

Spectral resolution of Cauchois-Johansson spectrometer

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Abstract Spectral resolution of a Cauchois-Johansson spectrometer is analyzed analytically and studied experimentally, using an X-ray tube. Widening of Mo K-alpha spectra, taken in the transmission regime are discussed. Spectral resolution is shown to be $\delta\lambda/\lambda \approx 1.7 \times 10^{-3}$. This value is explained by the influence of crystal thickness and diffraction defocusing of line.

Key words resolution • spectrograph • X-rays

Introduction

Spectrometers, based on the Cauchois-Johansson optical scheme [2], have some advantages in comparison with Cauchois-Johann devices: i) position of the line does not depend on the position of source, ii) the line width does not depend on the size of X-ray source. Therefore, Cauchois-Johansson devices can be successfully used to measure the X-ray emission from extended sources or sources moving during exposure time.

The main characteristics of any spectroscopy device are the energy range as well as spectral and spatial resolutions. The energy range of a Cauchois-Johansson device was discussed in [2]. The goal of the paper is to analyze the spectral resolution of a Cauchois-Johansson spectrometer, trying to take into account theoretically all possible defocusing components. We pay attention that to carry out the full experimental study of spectral resolution of a given device is a complicated task. In this paper we only made a first step in this direction, we investigated the width of lines, emitted by a point source, placed inside a Rowland circle. This experimental geometry is typical for some Z-pinch, laser produced plasma, vacuum sparks.

Spectral resolution

To understand the relative advantages of a Cauchois-Johansson device, we analyze the spectral resolution of a prototype-Cauchois-Johann device, comparing then with the spectral resolution of Cauchois-Johansson itself. We assume that a crystal and a detector are made mechanically correct and both are exactly mounted on the Rowland circle.

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The total width of line δX on the detector plane for Cauchois-Johann scheme can be expressed as:

$$(1) \delta X = \left((\delta x_{\text{geom}})^2 + (\delta x_{\text{diff}})^2 + (\delta x_d)^2 + (\delta x_{\text{th}})^2 + (\delta x_s)^2 + (\delta x_{\text{rad}})^2 \right)^{\frac{1}{2}}$$

where (δx_{geom}) – width component due to geometrical defocusing, (δx_{diff}) – width component due to rocking curve of bent crystal, (δx_d) – width component due to change of d after bending, (δx_{th}) – width component due to the thickness of crystal, (δx_s) – component due to the source size, (δx_{rad}) – radiative width of line, known from tables [1].

Geometrical defocusing of lines δx_{geom} for bent crystals can be measured optically by irradiation the crystal with a divergent beam and estimation of the focal spot size. This type of defocusing is essential for Johann devices and Cauchois-Johann devices in the cases of i) extended X-ray sources, ii) sources moving during exposure.

For i), ii) the entire crystal surface, or at least the main part of it, reflects the line. In these cases, geometrical defocusing is more essential than geometrical defocusing in other geometries of experiments, where a smaller part of crystal reflects the line. Moreover, for i)–ii) δx_{geom} is typically much larger, than δx_{diff} , δx_d , δx_{th} , δx_{rad} . The geometrical defocusing component on the detector plane is:

$$(2) \delta x_{\text{geom}} = R_{\text{cr}} \cdot \delta \theta_{\text{geom}}$$

Formula (2) can be used for any kind of defocusing after substitution of the corresponding $\delta \theta$ component. Angular geometrical widening $\delta \theta_{\text{geom}}$ for Cauchois-Johann [2] is:

$$(3) \delta \theta_{\text{geom}} = \left(\frac{\gamma^2}{2} \right) (\text{tg}(\theta - \gamma) + \gamma) \cong \left(\frac{\gamma^2}{2} \right) \text{tg} \theta \cong \left(\frac{\gamma^2}{2} \right) \theta$$

Here $\gamma^2 = (L/R_{\text{cr}})^2$, R_{cr} – radius of crystal reflecting planes, L – crystal length, reflecting the line. L depends on the size of the X-ray source – the larger the size the larger is the value of L . Corresponding geometrical resolution component is:

$$(4) \left(\frac{\delta E}{E} \right)_{\text{geom}} = \left(\frac{\delta \lambda}{\lambda} \right)_{\text{geom}} = \text{ctg} \theta \cdot \delta \theta_{\text{geom}} \cong \frac{\gamma^2}{2}$$

From (4) it is seen that $(\delta \lambda / \lambda)_{\text{geom}}$ depends on the source size (γ depends on it) and does not depend on the Bragg angle.

In analogy with the previous consideration, the diffraction widening can be estimated as:

$$(5) \delta x_{\text{diff}} = R_{\text{cr}} \cdot \delta \theta_{\text{diff}}$$

and correspondingly:

$$(6) \left(\frac{\delta \lambda}{\lambda} \right)_{\text{diff}} = \text{ctg} \theta \cdot \delta \theta_{\text{diff}}$$

where $\delta \theta_{\text{diff}}$ is a half the width of a rocking curve of a cylindrical crystal, which can be measured by a two crystal diffractometry approach. For flat quartz crystals $\delta \theta_{\text{diff}}$ is usually within 1–10 arcseconds and depends on the cut, wavelength, quality of crystal, etching of crystal. For bent crystals $\delta \theta_{\text{diff}}$ also depends on the radius of curvature and the thickness of the crystal. From data presented in [3], it follows that $\delta \theta_{\text{diff}} \approx 50\text{--}100$ arcsec for bent crystals with radii 250–500 mm.

The origin of defocusing due to changing of d after bending for transmission type crystal is given in [2]. The defocusing component $\delta \theta_d$ on the detector plane is expressed as:

$$(7) \delta x_d = R_{\text{cr}} \delta \theta_d$$

where $\delta \theta_d$ – angular defocusing of the line due to changing of d after bending. From [2]:

$$(8) \delta \theta_d = \left(\frac{h}{R_{\text{cr}}} \right) \cdot \text{tg} \theta$$

where h – thickness of transmission crystal, so from (7), (8) it follows:

$$(9) \delta x_d = h \cdot \text{tg} \theta$$

The corresponding resolution component is

$$(10) \left(\frac{\delta \lambda}{\lambda} \right)_d = \text{ctg} \theta \cdot \delta \theta_d = \frac{h}{R_{\text{cr}}}$$

It is seen, that $(\delta \lambda / \lambda)_d$ also does not depend on the Bragg angle.

The δx_{th} is estimated here for the first time. Fig. 1 illustrates the origin of this type of widening. The physical sense is as follows: an infinitely narrow parallel X-ray beam falling on the transmission crystal with the finite thickness h , becomes wider after passing the crystal. For simplicity the above calculations are given for a flat crystal. The obtained values can be considered as the upper limit for bent crystals, for which the result should be more optimistic due to the focusing of the line.

In Fig. 1, X-ray with unit intensity comes at the Bragg angle θ , h being the thickness of crystal. Let on the way from cross section 1 to cross section 11 an X-ray loses by a half of intensity, Fig. 1 shows a simplified scheme for 5 reflections of the X-ray. After passing the crystal, the initial X-ray is transported into 5 X-rays with relative intensities $J_k = C_4^k / 2^5$, $k = 0 \dots 4$. In general case

$$(11) J_k = \frac{C_{N-1}^k}{2^N}, \quad k = 0, \dots, (N-1)$$

If $N \gg 1$ it is possible to use an approximation [4]:

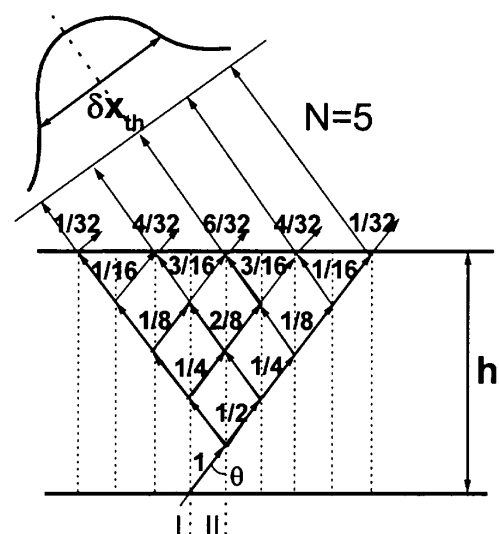


Fig. 1. Origin of the line defocusing dx_{th} influenced by the crystal thickness h .

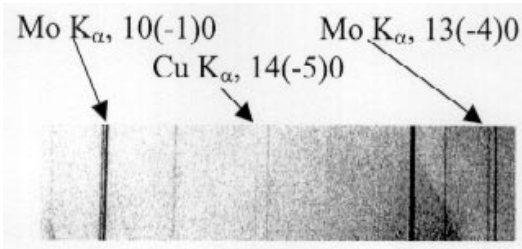


Fig. 2. Mo K_α lines, taken in the transmission regime in the second order of reflection from 10(-1)0 cut and in the first order from 13(-4)0 cut, Cu K_α lines taken in the transmission regime in the first order of reflection from 14(-5)0 cut.

$$(12) J_k \cong \left(\frac{1}{2}\sqrt{2\pi}\right) \cdot \left(\frac{1}{\sigma_k}\right) \exp\left(-\frac{\left(\frac{N-1}{2}-k\right)^2}{2\sigma_k^2}\right)$$

where $\sigma_k = (\sqrt{N-1})/2$, $k = 0, 1, \dots, N-1$. Taking into account that $\sigma_k \approx 1.2\sqrt{N}$ and $N = h\delta\theta/d$ we find a simple formula:

$$(13) \delta x_{th} \approx 10 \text{ tg } \theta \cdot \left(\frac{h \cdot d}{\delta\theta}\right)^{\frac{2}{3}}$$

where h is in μ , d is expressed in \AA , δx_{th} is in μ , $\delta\theta$ is in angular seconds. For an example: $h = 200 \mu$, $d = 1 \text{\AA}$, $\delta\theta = 20 \text{ arc}$, $\theta = 30^\circ$, $\delta x_{th} = 18 \mu$, i.e. ten times less than the crystal thickness.

It was shown in [2] that for the Cauchois-Johansson optical scheme $\delta x_{geom} = \delta x_s = 0$, therefore for the total widening of the line one can use the formula:

$$(14) \delta X = ((\delta x_{diff})^2 + (\delta x_d)^2 + (\delta x_{th})^2 + (\delta x_{rad})^2)^{1/2}$$

where δx_{diff} in the correct case should be taken from two crystal diffractometry measurements, δx_d can be estimated using (9), δx_{th} can be estimated, using (13) and can be neglected in our case.

Results of calibration

The investigated spectrometer uses a 500 mm radius cylindrical quartz crystal, made as described in [2], i.e. it has $2d = 4.9 \text{\AA}$ for transmission geometry and $2d = 8.5 \text{\AA}$ for reflection geometry. Crystal sizes are $L \times H \times T = 65 \times 10 \times 0.3 \text{ mm}$. Registered angle range is 25–75 degrees.

Calibration was made with an X-ray tube, $I = 30 \text{ mA}$, $U = 38 \text{ kV}$, equipped with a Mo anode. The anode to crystal distance was 40 mm, exposition time was 1 hour, X-ray source size was 0.1 mm. Fig. 2 shows the Mo K_α spectra, reflected from 13(-4)0 inclined cut and from 20(-2)0 inclined cut. The Cu K_α spectrum was also observed, reflected from 14(-5)0 inclined cut. The Cu K_α lines are the result of fluorescence from an Cu envelope of the X-ray tube, so the source of the Cu lines is extended and has a 7 mm diameter size. Fig. 3 presents the densitogram of Mo K_α lines, $\lambda_1 = 0.7092 \text{\AA}$, $\lambda_2 = 0.7136 \text{\AA}$, reflected in the first order of reflection from 13(-4)0 cut. For this cut $d = 1.18 \text{\AA}$, $\theta_{\lambda_1} = 17.5^\circ$, dispersion on the detector plane is $(\delta\lambda/\delta x) = (\lambda \cdot \text{ctg } \theta)/R_{cr} = 0.0045 \text{\AA/mm}$. From Fig. 3 it follows that total width of line λ_1 is $\delta\lambda_1 = 1.16 \text{ m\AA}$. Its radiative width, taken from tables [4] $\delta\lambda_{1rad} = 0.29 \text{ m\AA}$. Using formula (10) we obtain $\delta\lambda_{1d} = 0.43 \text{ m\AA}$. Excluding $\delta\lambda_{1d}$ and $\delta\lambda_{1rad}$ from $\delta\lambda_1$ we estimate $\delta\theta_{diff} \approx 90 \text{ arcsec}$. Fig. 4 shows a densitogram of Mo K_α spectrum, reflected from the second order of reflection from the 10(-1)0 cut. The principal values are: $d = 4.2548 \text{\AA}$, $\delta\lambda_1 = 3.4 \text{ m\AA}$, $\delta\lambda_{1d} = 1.7 \text{ m\AA}$, $\theta_{\lambda_1} = 9.6^\circ$, $(\delta\lambda/\delta x) = 0.032 \text{\AA/mm}$. By analogy with previous calculations we obtain $\delta\theta_{diff} \approx 160 \text{ arcsec}$. We assume that so large widening can be associated not only with the diffraction component but also with a probable high mosaicity of the crystal, which can play a more essential role in the transmission geometry at small Bragg angles. The shape of the line with a flat top testifies for that.

The spectral resolution $\delta\lambda_1/\lambda_1$ for 13(-4)0 cut is 1.7×10^{-3} and the spectral resolution for the 20(-2)0 cut is 5×10^{-3} . The last value is measured at small Bragg angles, where the resolution is known to be not so high.

We make the conclusion, that the resolution of the device in transmission of the Cauchois-Johansson geometry mainly depends on the rocking curve of bent crystal and the thickness of crystal. For cylindrical crystals in transmission geometry we estimated an half width of the rocking curve and found it essentially wider than that of the flat crystal. It is a nontrivial problem to decrease $\Delta\theta_{diff}$, because this strongly depends on the mechanical distortion of the bent crystal.

We would like to mention that the full investigation of the spectral resolution of the given device is not possible to present within so short paper. For example, we assumed

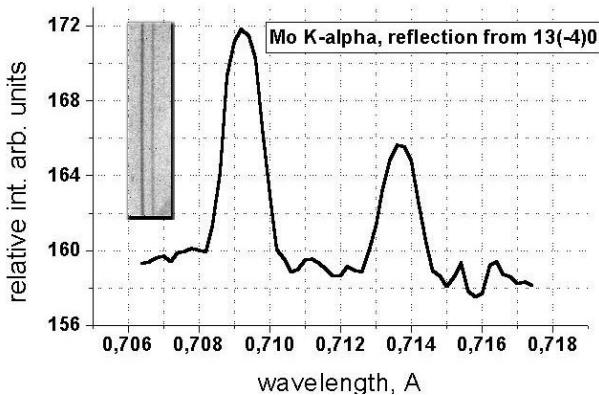


Fig. 3. Densitogram of Mo K_α lines, reflected from 13(-4)0 cut of quartz crystal.

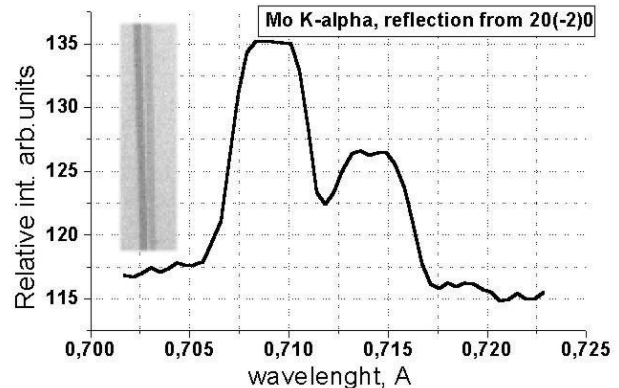


Fig. 4. Densitogram of Mo K_α lines, reflected from 20(-2)0 cut of quartz crystal.

here that an optical quality of the crystal surface is ideal. In reality it is necessary to investigate the optical quality and to estimate geometrical aberrations. A very important matter are local inhomogeneities of the crystal and its local mechanical tensions which can essentially influence the width of the line. To get more detailed characterization of the spectral resolution of our device we also plan to use an extended X-ray source. The data obtained in that geometry will be a subject for future publication.

Conclusions

The spectral resolution of the Cauchois-Johansson spectrometer was investigated analytically and experimentally, using an X-ray tube. It was shown that the spectral resolution of this kind of device is mainly determined by the rocking curve of the bent crystal and the crystal thickness. For the cylindrical quartz crystal with the radius $R = 500$ mm and the thickness of crystal 0.3 mm, the spectral reso-

lution is 1.7×10^{-3} for 13(-4)0 cut and 5×10^{-3} for 20(-2)0 cut. We experimentally estimated the rocking curve of this bent crystal as 80–90 arcsec. This value is about ten times larger than the rocking curve of a flat quartz crystal. To increase the resolution of the device it is necessary to decrease crystal thickness and mechanical tension inside bent crystal, which lead to widening of rocking curve.

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