Reflectivity and imaging capabilities of spherically bent crystals studied by ray-tracing simulations

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Abstract. Spherically bent crystals are widely used in focusing monochromators, spectrometers and other x-ray optical systems. In particular, they are used as dispersive elements in focusing spectrometers with spatial resolution, applied in high energy density diagnostics and warm dense matter studies. In this case, plasma parameters are obtained via measurements of relative intensities of characteristic spectral emission lines for multiply charged ions, which are affected by an instrumental function. Here we develop and use the ray-tracing computer simulations to study reflectivity properties of spherically bent crystals in a particular experimental conditions and to provide the method to adjust and validate the measured spectral line intensities on quantitative basis.

1. Introduction
Spherically bent crystals are widely used in focusing monochromators, spectrometers and other x-ray optical systems. In particular, they are used as dispersive elements in focusing spectrometers with spatial resolution (FSSR). These spectrometers provide diagnostic of high energy density states of the matter including femtosecond relativistic laser plasma, plasma jets and shock waves in nanosecond laser plasma, strongly coupled plasma created by swift heavy ion beams, etc [1–3].

Plasma parameters are obtained via measurements of relative intensities of characteristic spectral emission lines for plasma multiply charged ions. The measured intensity of each spectral component is affected by an instrumental function determined by both a particular area on the spherically bent crystal surface where this spectral line is reflected, and the crystal reflectivity function. The strongest influence of the instrumental function on the recorded spectrum should be observed when the reflection area is located near the boundary of the crystal aperture.

The main goal of the work is to develop a method for initial signal reconstruction taking into account the instrumental function for a specific spectral components and the spectrometer configuration. It allows increasing the accuracy of measured parameters of the investigated plasma source and to measure absolute values of the intensity of plasma x-ray radiation.

2. Results
Areas, where spectral lines are reflected, are determinate by geometry of optical system, crystal and reflectivity function. Reflectivity function defined by many parameters such as scattering angle of radiation, material and geometry of crystal [4]. Using ray-tracing simulation the effect of reflectivity function was studied for spherically bent crystal of quartz with curvature radius
Figure 1. Rocking curve for spherically bent quartz crystal with curvature radius of 150 mm and Bragg angle of 46°. Dotted line represents rocking curve for plane alpha-quartz plate at the same Bragg angle. Dashed line shows the approximation of the rocking curve by set of trapezoids.

Figure 2. Calculation results for different Bragg angle and approximations of reflectivity function. Solid lines calculated with rocking curve for spherically bent quartz crystal with \(2d = 2.465\) Å. Calculation with the approximation of trapezoids is given by dash lines. Dotted lines shows the influence of FWHM of rocking curve on the reflectivity of the crystal. Dash-dot lines calculated with Gaussian function. In all calculation position of x-ray source and spherical crystal corresponds to FSSR scheme at 1D spatial resolution mode [1, 2].

The rocking curve was approximated by Gaussian function or by set of trapezoids, see figure 1. Such type of approximation was chosen due to rocking curve of plane alpha-quartz has the same profile [5]. In general, reflectivity functions for spherically bent crystal are similar in profile in wide range of parameter and we can successfully approximate it by one or three trapezoids.

Calculations for different Bragg angle, x-ray source size and distance to the mirror are carried out with different reflectivity function and presented at Figure 2. According to this calculation it can be said that approximation by Gaussian function gives less reflectivity than that one obtained with the approximation by single trapezoid with underestimation of 6% at the central wavelength, and of about 1% at the edge of the crystal. However, with the approximation by using three trapezoids the discrepancy with exact values of less than 0.5% was achieved. Results are the same for the different angles, source size, and distance to the radiation source.
Figure 3. Ray tracing result for different system configuration. Distance from x-ray source and scattering angle was varied. Result of simulation for scattering angle 46° and source distance 3000 mm (solid line), 2500 mm (dash line) and 1500 mm (dotted line) are presented on the first picture. Calculation for scattering angle 67° carried out for next source distance: 160 mm (dotted line), 200 mm (solid line) and 400 mm (dash line); for scattering angle 88°—150.2 mm (solid line), 300.4 mm (dotted line) and 450.6 mm (dash line). In all calculation, used quartz spherically bent crystal with \(2d = 2.465 \text{ Å}\). Reflectivity function is approximated by three trapezoids.

Figure 4. Projection of reflection zone for spherically bent quartz crystal for different wavelength and two scattering angle. Rectangle represent area of spherically bent quartz crystal with curvature 150 mm and size 5 mm × 2 mm.

The FWHM of rocking curve effects on reflection efficiency. Linear dependence from FWHM was obtained in wide range of Bragg angle and type of rocking curve. Results of simulations for three angles are represented in Figure 2.

Ray tracing simulations for different scattering angle and distance to the x-ray source shows that in range of scattering angle close to 46° the reflectivity does not depend strongly on the distance to the source. In this case, the distance to the source determines the range of reflected wavelengths. The distance to x-ray source sufficiently effects the reflectivity when the scattering angle increases. At small distance one can observe the reduction of reflection range and increasing reflectivity for waves reflected from the center of the crystal. Obviously, the highest reflectivity is observed for the angles close to 90°. In this case, the waves in the narrow bandwidth are effectively reflected from bent crystal. Increasing distance to the light source decreases the reflection range and changes the reflectivity curve (figure 3, 88°). These properties of reflectivity can be explained by geometry of reflection zone in spherically bent crystal.
Figure 5. Experimental spectra of Fe target irradiated by high power laser pulses (20 J, 2 ps). Spherically bent crystal of quartz in orientation [3140] with $2d = 2.3604 \, \text{Å}$, curvature 150 mm and the aperture of 33x12 mm, was used as dispersive element. The source was at 450 mm from the mirror and scattering angle was equal to 52.8°. of the inset shows the shape if reflection zones for Fe $L_{\alpha}$, $He_{\alpha}$, intercombination, $K_{\alpha_1}$ and $K_{\alpha_2}$ spectral lines at the crystal surface. Black curve represents the spectra adjusted according to the reflection efficiency calculated for each spectral line.

crystal (figure 4). Reflection zones for 46° are small and strictly limited by the aperture of the crystal. In contrast, the zone for the waves reflected from the center of the crystal at 88° incidence is much wider and almost fits to the given aperture of the crystal. Correspondingly, the reflected wavelength range is strictly limited.

The ray-tracing code is applied to analyze the experimental spectra of Fe target irradiated by high power laser pulses (of 20 J energy and 2 ps pulse duration). The spectra was measured from the rear side of 10 um foil target using quartz spherically bent crystal (interplanar distance of $2d = 2.3604 \, \text{Å}$, curvature radius of $R = 150 \, \text{mm}$) aligned at central Bragg angel of 52.8°.

The measured spectrum is shown in figure 5 as gray line and consists of $L_{\alpha}$, $He_{\alpha}$, $K_\alpha$ spectral components. The ray tracing simulation run for particular spectrometer configuration demonstrates the significant changes in the crystal reflectivity properties for different spectral lines. The changes in the reflectivity are caused mainly by cutting of the effective reflection zones for a certain spectral component at the edge of crystal aperture, as it introduced in the inset in figure 5. Using the reflectivity factor calculated across the observed spectral range, the actual intensities of the observed spectral components were adjusted. The obtained corrected spectrum is shown as black line.

3. Conclusion

Using ray-tracing code, we studied the dispersion of the spherically bent quartz crystal. The influence of the following parameters was considered: the position of x-ray source, the size of the source, and the crystal surface reflectivity function. Different types of approximation were studied. The approximation of crystal reflectivity function by three trapezoids allows performing calculation with good precision in all range of angles, source size and distance from the crystal. Moreover, the dependence reflectivity on scattering angle and distance from light source was examined. Intensity of reflection low depend on distance to light source for angle in range near 46°. For angles near 88° only small range reflected from crystal, but it have big intensity. The ray-tracing code is applied to analyze the experimental spectra of Fe target irradiated by
high power laser pulses (of 20 J energy and 2 ps pulse duration). Using the reflectivity factor calculated across the observed spectral range, the actual intensities of the observed spectral components were adjusted.

The further development of the code is arranged in order to provide a convenient tool to taking into account the instrumental function of FSSR diagnostics and to reconstruct quantitatively the real intensities of characteristic x-ray radiation of high energy density matter.

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