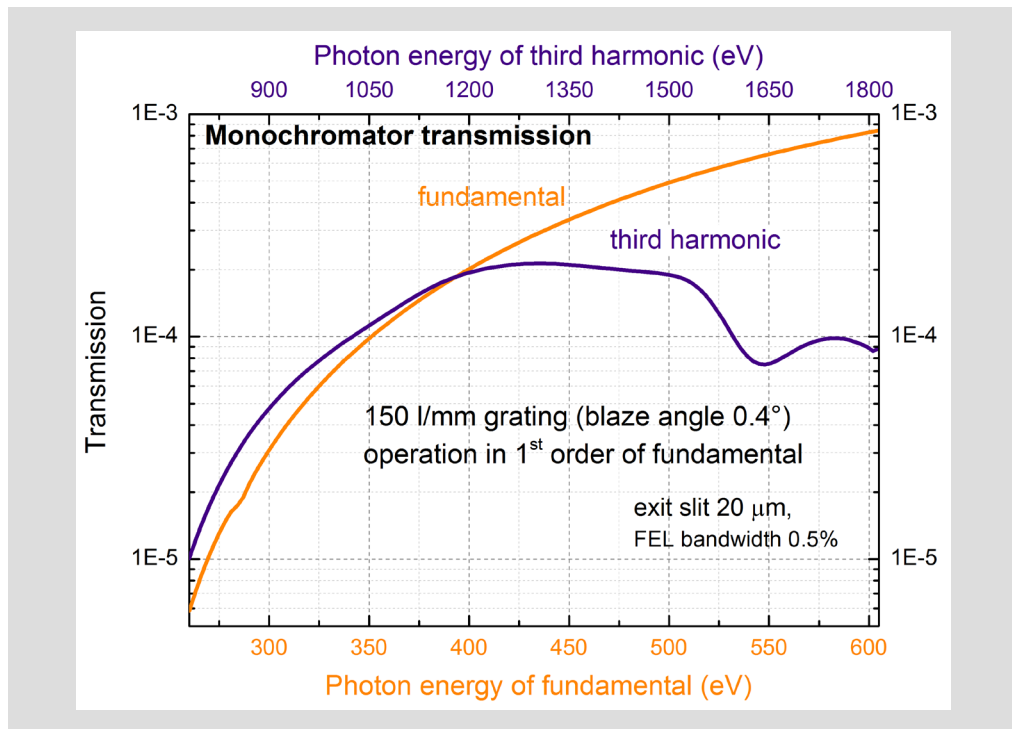
## 4 Third harmonic

The higher harmonics, although of considerably lower intensity than the fundamental, will be produced by the SASE3 undulator. The harmonics, if not suppressed, could be harmful to the experiments. The monochromator provides spatial filtering of harmonics, ensuring spectrally clean beam at the experiment. On the other hand, the harmonics could be used for two-colour X-ray pump – X-ray probe experiments; such a possibility was proposed [2] in a scheme similar to the 0<sup>th</sup> order – 1<sup>st</sup> order beam splitter discussed above. To investigate the feasibility of such experiments, an analysis of the possible working range, efficiency, transmission and spatial separation is presented in this section. The third harmonic, expected to be the most efficient among the higher harmonics, is discussed.

The constraints on the operational range are given by transmission by optics. Here, only the pre-mirror and the grating are considered. The resulting transmission is presented in Figure 27 and Figure 28 for 50 l/mm and 150 l/mm gratings, respectively. The transmission can be increased substantially (up to more than an order of magnitude) by opening the exit slit, provided the experiment accepts a larger spot size and bandwidth.



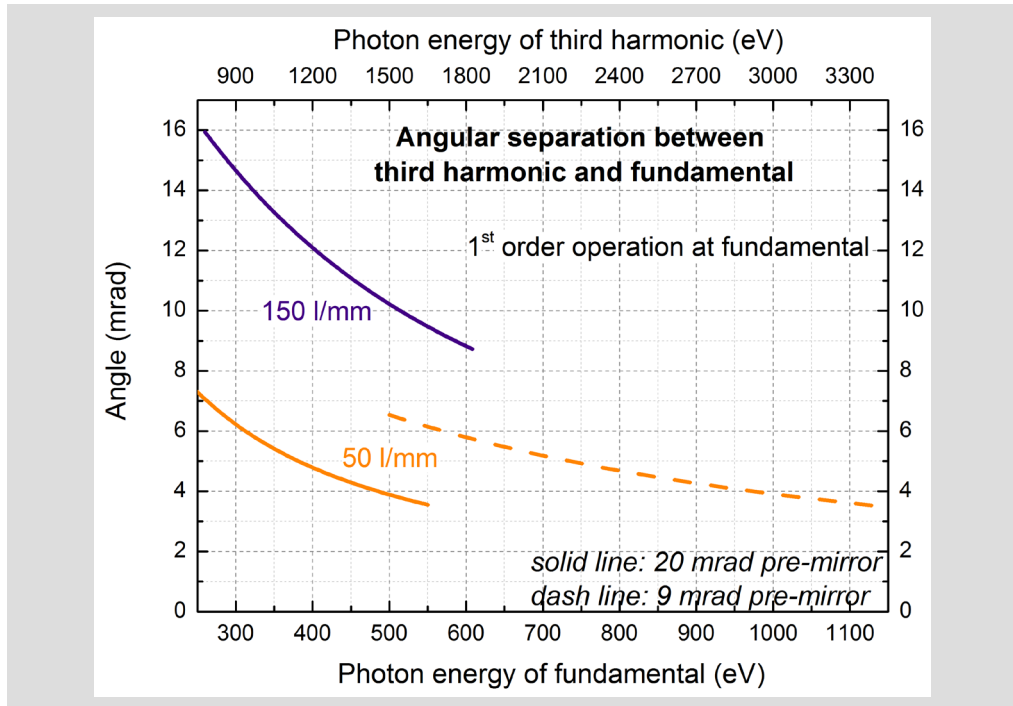
**Figure 27:** Monochromator transmission of the fundamental and the third harmonic for the 50 l/mm grating (blaze angle  $0.1^\circ$ ) operating in the 1<sup>st</sup> diffraction order of the fundamental. The exit slit is set to 20  $\mu\text{m}$ .



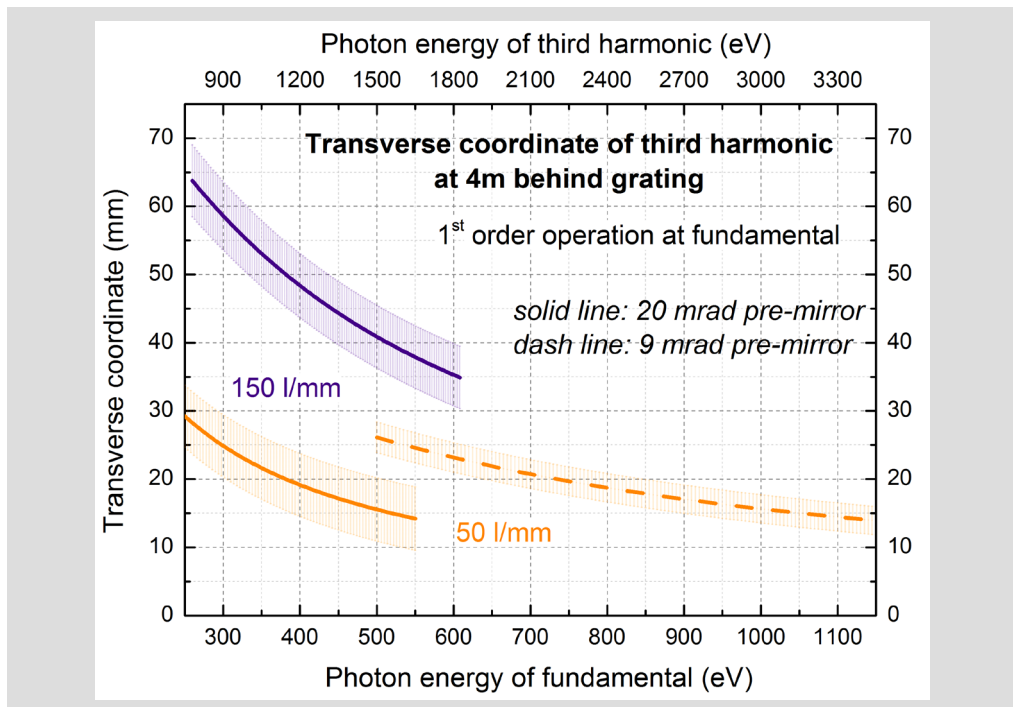
**Figure 28:** Monochromator transmission of the fundamental and the third harmonic for the 150 l/mm grating (blaze angle  $0.4^\circ$ ) operating in the 1<sup>st</sup> diffraction order of the fundamental and for the low-energy pre-mirror. The exit slit is set to  $20\ \mu\text{m}$ .

The angular separation between the third harmonic and the fundamental is presented in Figure 29. The transverse coordinate and maximal transverse beam size at 4 m behind the grating is presented in Figure 30. The angular separation is large enough to allow the full separation of the third harmonic from the fundamental at a distance 3 m behind the grating (Figure 31). A condition of the third harmonic separation, along with keeping an open aperture of 20 mm, is fulfilled at a distance of 4.2 m (Figure 32).

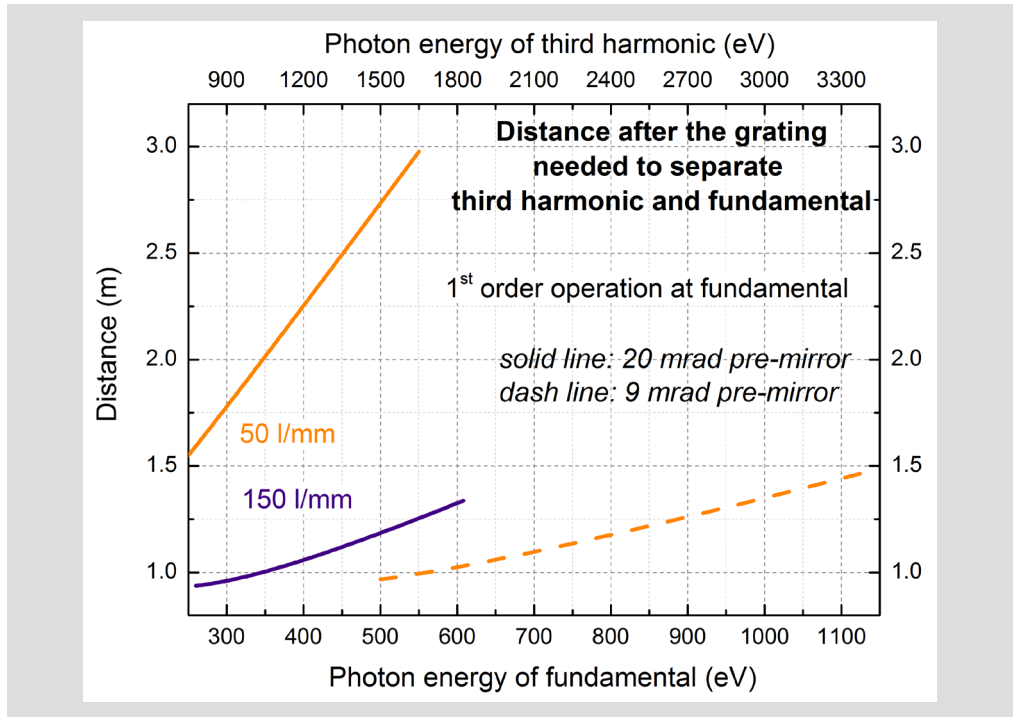




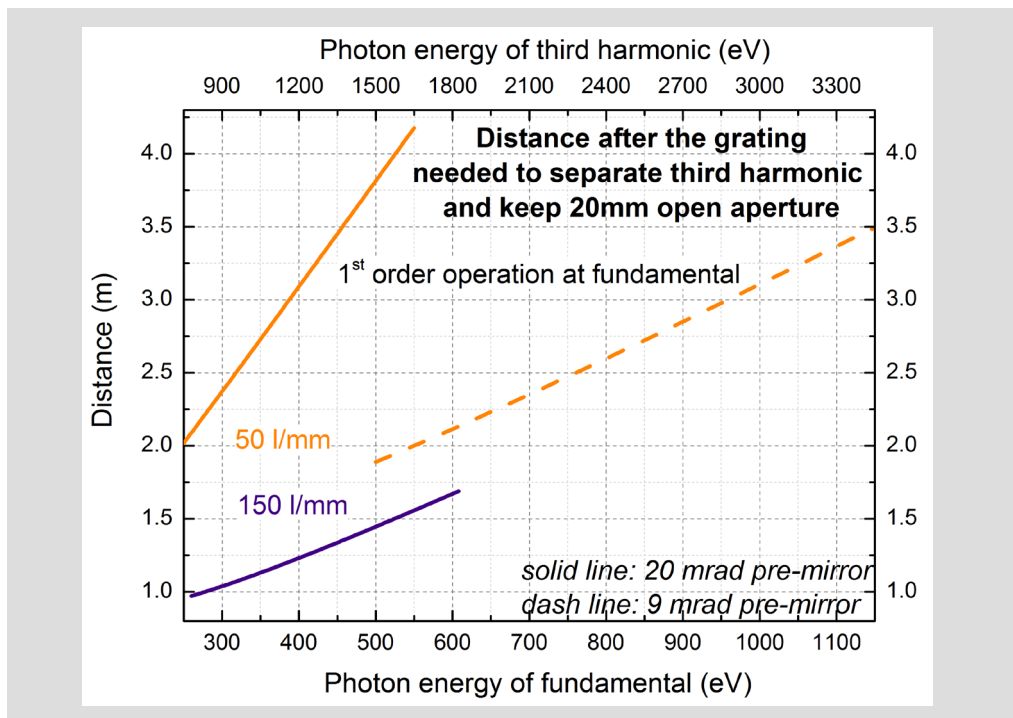
**Figure 29:** Angular separation between the third harmonic and the fundamental for operation in the 1<sup>st</sup> diffraction order of the fundamental



**Figure 30:** Transverse coordinate of the third harmonic for operation in the 1<sup>st</sup> diffraction order of the fundamental at 4 m behind the grating. Maximal beam size of the third harmonic given by the open aperture of the grating is shown as shaded area.



**Figure 31:** Distance after the grating needed to separate the third harmonic from the fundamental



**Figure 32:** Distance after the grating needed to separate the third harmonic and keep a 20 mm open aperture for the fundamental

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