



# Remarks on a Johann spectrometer for exotic-atom research and more<sup>☆</sup>



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## ABSTRACT

General properties of a Johann-type spectrometer equipped with spherically bent crystals are described leading to simple rules of thumb for practical use. They are verified by comparing with results from Monte-Carlo studies and demonstrated by selected measurements in exotic-atom and X-ray fluorescence research.

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## 1. Introduction

The advent of high-intensity pion and antiproton beams allowed to perform ultimate precision measurements of exotic-atom X-rays by means of crystal spectrometers. Vice versa, also fluorescence studies of standard atoms and ions benefit from adapting and developing further established methods of X-ray diffraction to the needs of exotic-atom spectroscopy.

Exotic atoms are formed when a heavier negatively charged particle like a muon, pion, or antiproton is bound in the Coulomb field of a nucleus. Because of their large mass the dimensions of such atoms are closer to nuclear than to atomic scales. The study of the elementary systems formed with hydrogen, *i. e.* muonic, pionic, and antiprotonic hydrogen ( $\mu\text{H}$ ,  $\pi\text{H}$ , and  $\bar{p}\text{H}$ ), requires the measurement of X-rays with energies in the few keV range. The X-rays stem from the final steps of a de-excitation cascade of the exotic atom, which is formed in high-lying atomic states. Hence, measurements reveal properties of the interplay of the captured particle with remaining electrons in high-lying and nuclear properties from the low-lying transitions. A more detailed description of such systems may be found in ref. [1].

A variety of problems may be tackled by ultimate resolution spectroscopy of fluorescence radiation. Examples are the dependence of X-ray line shapes on the chemical environment [2,3], the relationship of various precise X-ray standards [4,5,6], or studies of highly-charged ions [7,8] which in turn allow decisive tests of methods used for QED calculations [9].

In order to minimise absorption losses in the crystal material, measurements in the few keV range require the use of reflection-type spectrometers, and only silicon and quartz crystals fulfil the requirements for ultimate-resolution spectroscopy. Their resolving power is of the order of  $10^4$ . Consequently, the integrated reflectivity  $R_I$  of such a crystal material is typically about  $100 \mu\text{rad}$  in first order diffraction.

In spite of the high beam intensity provided by modern particle accelerators, an inherent challenge in exotic-atom research is the low count rate together with demanding background conditions. Typical count rates of exotic-atom X-rays are in the range of 20–100 per hour where the flux of pions amounts to a few  $10^8/\text{s}$  (Paul Scherrer Institut, Switzerland [10]) and up to  $10^6/\text{s}$  for antiprotons (at LEAR, CERN [11] until shut down by the end of the year 1996). Such high fluxes produce an enormous beam-induced background level.

Therefore, an apparatus for ultimate-resolution spectroscopy constitutes a compromise between conserving the intrinsic resolution of ideal single crystals and sufficiently high efficiency to achieve acceptable measurement times together with mechanical long-term stability.

The experimental approach consists of a Johann-type Bragg spectrometer equipped with spherically bent silicon and quartz crystals. Such a set-up allows to record simultaneously a finite energy interval according to the width of the X-ray source when using a correspondingly extended X-ray detector. Large bending radii of about 3 m minimise aberrations and result in a sufficient distance to the X-ray source allowing for an effective shielding of the X-ray detector.

The paper discusses general features of such spectrometers using a simple geometrical picture giving at hand rules of thumb to assess a typical set-up (Section 2). The validity of approximations is exemplified by means of experimental results and by Monte-Carlo studies (Section 3). The mechanical set-up is sketched in Section 4. Examples from exotic-atom spectroscopy are referenced for light antiprotonic and pionic

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atoms as well as applications in the field of X-ray fluorescence (Section 5).

## 2. Imaging properties

Crystal spectrometers exploit the fact, that a regular atomic lattice diffracts intensity only for wavelengths  $\lambda$  fulfilling the Bragg condition

$$n\lambda = 2d \left[ 1 - \left( \frac{2d}{n\lambda} \right)^2 \delta \right] \cdot \sin\Theta_B, \quad (1)$$

where  $n$  is the order of diffraction,  $d$  the lattice spacing perpendicular to the diffracting plane, and  $\Theta_B$  the Bragg angle. The correction term  $\delta = 1 - n_r$  takes into account the change of the index of refraction inside the crystal material with  $n_r$  being the real part of the index of refraction [12].  $\delta$  itself depends on  $\lambda$  and is of the order  $10^{-3}$  in the considered energy range [13,14]. Energy  $E$  and wavelength  $\lambda$  are related by  $E = \frac{hc}{\lambda}$ .

In the so called Johann-type set-up the diffracting planes are bent to a radius  $R_c$ . The benefit of the focusing properties of such curved crystal spectrometers was described first for the cylindrical case [15,16]. The major advantage is the possibility to measure simultaneously a complete energy interval given a (preferentially homogeneous) extended source together with an extended detector (Fig. 1). Different wavelengths are accepted from different locations of the source which correspond to different locations in the focal plane. Consequently, the impact point of the diffracted X-rays in the detector plane constitutes a wavelength or energy spectrum in the direction of dispersion.

Varying  $\Theta_B$ , i. e.  $\lambda$ , the location of the minimum width of a bundle reflected under  $\Theta_B$  from a curved mirror is a circle with diameter  $R_c$ , the Rowland circle. The distance of the crystal centre to the focal point on the Rowland circle is given by  $R_c \cdot \sin\Theta_B$  (focal condition).

From the angular dispersion,  $\frac{d\lambda}{d\Theta} = \frac{\lambda}{\tan\Theta_B}$  (neglecting the index of refraction shift), one derives the (local) dispersion in a detection plane at the focus  $F$  to be  $\frac{d\lambda}{dx} = \frac{d\lambda}{d\Theta} \cdot \frac{1}{R_c \cdot \sin\Theta_B}$ , where  $x$  is the direction of dispersion in the plane perpendicular to the direction  $\overline{CF}$  (see Fig. 2). In terms of the X-ray energy  $E$ , the relations are  $\frac{dE}{d\Theta} = -\frac{E}{\tan\Theta_B}$  and  $\frac{dE}{dx} = \frac{dE}{d\Theta} \cdot \frac{1}{R_c \cdot \sin\Theta_B}$ .

In reality, pure specular reflection must be extended to a finite angular range around the Bragg angle  $\Theta_B$  determined by a given wavelength  $\lambda$ . In this range, the acceptance of the crystal is weighted according to the shape of the rocking curve. The rocking curve, characterised by its width  $\omega_c$  at full width half maximum (FWHM), represents the angular spread of the diffraction pattern for a particular crystal plane (Fig. 4).  $\omega_c$  may be regarded as the intrinsic resolution of a plane crystal. The integral of the rocking curve, the integrated reflectivity  $R_i$ , represents the

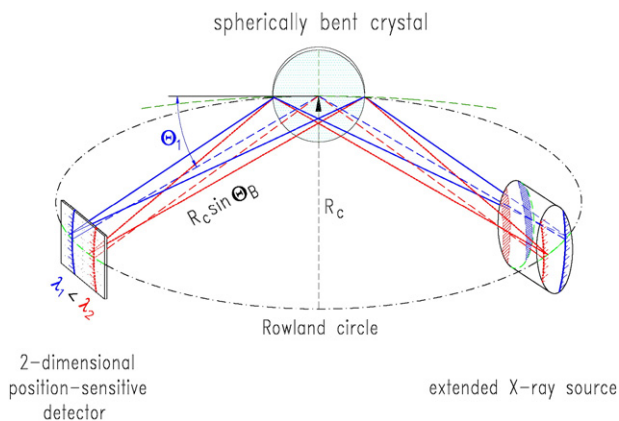


Fig. 1. Source and image locations of two different wavelengths  $\lambda_1 < \lambda_2$  for a Johann-type set-up (symmetric Bragg case). A spherically bent Bragg crystal allows in addition partial vertical focussing.

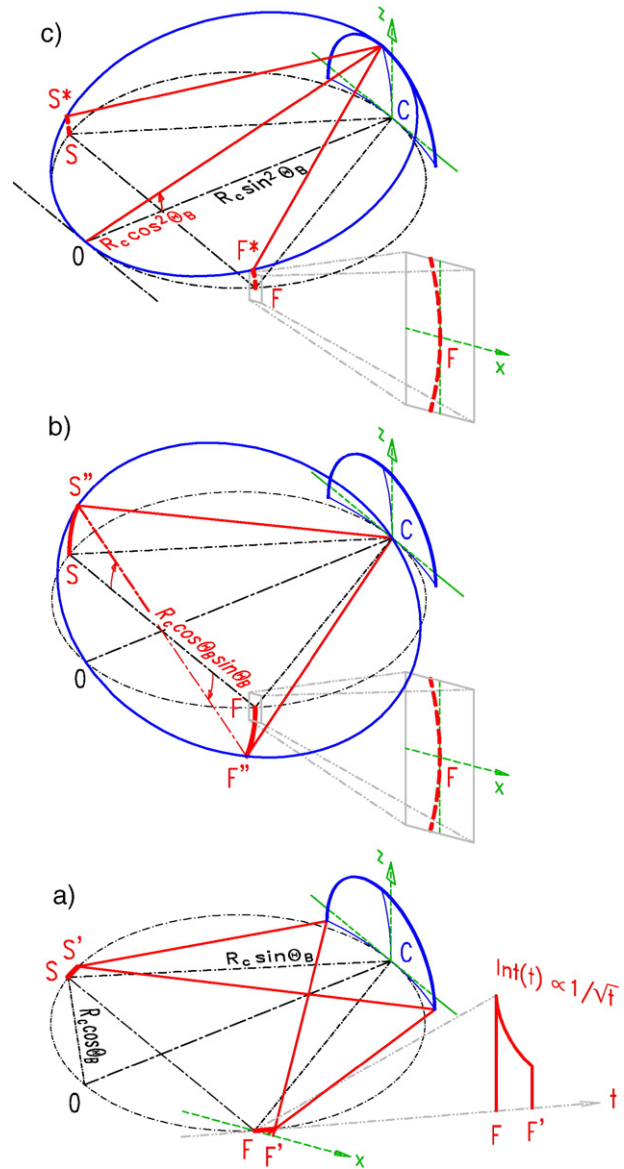


Fig. 2. Johann shift and symmetries in spherical-mirror imaging (see text).

total reflected intensity. The rocking curve can be calculated by means of diffraction theory, e.g., by using the code XOP [17].

A complication when using Johann set-ups is a precise absolute angular calibration. It requires the exact knowledge of the orientation of the reflecting plane which meets enormous technical difficulties. Therefore, using a calibration line with a Bragg angle as close as possible is mandatory for ultimate energy determination. The calibration is then achieved by the angular distance measured by means of the position difference in the direction of dispersion  $x$ .

For cylindrically bent crystals, the image height is approximately twice the crystal height plus the source height. Vertical focussing is achieved by crystal bending in the vertical direction  $z$  as realised in the so called v. Hámos geometry [18]. The (vertical) bending radius required is  $R_c \cdot \sin^2\Theta_B$ , i. e. simultaneous complete focussing is achieved for spheres only in the limit of back reflection  $\Theta_B = 90^\circ$ . However, the ideal case of an elliptical surface of highest quality meets very demanding fabrication techniques and, in addition, fixes the geometry to one particular Bragg angle. Therefore, spherical bending is commonly used. For small Bragg angles  $\Theta_B$ , the image height is still comparable with the one of a cylindrically bent crystal, but with increasing  $\Theta_B$  significant vertical focussing can be achieved (see Figs. 3 and 4). A detailed analytical

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