Aberration-free imaging of inelastic scattering spectra with x-ray echo spectrometers

Manuel Sánchez del Río and Yuri Shvydko

1ESRF, The European Synchrotron, Grenoble, France
2Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois, USA

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We study conditions for aberration-free imaging of inelastic x-ray scattering (IXS) spectra with x-ray echo spectrometers. Aberration-free imaging is essential for achieving instrumental functions with high resolution and high contrast. Computational ray tracing is applied to a thorough analysis of a 0.1-meV/0.07-nm$^{-1}$-resolution echo-type IXS spectrometer operating with 9-keV x-rays. We show that IXS spectra imaged by the x-ray echo spectrometer that uses lenses for the collimating and focusing optics are free of aberrations. When grazing-incidence mirrors (paraboloidal, parabolic Kirkpatrick-Baez, or parabolic Montel) are used instead of the lenses, the imaging system reveals some defocus aberration that depends on the inelastic energy transfer. However, the aberration-free images can be still recorded in a plane that is tilted with respect to the optical axis. This distortion can be thus fully compensated by inclining appropriately the x-ray imaging detector, which simultaneously improves its spatial resolution. A full simulation of imaging IXS spectra from a realistic sample demonstrates the excellent performance of the proposed designs.

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I. INTRODUCTION

X-ray echo spectroscopy [1], a space-domain counterpart of neutron spin echo [2], was introduced recently to overcome the limitations in spectral resolution and weak signals of the traditional inelastic hard x-ray scattering (IXS) probes. X-ray echo spectroscopy is an extension into the hard x-ray domain of the approach proposed [3] and demonstrated in the soft x-ray domain [4]. X-ray echo is refocusing the defocused x-ray source image. Defocusing and refocusing systems are the main components of x-ray echo spectrometers. They are composed of focusing and dispersing optical elements, where the latter are asymmetrically cut crystals in Bragg diffraction. The optical elements have to be complemented by the x-ray source, sample, and x-ray position-sensitive detector, as schematically shown in Fig. I. Refocusing takes place only when the defocusing and the refocusing systems compose a time-reversed pair. This implies that a virtual source placed into the detector plane produces the defocused image in the sample plane with the same linear dispersion rate as the real source.

When the defocused x-rays are scattered inelastically from the sample with an energy transfer $\epsilon$, they pass through the refocusing system that refocuses them on the detector, but with a lateral shift with respect to the optical axis that is proportional to $\epsilon$, see Fig. I(v). This property enables echo spectrometers to image IXS spectra with a spectral resolution solely determined by the sharpness of the refocused image of the source, and completely independent of the spectral composition of x-rays incident on the sample. The spectral resolution of x-ray echo spectrometers is therefore decoupled from the spectrometer bandwidth, x-ray monochromatization is not required, and the IXS refocusing (imaging) system is broadband. These features of echo spectrometers are in a striking contrast to present-day narrow-band scanning IXS spectrometers (see [5] for a review), whose spectral resolution is determined by the smallness of the monochromator and analyzer bandwidths. As a result, broadband imaging echo-type IXS spectrometers have the potential of increasing the signal strength by orders of magnitude, thus reducing acquisition times and substantially improving spectral resolution.

The ability of the refocusing system to produce sharp and undeformed images for each inelastic $\epsilon$-component is critical for achieving the high-resolution and high-contrast instrumental functions of echo-type spectrometers. This is, however, a challenge, because the defocused source image on the sample and the refocused IXS image on the detector are spread laterally with respect to the optical axis. Therefore, x-ray echo spectrometers must be truly aberration-free imaging systems capable of producing sharp images when the focusing elements are illuminated both on-axis or off-axis.

The theory of x-ray echo spectrometers developed in [1,6] is based on paraxial analytical ray tracing, which uses ray transfer matrix analysis. It predicts aberration-free imaging, provided ideal (perfectly focusing and non-absorbing) parabolic x-ray lenses are used, which make sure that the collimating and focusing elements form a truly imaging optical system. This conclusion is also supported by computational wave propagation studies [7] performed with SRW code [8] for a 0.1-meV-resolution x-ray echo spectrometer with the parameters from [1].

Real parabolic x-ray compound refractive lenses (CRL) [9] have small effective aperture for the x-ray echo spectrometers because of photo absorption. Curved grazing incidence mirrors may feature much larger apertures.
Here, we review the principles of x-ray echo spectrometers, and the optical scheme defining in detail the configuration and elements used in the numerical simulations.

### II. PRINCIPLES, OPTICAL DESIGN, AND PARAMETERS OF X-RAY ECHO SPECTROMETERS

The optical scheme of the x-ray echo spectrometer considered here is shown in Fig. 1. Its performance was discussed in detail and substantiated by analytical ray tracing in [6].

As a result of propagation through the defocusing system $\hat{O_D}$, x-rays from the source with a vertical size $\Delta x_0$ in reference plane 0 are focused on the sample in reference plane 1 with an image size $\Delta x_1 = A_D \Delta x_0$ ($A_D$ is a magnification factor), albeit, with the focal spot location dispersed in vertical direction $x$ for different spectral components with a linear dispersion rate $G_D$.

All spectral components of the defocused source image can be refocused into a single spot (echo) with a size $\Delta x_2 = A_n \Delta x_1$ in the detector reference plane 2 by propagation through the refocusing system $\hat{O_R}$, provided it is a time-reversed counterpart of the defocusing system $\hat{O_D}$. The later means that x-rays from a virtual source of size $\Delta x_2$ in the detector plane being propagated in the reverse direction produce on the sample exactly the same defocused image as the image by the defocusing system. This is expressed by the refocusing condition

$$G_D + G_R/A_D = 0, \quad (1)$$

were, $G_R$ is a linear dispersion rate and $A_D$ a magnification factor of the refocusing system.
If inelastic scattering takes place on the sample with an energy transfer $\epsilon$, the dispersed signal is still refocused into a tight echo signal, but laterally shifted by $\Delta x_2 = G_R \epsilon$ in the detector plane, as shown schematically in Fig. 1(v). This effect enables imaging IXS spectra with an energy resolution

$$\Delta \epsilon = \Delta x_2 / |G_R| \equiv \Delta x_1 / |G_D|,$$

were $\Delta \epsilon$ corresponds to an energy transfer resulting in a lateral shift $\delta x$ that is equal to the image size $\Delta x_1$. One of the major purposes of the paper is to verify by detailed numerical simulations the capability of x-ray echo spectrometers to image IXS spectra with the spectral resolution given by Eq. (2).

The main components of the defocusing and refocusing systems are the dispersing elements $D_D$ and $D_R$ and focusing elements $F$, $F_1$, and $F_2$. The dispersing elements are characterized by the cumulative angular dispersion rates $D_{\cup D}$ and $D_{\cup R}$, cumulative asymmetry parameters $b_{\cup D}$ and $b_{\cup R}$, and spectral bandwidths $\Delta E_D$ and $\Delta E_R$, respectively, see Table I for details. The focusing elements are characterized by the focal lengths $f$, $f_1$, and $f_2$. These parameters determine the linear dispersion rate $G_D$ and the magnification factor $A_D$ of the defocusing system

$$A_D = -\sigma_D l_3 b_{\cup D} l_{12}, \quad G_D = \sigma_D D_{\cup D} b_{\cup D} l_{12} / l_{12},$$

$$1 / f = 1 / l_{12} + 1 / l_3, \quad l_{12} = l_1 / b_{\cup D} + l_2,$$

and of the refocusing system

$$G_R = \sigma_R D_{\cup R} f_2, \quad A_R = -b_{\cup R} f_2 / f_1.$$

Parameters $\sigma_X = +1$ if lenses are used as focusing elements, or alternatively $\sigma_X = -1$ for mirrors. Here $X=D$ or $X=R$.

Using Eq. (5), the spectral resolution $\Delta \epsilon$ given by Eq. (2) can be equivalently expressed through the parameters of the refocusing system as

$$\Delta \epsilon = |b_{\cup R}| \Delta x_1 / |D_{\cup R}| f_1.$$

In the present paper we are studying a particular case of an x-ray echo spectrometer with a 0.1-meV spectral and a 0.07 nm$^{-1}$ momentum-transfer resolution employing 9.1-keV x-rays with design parameters provided in [6]. The global optical parameters of the x-ray echo spectrometer are summarized in Table I and discussed in the following sections.

### B. From source to sample: defocusing system

The vertical source size is typically $\Delta x_0 \approx 25 \mu$m [full width at half maximum (FWHM)] for state of the art undulator synchrotron radiation sources. Assuming a focusing system with a magnification factor $|A_D| \approx 0.1$, we expect for the monochromatic beam size on the sample $\Delta x_1 = |A_D| \Delta x_0 \approx 2.5 \mu$m. Because the high-load monochromator (installed upstream of the defocusing system, not shown in Fig. 1) may degrade the wavefront, we use in our simulations a more conservative value $\Delta x_1 = 5 \mu$m. This value together with the design spectral resolution $\Delta \epsilon = 0.1$ meV of the x-ray echo spectrometer determine via Eq. (2) the required value of the linear dispersion rate $|G_D| = 50 \mu$m/meV.

Focusing element $F$ should possess properties of the true imaging system. We assume it to be a paraboloidal compound refractive lens (CRL), in a good approximation the truly imaging optic [9]. Its focal length $f = 1.446$ m can be realized using 17 double-convex 2D Beryllium lenses of 200 $\mu$m radius of curvature. This chosen configuration gives an effective geometrical aperture of 660 $\mu$m, comparable to the size of the intercepted undulator beam.

In our studies, we fix the value of $f$ as well as the source-to-sample distance $l = l_1 + l_2 + l_3 = 35$ m. The values of other parameters of the defocusing system, see Table I, such as $D_{\cup D}$, $b_{\cup D}$, $l_1$, $l_2$, $l_3$, and $A_D$ are not

| Defocusing system | Refocusing system |
|-------------------|-------------------|
| $G_D$  | $l_1$  | $l_2$  | $l_3$  | $A_D$  | $D_{\cup D}$  | $b_{\cup D}$  | $f$  |
| $G_R$  | $A_R$  | $f_1$  | $D_{\cup R}$  | $b_{\cup R}$  | $f_2$  | $A_D$  | $A_R$  |
| $\mu$m | meV | m | m | m | meV | m | m | m | meV | m |
| 50  | 35  | 32.55 | 0.73 | 1.72 | -0.095 | -31.7 | 1.96 | 1.45 | 1.0 | -0.4 | -125 | 0.27 | 1.471 | 0.095 |

TABLE I: Global optical parameters of an x-ray echo spectrometer with a 0.1-meV spectral and a 0.07 nm$^{-1}$ momentum-transfer resolution. See Fig. 1 for the optical scheme and the text for notations. The following parameters are fixed: monochromatic source size on the sample $\Delta x_1 = 5 \mu$m, the source to sample distance $l = l_1 + l_2 + l_3$, and the focal lengths $f$, $f_1$. Other parameters are chosen to ensure the 0.1-meV design spectral resolution, Eqs. (2) and (6), to fulfill the refocusing condition, Eq. (1) and Eqs. (3)-(4). The central photon energy of the incident x-rays on the sample is $E_0 = 9137.01$ eV, defined by (008) Bragg reflections from the Si crystals in the dispersing elements.
unique, but are chosen to be practical and to meet the constraints imposed by Eqs. 1-4.

The dispersing element $D_D$ is chosen to meet the values of $D_{\cup D}$ and $b_{\cup D}$ provided in Table I. The required big angular dispersion rate $D_{\cup D} = -31.7 \mu$rad/meV can be achieved only by using multi-crystal systems featuring the enhancement effect of angular dispersion $\varepsilon_D$.[1][15][16] Figure 2 shows the optical scheme and spectral transmission function of the four-crystal dispersing element considered in the present studies (see [5] for more details).

1 Diffraction gratings are not practical dispersing elements in the hard x-ray regime. Instead, crystals in Bragg diffraction can function as gratings, dispersing x-rays into spectral fans with photons of different energies propagating at different angles [17-19]. The grating effect takes place only in asymmetric Bragg diffraction, with the diffracting atomic planes at a nonzero angle $\eta \neq 0$ to the entrance crystal surface. Bragg diffraction ensures high reflectivity, while the asymmetric cut results in electron density periodic modulation along the crystal surface responsible for the grating effect of angular dispersion.

C. From sample to detector: refocusing system

The refocusing system is composed of a pair of focusing elements $F_1$, $F_2$, and a dispersing element $D_R$ placed in between, see Fig. 1.

The focal length of $F_1$ is chosen to be $f_1 = 0.4$ m, defined by the required momentum transfer resolution of $\Delta Q = 0.07$ nm$^{-1}$, see [6]. According to Eq. 4, this value of $f_1$ together with the design spectral resolution $\Delta \varepsilon = 0.1$ meV and the fixed value of the secondary monochromatic source size $\Delta x_s = 5 \mu$m requires that $D_{\cup R}/b_{\cup R} = -125 \mu$rad/meV. Here, the negative sign results from Eqs. 1 and 5.

The optical scheme of a four-crystal dispersing element with the required value of $D_{\cup R}/b_{\cup R}$ and its spectral transmission function are presented in Fig. 3.

The refocusing system is designed to provide 1:1 imaging (magnification factor $A_R = -1$) of the secondary source in the intermediate image plane 1 to image plane 2. This is favored by the Abbe sine condition, see discussion in [6] for details. This condition along with the previously defined values of $f_1$ and $b_{\cup R}$ require $f_2 = 1.471$ m, see

\begin{align*}
\text{D}_1: \text{CDDW}(\pi+,-0,+,0-) \\
C = \text{Si}(111) \\
D_1 = \text{Si}(800) \\
D_2 = \text{Si}(800) \\
W = \text{Ge}(111)
\end{align*}

\begin{align*}
\text{D}_2: \text{CDDW}(\pi+,0-,0+,0-) \\
C = \text{Ge}(111) \\
D_1 = \text{Si}(800) \\
D_2 = \text{Si}(800) \\
W = \text{Ge}(111)
\end{align*}
Eq. (5). In fact, the significance of the 1:1 magnification for aberration-free imaging of the IXS spectra is one of the central questions to be addressed by numerical simulations. Deviations from 1:1 imaging will be studied as well. The specific case of $A_r = 1$ requires $G_r = G_o = -50 \mu m/meV$ and $\Delta x_2 = |A_o|\Delta x_o \equiv \Delta x_2 \approx 5 \mu m$.

We study IXS imaging with different types of focusing elements $F_1$ and $F_2$: ideal lenses, 2D paraboloidal compound refractive lenses [9], 2D paraboloidal mirrors [20], or compound 2D mirror systems composed of 1D parabolic mirrors, such as Kirkpatrick-Baez (KB) [21] or Montel [22]. The mirrors are considered to be coated with laterally graded multilayers similar to those used in [23, 24], providing a large glancing angle of incidence $\varphi \approx 20 – 30$ mrad. Due to the large $\varphi$, the mirrors are compact, have a large geometrical aperture, and most importantly mitigate aberrations, as discussed in [6]. Impacts of the magnitude of $\varphi$ and of the mirrors’ slope errors on the IXS imaging will be studied.

D. Description of the sample, a secondary source for the refocusing system

X-rays scattered from the sample are seen by the refocusing system as emanating from a secondary three-dimensional source. Studies [1, 6, 7] show that the performance of the refocusing system is relatively insensitive to the secondary source position along the optical axis. In particular, the tolerance on the position variation is at least a few millimeters in the present case of the 0.1-meV spectrometer. Therefore, if the sample thickness is much smaller, the secondary source can be considered with high accuracy to be flat and distributed only in plane $(x, y)$. Such an approximation is used here.

The defocusing system focuses each spectral component $E$ to a spot of a vertical size $\Delta x_1$, see Figs. 1(v)–(v), with the locations linearly dispersed as

$$x_i(E) = G_o(E - E_o).$$

In the elastic scattering process, the photon energy of the secondary source is the same as that of the incident one, as indicated in Fig. 1(v). To simulate inelastic scattering with an energy transfer $\epsilon$, we modify the energy of the x-ray scattered by the sample as

$$E_o \rightarrow E_o + \epsilon.$$

This presentation may mean that inelastic x-ray scattering with an energy transfer $\epsilon$ takes place in all scattering points simultaneously, as indicated in Fig. 1(v). This is not actually the case. However, this presentation is still valid if a time-averaged picture is assumed.

Because the angular acceptance of the refocusing system is limited to $\Delta \theta_r \simeq 260 \mu rad$ [6], it can “see” only $\Delta \theta_r f_1 \simeq 100 \mu m$ of the secondary source. We restrict therefore the total vertical size of the secondary source in our simulations to $\Delta X_i = 150 \mu m$, see Fig. 4(a). This corresponds to a maximal spectral variation of $E - E_0 = \pm 1.5$ meV in the incident beam, see Fig. 4(b).

If the scattering angle $\Phi$ is small, as shown in Fig. 1(h), the horizontal secondary source size is equal to the horizontal focal spot size on the sample, which can be just a few micrometers. However, with a finite penetration length $L_z$, the horizontal secondary source size $\Delta Y_i / L_z \approx \sin \Phi$ grows with $\Phi$, as shown in the inset of Fig. 1(h). For practical reasons, which cover many cases, we assume in our simulations $\Delta Y_i = 300 \mu m$.

Each point on the sample is a secondary source emitting isotropically (a spherical wave). But only a small part of the radiation will be accepted by the refocusing system (defined by the numerical aperture of the system and possible use of secondary slits to control the momentum resolution. Here we limit the angular spread of the photons from the sample to 1.5 mrad in both the vertical $\Upsilon_y$ and horizontal $\Upsilon_x$ planes. This is consistent with the required momentum transfer resolution $\Delta Q = \Upsilon Q = 0.07 \: \text{nm}^{-1}$ for the 0.1-meV spectrometer, where $\Upsilon = \max[\Upsilon_y, \Upsilon_x]$.

III. IXS IMAGING WITH LENSES

In the first step, we study how the extended two-dimensional x-ray source dispersed in the vertical direction in reference plane 1, see Figs. 1 and 3, is imaged in reference plane 2 by the refocusing system composed of non-absorbing perfect paraboloidal lenses used as the collimating $F_1$ and focusing $F_2$ optical elements and of the CDDW dispersing element in between.

According to Fig. 1 we expect the refocusing system to focus all vertically dispersed monochromatic components into one spot, with the linear dispersion annihilated. In the perfect case, the vertical distribution should be Gaussian with a width $\Delta x_y$ equal to the monochromatic source
size $\Delta x_1 = 5 \, \mu m$, assuming the designed 1:1 imaging in the vertical plane, which takes into account the combined effect of lenses and crystals ($A_y = -b_{y,f} f_2 / f_1 = -1$). The source image size in the horizontal direction is defined by the focal lengths of the lenses only: the magnification factor is $f_2 / f_1 = 3.678$, thus the image size in the horizontal plane is $\Delta Y = \Delta Y_2 (f_2 / f_1) = 1103 \, \mu m$. This picture turns out, however, to be incomplete.

Figure 5(a) shows the cross section of the beam calculated in image plane 2 in the case of elastic scattering ($\varepsilon = 0$), related to Fig. 1(v) $\xi_0$. Its horizontal width $\Delta Y_2$ agrees with $\Delta Y_2$ (we are using tilde throughout the paper to indicate values calculated numerically). The vertical profile at any $y_2$ has a distribution which fits perfectly to the Gaussian function with a width $\Delta \tilde{x}_2 \approx 4.95 \, \mu m$ (FWHM), which is very close to that expected from the paraxial theory image vertical size $\Delta x_2 = 5 \, \mu m$. However, the whole image is curved to a parabolic shape. This happens due to Bragg reflections from the crystals in the dispersing element $D_{\mu} = \xi_0$; see [6][7] for details.

A 1D (strip) detector would measure a distribution shown in Fig. 5(b) with a vertical spread $\Delta \bar{x} \approx 32 \, \mu m$ much larger than $\Delta x_2 = 5 \, \mu m$, and therefore would result in an asymmetric and much broadened instrumental spectral function. The detrimental effect of the curvature is significant only if the horizontal secondary source size is large, as in the case considered here of $\Delta Y_2 = 300 \, \mu m$.

The problem can be mastered by using a 2D pixel detector and the following data evaluation [8]. The image in Fig. 5(a) is flattened by subtracting the best fit parabola $x_2 = \Pi y_2^2 + x_2 (0)$ and integrating over $y_2$. The resulting reduced vertical profile, shown in Fig. 5(c), fits to a Gaussian function over an intensity range of at least four orders of magnitude with a width $\Delta \tilde{x}_2 = 4.95 \pm 0.02 \, \mu m$ (FWHM), which is in a very good agreement with the expected $\Delta x_2 = 5 \, \mu m$.

Further simulations show that this picture remains valid also in the case of inelastic x-ray scattering with nonzero energy transfer $\varepsilon \neq 0$. What changes is the position of the image, which shifts linearly with $\varepsilon$ in the vertical direction along $x_2$ with a linear dispersion rate $G_{\mu} = -49.4 \, \mu m/meV$, see Figs. 6(a)-(b), in agree-
ment with that predicted by the paraxial theory $G_n = -50 \mu m/meV$. The reduced image size and therefore the spectral resolution of the spectrometer is independent of $\varepsilon$, see Fig. 3(c). The results of Figs. 3(a)-(c) confirm one of the key properties of x-ray echo spectrometers: their capability of imaging IXS spectra with high resolution and contrast.

Figure 3(d) demonstrates another important feature: the curvature $\Pi$ of the best-fit parabola to the image profile is practically independent of $\varepsilon$. This is in agreement with the theory [6], which predicts that $\Pi = U A \beta / 2 f_x^2$, where $U = f_j (1 - b_i b_i) / |b_i b_i b_j| \cos \theta_j$, and therefore that $\Pi$ is an invariant of the refocusing system, independent of the IXS energy transfer $\varepsilon$. Due to this, the curvature $\Pi$ can be determined in practice from the elastic signals, and thus to overcome degradation of the spectral function and resolution due to the large horizontal size of the secondary source. With the parameters of the spectrometer considered here we calculate $\Pi = 102 m^{-1}$ and $\Delta X_2 = \Pi (\Delta Y f_j^2 / 2 f_x^2) = 31 \mu m$, which are close to $\Pi = 104.4 m^{-1}$ and $\Delta X = 32 \mu m$ calculated numerically for the ideal lenses, see Figs. 5(a) and 5(c).

The picture does not change if realistic absorbing parabolic compound refractive lenses are used instead of the ideal lens. The appropriate results of simulations are shown by dashed lines in Figs. 3(b)-(d). The only major difference is in the signal strength, which is reduced by a factor of 41 (assuming $\Upsilon_x \times \Upsilon_y = 1.5 \times 1.5 \, \text{mrad}^2$ angular divergence of x-rays from the source) because of the geometrical aperture reduced by photo-absorption.

Here we conclude that the refocusing system composed of parabolic lenses represents an aberration-free imaging system capable of making sharp images of IXS spectra.

Focusing mirrors certainly may feature a significantly larger numerical aperture; however, would they be also able to produce aberration-free IXS images?

IV. IXS IMAGING WITH MIRRORS

Unlike paraboloidal lenses, curved grazing incidence mirrors are in general not good x-ray imaging devices. Some particular combinations of two or more reflectors may comply with the Abbe sine condition and perform as good imaging systems. A prominent example is the Wolter-type mirror pairs [10, 11]. The two mirrors that play the role of collimating and focusing elements in the refocusing system of the x-ray echo spectrometer with the dispersing system in between may perform similarly to a Wolter-type imaging system. In particular, a paraboloidal double-mirror system in a collimating-plus-focusing configuration has the great advantage of producing parallel x-rays between the two reflections, which is perfect for the proper performance of a plane dispersive system (“diffraction grating”) inserted in between [23]. The Abbe sine condition is perfectly fulfilled for the 1:1 1D-imaging case with no dispersing element in between [6]. However, the question still remains open whether perfect imaging can be achieved if a dispersing system is included, and whether this is valid in the 2D case, as x-ray spectrometers require.

We study in this section IXS imaging with three different grazing incidence mirror systems composed of (i) two 2D paraboloidal mirrors [20], (ii) two Kirkpatrick-Baez (KB) systems [21] each formed by cylindric parabolic mirrors, and (iii) two Montel [22] systems, made as well of cylindric parabolic mirrors.

A. Elastic scattering $\varepsilon = 0$

We start with the refocusing system composed of two 2D paraboloidal mirrors and the CDDW dispersing element in between. The setting of the two paraboloids is not unique. They can be in a parallel or antiparallel configuration. Extending the nomenclature used for crystal systems, we can label these mirror configurations as $(-||+)$ and $(-||-)$, respectively. Here, plus corresponds to the x-ray beam reflected counterclockwise from an optical element, and minus clockwise. Importantly, the relative position of the CDDW system must be properly chosen to match the sign of the linear dispersion rate $G_\sigma$ on the sample in reference plane 1 [the first crystal may reflect counterclockwise (+) or clockwise (−)], which is critical to obeying the refocusing condition Eq. (1).

Table II shows graphs of four possible unique mirror-crystal configurations fulfilling the refocusing condition. Each configuration is coded by a sequence of signs. The left and right outer signs correspond to mirrors $F_1$ and $F_2$, respectively. The crystals are additionally characterized by the azimuthal angles of incidence $\pi$ or 0, see [10, 11] for details. Configurations with all signs reversed including the $G_\sigma$ sign represent four equivalent configurations.

Table II presents results of the ray tracing simulations: the images and the reduced image profiles (similar to those in Fig. 5(a)-(e)). The simulations are performed for two different numerical apertures: $\Upsilon_x = \Upsilon_y = 1.5 \, \text{mrad}$ (nominal case of the 0.07 nm$^{-1}$ momentum transfer resolution) and $\Upsilon_x = 1.5 \, \text{mrad}$; $\Upsilon_y = 10 \, \text{mrad}$ (a larger horizontal aperture). Table II also provides calculated values of the vertical image size $\Delta X_2$, the reduced image size $\Delta \tilde{x}_2$, and of the spectral resolution $\Delta \tilde{\varepsilon}$.

Only the $(-||-)$ mirror configurations I and II result in sharp reduced images with Gaussian profiles and image sizes of $\Delta \tilde{x}_2 \approx 5 \, \mu m$ in agreement with those expected from the paraxial theory value of $\Delta X_2 = 5 \, \mu m$, both for $\Upsilon_x = 1.5 \, \text{mrad}$ and 10 mrad. The imaging properties of systems III and IV are worse but still almost as good for $\Upsilon_x = 1.5 \, \text{mrad}$. However, major aberrations explode with increasing the horizontal numerical aperture to 10 mrad. According to Table II results, configuration I is the best, providing the smallest image size $\Delta X_2$, the smallest reduced image size $\Delta \tilde{x}_2$, and therefore the best spectral resolution $\Delta \tilde{\varepsilon}$, in agreement with the design value and with the lens case.
TABLE II: Beam cross sections in image plane 2 calculated for the elastic scattering case $\varepsilon = 0$ for the refocusing system of the x-ray echo spectrometer in four different mirror-crystal configurations with paraboloidal mirrors as collimating and focusing elements. Two cases of the numerical apertures $\Upsilon_v \times \Upsilon_h$ are considered. Numerical values are provided for the vertical image size $\Delta X_2$ in image plane 2, reduced image size $\Delta \tilde{x}_2$, and the spectral resolution $\Delta \tilde{\varepsilon}$. The configuration graphs show side views of the beam trajectories (optical axes). The numbers in square brackets correspond to calculations with the horizontal numerical aperture increased to $\Upsilon_h = 10$ mrad. The numbers highlighted in gray correspond to best imaging cases.

| Configurations | I | II | III | IV |
|----------------|---|----|-----|----|
| $x \ [m]$ | | | | |
| $z \ [m]$ | | | | |
| $(-|\pi,\pi,\pi+,0+|)$ | | | | |
| $G_D < 0$ | | | | |
| $x \ [m]$ | | | | |
| $z \ [m]$ | | | | |
| $(−|\pi,+\pi,\pi−,0−|)$ | | | | |
| $G_D > 0$ | | | | |
| $\Delta \tilde{\varepsilon} \ [\mu eV]$ | $105.5 \pm 0.3$ | $108.7 \pm 0.3$ | $151.6 \pm 0.4$ | $583 \pm 2$ |
| $\Delta X_2 \ [\mu m]$ | $24.29 \pm 0.04$ | $40.73 \pm 0.08$ | $40.1 \pm 0.2$ | $30.55 \pm 0.09$ |
| $\Delta \tilde{x}_2 \ [\mu m]$ | $5.28 \pm 0.01$ | $5.43 \pm 0.01$ | $7.58 \pm 0.02$ | $7.56 \pm 0.01$ |
| $\Delta \tilde{\varepsilon} \ [\mu eV]$ | $105.5 \pm 0.3$ | $108.7 \pm 0.3$ | $151.6 \pm 0.4$ | $583 \pm 2$ |

Table III shows results of similar calculations for the refocusing system, in which the two paraboloidal mirrors are replaced by two KB-mirror systems. The vertical focusing mirrors (VFM) are placed as the paraboloidal mirrors at distances $f_1$ and $f_2$ from reference planes 1 and 2, respectively, while the horizontal focusing mirrors (HFM) are at 50 mm and 100 mm downstream the VFMs, respectively, with the focal lengths of the HFMs appropriately corrected. Remarkably, the refocusing system composed of the KB-mirror systems produce sharp images in all four possible configurations (as the paraboloidal mirrors in the best configuration I).

The refocusing system comprising Montel mirrors performs in all four possible configurations very similar to the KB-mirror case, provided the $\Upsilon_v=1.5$ mrad numerical aperture case is considered (see Table VII of Appendix A). However, the Montel mirrors are more sensitive to the horizontal divergence, producing significantly worse results in the $\Upsilon_v=10$ mrad numerical aperture case especially in configurations I and IV. The better performance of the KB-mirror compared to the Montel-mirror systems maybe due to the fact that the VFM and HFM in the KB case are perfectly aligned along the optical axis (x-ray trajectory). In contrast, VFM and HFM are orthogonal to each other in the Montel case, composing a system with an ill-defined optical axis.

The performance of the refocusing systems composed of KB mirrors appears to be also least sensitive to increasing the vertical numerical aperture $\Upsilon_v$ as the results of the calculations of the reduced image size $\Delta \tilde{x}_2$ and of the spectral resolution $\Delta \tilde{\varepsilon}$ show, presented in Table IV. The image size and spectral resolution degrade roughly by a factor of two from $\Delta \tilde{\varepsilon}=0.1$ meV to $\simeq 0.2$ meV with increasing $\Upsilon_v$ from the nominal 1.5 mrad to 10 mrad.
TABLE III: Similar to Table II however, with the results calculated for KB-mirror systems as collimating and focusing elements.

| Configurations | I               | II              | III             | IV              |
|----------------|-----------------|-----------------|-----------------|-----------------|
| $x$ [m]        | $z$ [m]         | $x$ [m]         | $z$ [m]         | $x$ [m]         |
| $(-|\pi-\pi-\pi+,0+|-)$ | $G_D < 0$       | $(-|\pi+\pi+,0-|-)$ | $G_D > 0$       | $(-|\pi+\pi+,0-|-)$ | $G_D > 0$ |
| $G_D < 0$      | $G_D > 0$       | $G_D < 0$       | $G_D > 0$       |

$\Upsilon_v = 1.5 \text{ mrad}$
$\Upsilon_h = 1.5 \text{ mrad}$

$\Delta \tilde{x}_2 [\mu m]$ | 26.92±0.02 [33.32±0.02] | 26.88±0.02 [33.18±0.02] | 27.16±0.02 [36.77±0.02] | 27.19±0.02 [36.88±0.02] |
$\Delta \tilde{\xi} [\mu m]$ | 5.11±0.01 [5.35±0.01] | 5.11±0.01 [5.35±0.01] | 5.13±0.01 [5.35±0.01] | 5.13±0.01 [5.34±0.01] |
$\Delta \tilde{\varepsilon} [\mu eV]$ | 102.2±0.2 [107.0±0.2] | 102.1±0.3 [106.8±0.3] | 102.7±0.2 [107.0±0.1] | 102.6±0.2 [106.8±0.2] |

Note that the calculations are performed with mirrors and crystals long enough to accept the full beam.

In summary, in the elastic scattering case, the refocusing systems composed of focusing mirrors perform in the best mirror-crystal configurations very similarly to the systems composed of lenses. Whether this is still true for the inelastic scattering case, we study in the next section.

B. Inelastic scattering $\varepsilon \neq 0$

1. Aberrations in the image plane

In the case of lenses, the reduced image size in plane 2 does not change if inelastic scattering ($\varepsilon \neq 0$) takes place. This is no longer the case if mirrors are used instead of lenses. Indeed, the reduced image size in reference plane 2 plotted versus $\varepsilon$ in Fig. 7 appears to grow quadratically with $\varepsilon$: $\Delta \tilde{x}_2(\varepsilon) - \Delta \tilde{x}_2(0) \propto \varepsilon^2$. Thus the mirror systems behave very differently compared to the lens systems: the spectral resolution degrades with $|\varepsilon|$. This degradation can be reduced or even eliminated if the vertical numerical aperture $\Upsilon_v$ is diminished substantially by a factor 10 or 100. This, however, would reduce the photon flux in the detector to unacceptably low values. Interestingly, the horizontal numerical aperture does not have the same effect, except for Montel mirror systems, which are very sensitive to large $\Upsilon_h$.

The different behavior of the mirror- and lens-based systems may be related to focusing element $F_2$. While collimating element $F_1$ functions in the same way both in the elastic and inelastic scattering regimes, see Figs. 1(v_e)-(v_i). In contrast, it is not the case for focusing element $F_2$, as the incidence angle changes with $\varepsilon$ for it. This is probably of no significance if lenses are used as $F_2$, for which the incidence angle is close to normal. However, this appears to be important if grazing incidence mirrors are used instead.

To gain more insight into the problem of spectral resolution degradation with $\varepsilon$, we study here the reduced image size dependence on the focal length $f_2$. The results are shown in Fig. 8. If the numerical aperture of
FIG. 7: Reduced vertical image size $\Delta x_2$ in reference plane 2 as a function of the energy transfer $\epsilon$, calculated for the refocusing system with (a) the paraboloidal mirrors (b) KB-mirror systems, and (c) Montel systems, all in configuration I (see Table II) for different values of the numerical apertures $\Upsilon_h$ and $\Upsilon_v$.

The results of the studies presented in Fig. 8 provide another example of the superior performance of KB optical systems $F_2$ calculated for the refocusing system with (a) the paraboloidal mirrors, (b) KB-mirror systems, and (c) Montel systems, all in configuration I (see Tables II-III) for different values of the numerical apertures $\Upsilon_h$ and $\Upsilon_v$. Red lines show results of calculations for the ideal lens case, as a reference.
systems compared to Montel and paraboloidal mirrors. However, no optimal $f_1$ value can be found in any of the considered mirror cases, which would eliminate or mitigate the degradation of the spectral resolution with $\varepsilon$.

2. Defocus correction in an oblique image plane

In this section we show that the degradation of the reduced vertical size when passing from elastic ($\varepsilon = 0$) to inelastic ($\varepsilon \neq 0$) scattering is merely the defocus aberration that can be easily compensated.

For this, we calculate how the reduced image size changes along the optical axis for different values of $\varepsilon$. The results presented in Fig. 9 show that the smallest reduced image size (waist) for any $\varepsilon$ is in fact equal to the elastic image size $\Delta{\bar{x}}_2(\varepsilon = 0)$. However, it is attained with a shift $z_2(\varepsilon) - z_2(0)$ along the optical axis from the location $z_2$ of the nominal image plane. The waist size scales with the focal length $f_2$ in Figs. 9(a), (b), and (c), because it changes the magnification factor $A_\psi = -(b_{\psi R} f_2 / f_1)$, Eq. [3].

The waist position shifts linearly with $\varepsilon$ as $z_2(\varepsilon) - z_2(0) = \varepsilon / \gamma$, see Fig. 10. The slope $\gamma$ depends on focal length $f_2$ of mirror $F_2$ and on mirrors' incidence angle $\varphi$, as illustrated in Figs. 10(a) and (b), respectively. The slope $\gamma$ is independent of the CDDW-to-$F_2$ distance (the results of calculations are not shown).

The loci of the waists is therefore a line inclined to the optical $z$-axis by an angle $\psi = G_{\varphi \gamma}$. In particular, if $f_2 = 1.471$ m, which corresponds to the 1:1 imaging, the inclination of the IXS image plane is $\psi \approx \varphi$, see numerical values in the inset of Fig. 10(b). In a more general case, $\psi$ is still proportional to $\varphi$ but scales with the magnification factor of the refocusing system as $\psi \approx \varphi (b_{\psi R} f_2 / f_1)$, see values in the inset of Fig. 10(a).

The spectral resolution degradation in the nominal image plane 2, see Fig. 7, therefore can be compensated by inclination of the x-ray pixel detector by the angle $\psi$. Such an inclination may simultaneously improve the detector’s spatial resolution. For example, if the detector has a pixel size $p = 50 \ \mu$m, its projection on reference plane 2 and thus the spatial resolution becomes $p \psi \approx 1.5 \ \mu$m (for $\psi = 30$-mrad) or $p \psi \approx 1.3 \ \mu$m (for $\psi = 25$-mrad).

Figure 11 summarizes IXS imaging properties of the refocusing system composed of grazing incidence curved KB-mirror systems and the pixel x-ray detector in the oblique image plane. The properties are very similar to those of the system composed of paraboloidal lenses. The only difference is that the aberration-free imaging takes place in the oblique image plane at the angle $\psi$ to the optical axis. The imaging properties of the refocusing system composed of the paraboloidal or Montel-mirror

3 A similar approach is used in soft x-ray grating spectrometers, see, e.g., [25].

4 To be practical, the application of a high-Z sensor material is required with a photo-absorption length $L_\alpha \ll p$. A CdTe $50 \times 50 \times 50$-µm$^3$ pixel detector would be most optimal for this application. CdTe: $L_\alpha = 6.5 \ \mu$m for 9.1 keV photons, $L_\alpha = 11.4 \ \mu$m for 11.210 keV photons, $L_\alpha = 22.9 \ \mu$m for 14.41 keV. To image a beam with a 400-µm large vertical size (corresponds to a 8-meV spectral window of imaging), a 12.5-µm CdTe sensor would be required. Photon-counting pixel detectors with such sensors are state of the art [29].

FIG. 9: Reduced vertical image size $\Delta{\bar{x}}_2$ as a function of deviation $z - z_2$ from reference image plane 2, calculated for different energy transfer values $\varepsilon$ and for selected focal length values $f_2$ of imaging mirror $F_2$: (a) $f_2 = 0.4 \ \text{m}$, (b) $f_2 = 1.471 \ \text{m}$, and (c) $f_2 = 2.5 \ \text{m}$. Calculations are for the KB-mirrors case in mirror-crystal configuration I (see Table III), and for the numerical apertures $\Upsilon_\varphi = \Upsilon_\psi = 1.5$ mrad. See Fig. 14 of Appendix A for the similar results of the paraboloidal or Montel-mirror systems.
Energy transfer $\epsilon$ [meV] and the deviation $z(\epsilon) - z_2$ from reference plane 2 of the reduced image with the smallest size (waist). Calculated for the KB-mirrors case. (a) Derived from data in Fig. 9 for selected focal length values $f_2$. Mirrors' incidence angle is $\varphi = 30$ mrad, and numerical apertures $\Upsilon_v = \Upsilon_h = 1.5$ mrad. (b) Calculated with $f_2 = 1.471$ m (1:1 imaging) and selected values of glancing angle of incidence $\varphi$. See Fig. 15 of Appendix A for the results of the paraboloidal or Montel-mirror systems.

TABLE V: Reduced image size (in $\mu$m) in the refocusing system of the x-ray echo spectrometer comprising mirror systems with different glancing angles of incidence $\varphi$. A slightly better resolution is found for KBs than for paraboloids and Montel systems.

| Mirror type / $\varphi$ [mrad] | 20  | 25  | 30  | 40  |
|-------------------------------|-----|-----|-----|-----|
| KB                            | 5.29| 5.17| 5.10| 5.05|
| Paraboloids                   | 5.54| 5.38| 5.27| 5.15|

Typically, the imaging property of a solitary mirror degrades with decreasing glancing angle of incidence because of the illumination of an increasing part of the optic. Here we study the effect of glancing angle of incidence $\varphi$ on the imaging properties of the refocusing system composed of mirror pairs and the CDDW dispersing element in between.

Table V presents results of calculations of the image size in case of KB and paraboloidal systems for selected values of $\varphi$. They show that the image size slightly increases and therefore the spectrometer resolution degrades when glancing angle decreases. The output intensity remains constant if mirrors are used long enough to accept the whole beam (data not shown). This means that larger $\varphi$ values are preferred. However, other considerations speak against large $\varphi$. Larger $\varphi$ requires multilayer coatings with smaller periods and eventually smaller reflectivity. Glancing angle of incidence $\varphi \simeq 30$ mrad is optimal for present-day technology, and therefore are used in the current simulations.

D. Effect of slope errors

Mirrors' slope errors will surely contribute to broadening the reduced image size and degrading the spectrom-
The normalized dynamical structure factor closely resembling glycerol at room temperature. As an example, we select a liquid sample with properties echo spectrometer to image IXS spectra of real samples. It is preferable from this point of view. Therefore, using mirrors with smaller focal lengths is the critical optic requiring such a small slope error that it is mirror $F_2$ with the largest focal length $f_2$ that is the critical optic requiring such a small slope error value. Therefore, using mirrors with smaller focal lengths is preferable from this point of view.

V. IMAGING IXS SPECTRA OF “GLYCEROL”

Finally, in this section we study the ability of the x-ray echo spectrometer to image IXS spectra of real samples. As an example, we select a liquid sample with properties closely resembling glycerol at room temperature.

The IXS spectra in liquids are typically modeled by the normalized dynamical structure factor

$$S(Q,\varepsilon) = \frac{S(Q)}{S(Q)} = f_Q \delta(\varepsilon) + \frac{1-f_Q}{\pi} \frac{\Gamma_Q \Omega_Q^2}{(\varepsilon^2-\Omega_Q^2)^2 + \varepsilon^2 \Gamma_Q^2}. \quad (10)$$

which is a sum of the delta function for the elastic component and the damped harmonic oscillator for the inelastic component measured at selected momentum transfer $Q$. The sound velocity $v_s = 2.8 \text{ km/s}$, reduced broadening $B = 3 \text{ m}^2\text{meV}$, and the elastic line fraction $f_Q = 0.7$ are assumed to be constant for simplicity, i.e., $Q$-independent, which is in fact not necessarily the case in practice. This assumption represents merely an interpolation of the known data for glycerol liquid into the yet unexplored range of $Q < 0.5 \text{ nm}^{-1}$. The graphs in the lower row of Fig. 13 show in red the normalized dynamical structure factor $S(Q,\varepsilon)/S(Q)$ of the “glycerol” calculated for selected $Q$ values using Eqs. (10)-(11).

The elastic line in green is a Gaussian with FWHM of 0.1 meV – equivalent to the resolution function of the x-ray spectrometer.

As in the simulations presented in the previous sections, the sample introduced a constant energy transfer $\varepsilon = 0$ for elastic and $\varepsilon \neq 0$ for inelastic cases. Now, each ray will be affected by a random $\varepsilon$ sampled by $S(Q,\varepsilon)/S(Q)$, thus simulating the real effect of the photon energy change by the sample with a probability determined by the ideal IXS spectrum of Eq. (10).

The real IXS spectra measured in experiments represent a convolution of $S(Q,\varepsilon)/S(Q)$ with the instrumental function. This convolution is naturally included in the ray tracing simulations. The graphs in the upper row of Fig. 13 present the “glycerol” IXS spectra obtained by the ray tracing through the refocusing system of the x-ray echo spectrometer equipped with the ideal lenses. The system equipped with the paraboloidal mirrors produces almost identical results (not shown). However, in the latter case, the detector plane has to be inclined by an angle of $\varphi = 30.5 \text{ mrad}$ with the optical axis. Recall that the spatial image produced in the detector is reduced by removing the parabola calculated for the elastic scattering with parameters provided in Fig. 6 for the lenses and in Fig. 11 for KB-mirror systems.

The ray tracing results practically reproduce the spec-
The curved images of all elastic and inelastic components are composed of lenses. The refocusing system of the x-ray echo spectrometer is preserved in all configurations also with the horizontal numerical aperture increased to $\Upsilon_h = 1$ mrad. However, the KB and Montel mirror systems provide sharp images both in the $(−||−)$ mirror configurations, while the paraboloidal mirrors work properly only in the $(−||−)$ configuration. KB-mirror systems appear to be the best choice for the refocusing system of the x-ray echo spectrometer composed of ideal lenses.

If curved grazing-incidence mirror systems are used instead (paraboloidal, parabolic KB, or parabolic Montel), the images of all $\varepsilon$-components still can be Gaussian and sharp when recorded on the detector plane tilted with respect to the optical axis. The inclination of this oblique image plane to the optical axis is equal to the grazing angle of incidence, in case of 1:1 imaging by the refocusing system. Compensation of the defocus aberration by inclining the x-ray imaging pixel detector simultaneously improves detector’s spatial resolution.

The refocusing system of the 0.1-meV-resolution x-ray echo spectrometer may feature sharp aberration-free images of IXS spectra using any considered mirror type assuming the numerical aperture is $\Upsilon = Y_h = 1.5$ mrad (required by spectrometer’s nominal momentum transfer resolution $\Delta Q = 0.07$ nm$^{-1}$). However, the KB and Montel mirror systems provide sharp images both in the $(-||-)$. KB-mirror systems appear to be the best imaging devices, as the high image quality by the KB systems is preserved in all configurations also with the horizontal numerical aperture increased to $\Upsilon_h = 1$ mrad. The paraboloidal mirrors can perform similarly, however, images reveal Gaussian profiles, if flawless optical elements are in use.

We show that all $\varepsilon$-components of IXS spectra are imaged aberration-free, featuring Gaussian profiles of constant width, provided the collimating and focusing optics of the refocusing system of the x-ray echo spectrometer are composed of lenses.
only in the 1:1 imaging case in the (−−) configuration. The performance of the KB-mirror systems is also least sensitive to the vertical numerical aperture Υv.

The instrumental function of echo-type IXS spectrometers has sharp high-contrast Gaussian tails. This is a great advantage over the long Lorentzian tails of the instrumental functions of present-day narrow-band scanning IXS spectrometers [5]. In practice, the contrast of the instrumental function will rely on the quality (smallness of the slope errors) of the mirrors of the x-ray echo spectrometers. The simulations show that slope errors better than 0.5 µrad are critical to avoid instrumental function degradation in the 30-mrad grazing incidence mirror case (Fig. 12) with a focal length of f2 = 1.4 m.

Initial design parameters of the x-ray echo spectrometer derived by analytical ray-tracing theory [6] are in a very good agreement with the results of the numerical simulations. In particular, no meaningful change in the resolution is observed if all the crystals are put at the same position, as the analytical theory assumes.

The results of the studies are applicable to hard x-ray imaging spectrographs [16], which represent a subsystem of x-ray echo spectrometers featuring a non-dispersed monochromatic secondary source on the sample.

The range of applications of echo-type IXS spectrometers and IXS spectographs of course includes resonant IXS (RIXS) [23], as a particular case.

VII. ACKNOWLEDGMENTS

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TABLE VI: Parameters of the CDDW-type in-line crystal optics designed as dispersing elements $D_D$, $D_R$ of the defocusing $\hat{O}_D$ and refocusing $\hat{O}_R$ systems of the 0.1-meV-resolution x-ray echo spectrometer. For each optic, the table presents crystal elements ($e=C,D_1,D_2,W$) and their Bragg reflection parameters: $(hkl)$, Miller indices of the Bragg diffraction vector; $H_e$; $\eta_e$, asymmetry angle; $\theta_e$, glancing angle of incidence; Bragg reflection intrinsic spectral width $\Delta E^{(s)}_e$ and angular acceptance $\Delta \theta^{(s)}_e$ in symmetric scattering geometry, respectively; $b_e$, asymmetry ratio; and $s_e D_e$, angular dispersion rate with deflection sign. For each optic, also shown are: angular acceptance $\Delta \theta_X$ ($X=D,R$) and spectral bandwidth $\Delta E_X$ as derived from the dynamical theory calculations, the angular spread of the dispersion fan $\gamma_X = |D_{\gamma_X}| \Delta E_X$, and the cumulative values of the asymmetry parameter $b_{\cup_X}$ and the dispersion rate $D_{\cup_X}$. X-ray photon energy is $E = 9.13708$ keV.

| Crystal element ($e$) | $H_e$ | $\eta_e$ | $\theta_e$ | $\Delta E^{(s)}_e$ | $\Delta \theta^{(s)}_e$ | $b_e$ | $s_e D_e$ |
|-----------------------|------|---------|----------|-------------------|----------------------|------|---------|
| [material]             |      |         |          |                   |                     |      |         |
| $D_D$: CDDW ($\pi+.0-,0+,0-$), Fig. 2 |
| 1 C [Si] | (1 1 1) | -10.5 | 12.5 | 1304 | 32 | -0.09 | -0.02 |
| 2 D_1 [Si] | (8 0 0) | 77.7 | 88 | 27 | 85 | -1.38 | -1.19 |
| 3 D_2 [Si] | (8 0 0) | 77.7 | 88 | 27 | 85 | -1.38 | +1.19 |
| 4 W [Si] | (1 1 1) | 10.5 | 12.5 | 3013 | 71 | -11.2 | -0.24 |
| Cumulative values $\Delta \theta_D$, $\Delta E_D$, $\Delta \theta_D^{(s)}$, $b_{\cup_D}$, $D_{\cup_D}$ $\mu$rad meV $\mu$rad meV |
| 57 | 3.5 | 112 | 1.91 | -31.7 |
| $D_R$: CDDW ($\pi+\pi+,\pi-,0-$), Fig. 3 |
| 1 C [Ge] | (1 1 1) | -10.5 | 12.0 | 3013 | 71 | -0.07 | -0.02 |
| 2 D_1 [Si] | (8 0 0) | -83.75 | 88 | 27 | 85 | -0.52 | -1.50 |
| 3 D_2 [Si] | (8 0 0) | -83.75 | 88 | 27 | 85 | -0.52 | +1.50 |
| 4 W [Ge] | (1 1 1) | 10.5 | 12.0 | 3013 | 71 | -14.75 | -0.31 |
| Cumulative values $\Delta \theta_R$, $\Delta E_R$, $\Delta \theta_R^{(s)}$, $b_{\cup_R}$, $D_{\cup_R}$ $\mu$rad meV $\mu$rad meV |
| 262 | 8 | 272 | 0.27 | -34.15 |

Very often the results of the calculations for different types of mirror systems look similar. Not to overwhelm the main part of the paper with too many details we move such data into the appendix containing a collection of supplementary tables and figures.

Table VI provides the crystal parameters of the dispersing elements. Table VII shows elastic signal imaging with the Montel mirror systems. Figure 14 and 15 show the inelastic waist vs. deviation from reference plane. Figure 16 shows the performance characteristics of paraboloid and Montel systems.
TABLE VII: Beam cross sections in image plane 2 calculated for the elastic scattering case $\varepsilon = 0$ for the refocusing system of the x-ray echo spectrometer in four different mirror-crystal configurations with Montel mirror systems as collimating and focusing elements. Two cases of the numerical apertures $\Upsilon_v \times \Upsilon_h$ are considered. Numerical values are provided for the vertical image size $\Delta\tilde{X}_2$ in image plane 2, reduced image size $\Delta\tilde{x}_2$, and for spectral resolution $\Delta\tilde{\varepsilon}$. The configuration graphs show side views of the beam trajectories (optical axes). The numbers in the square brackets correspond to calculations with the horizontal numerical aperture increased to $\Upsilon_h = 10$ mrad. The numbers highlighted in gray correspond to best imaging cases.

| Configurations | $\Upsilon_v = 1.5$ mrad | $\Upsilon_h = 1.5$ mrad | $\Upsilon_v = 1.5$ mrad | $\Upsilon_h = 10$ mrad |
|----------------|-------------------------|-------------------------|-------------------------|-------------------------|
| $\Delta\tilde{X}_2$ [\(\mu\text{m}\)] | 33.94±0.08 [42.7±0.2] | 34.16±0.03 [40.7±0.1] | 33.82±0.04 [49.1±0.1] | 34.66±0.08 [43.7±0.2] |
| $\Delta\tilde{x}_2$ [\(\mu\text{m}\)] | 5.65±0.01 [8.56±0.02] | 5.39±0.01 [6.49±0.02] | 5.38±0.01 [6.48±0.02] | 5.66±0.01 [8.40±0.02] |
| $\Delta\tilde{\varepsilon}$ [\(\mu\text{eV}\)] | 113.0±0.2 [171.2±0.4] | 107.9±0.3 [129.9±0.3] | 107.6±0.2 [129.7±0.3] | 113.2±0.3 [168.0±0.4] |

| I | II | III | IV |
|----|----|----|----|
| $G_D < 0$ | $G_D > 0$ | $G_D < 0$ | $G_D > 0$ |
FIG. 14: Reduced vertical image size $\Delta \tilde{x}$ as a function of deviation $z - z_2$ from reference image plane 2, calculated for different energy transfer values $\varepsilon$ and for selected focal length values $f_2$ of imaging mirror $F_2$: (a) $f_2 = 0.4$ m, (b) $f_2 = 1.471$ m, and (c) $f_2 = 2.5$ m. Presented here are results for I) paraboloids, and II) Montel mirror systems, with the numerical apertures $\Upsilon = 1.5$ mrad. All mirror systems feature very similar results. Mirror arrangement corresponds to configuration I in Tables II,III, and VII.
FIG. 15: Correspondence between the energy transfer $\epsilon$ and the deviation $z(\epsilon) - z_2$ from reference plane 2 of the reduced image with the smallest size. Calculated for paraboloidal mirrors case (left) and Montel mirrors case (right). To be compared with the data for the KB-mirrors case in Fig. 10. (a)-(a’) Derived from data in Fig. 14 for selected focal length values $f_2$. Mirrors’ incidence angle is $\phi = 30$ mrad and numerical apertures $\Upsilon_v = \Upsilon_h = 1.5$ mrad. (b)-(b’) Calculated with $f_2 = 1.471$ m (1:1 imaging) and selected values of glancing angle of incidence $\phi$. 
FIG. 16: Performance characteristics of the x-ray echo spectrometer with the refocusing system composed of paraboloidal mirrors (left column) and Montel mirror systems (right column): (a) Reduced image profiles calculated for various values of energy transfer $\varepsilon$ in inelastic x-ray scattering under the same conditions as in Fig. 5, however, with the IXS spectra imaged on the oblique image plane. (b) Image peak position $\tilde{x}_2$, (c) reduced image size $\Delta\tilde{x}_2$, and (d) curvature $\tilde{\Pi}$ of the best-fit parabola to the image profile as a function of $\varepsilon$. Compare with the similar results of Figs. 6 and 11 presented for the case of lenses and KB-mirror systems, respectively.