Comparison of double crystal (+n,-m) and (+n,+m) settings containing a fully asymmetric diffraction geometry of a bent perfect crystal with the output beam expansion

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Abstract. In this paper neutron diffraction properties of the dispersive double crystal (+n,-m) and (+n,+m) settings containing the bent perfect crystal Si(220) in symmetric diffraction geometry and the bent perfect crystal Si(311) in the fully asymmetric diffraction geometry with the output beam expansion are studied and compared. It has been found that the properties, namely, the width of the output double diffracted beam, of both settings strongly depends on the relative combination of curvatures of Si(311) crystal slab with respect to the curvature of the Si(220) one. Moreover, after the beam expansion the fully asymmetric diffraction geometry provides in both cases a highly collimated and highly monochromatic beam of a rather large cross-section of several square centimetres. Application possibilities, of such a beam, namely for neutron phase contrast radiography will be discussed.

1. Introduction

Several papers concerning studies of diffraction properties of bent perfect crystal (BPC) slabs in the fully asymmetric diffraction (FAD) geometry due to a possible use for highly efficient monochromators and analyzers were already published in the past [1-10]. Recently, we have decided to study another beneficial properties with the goal of obtaining an unconventional high-resolution neutron optics components. While in the past nondispersive (1,-1) double-bent-crystal settings were also studied [6-10], recent experimental investigations have been focused on studies of the properties of the monochromatic beam produced by a dispersive (or quasi-dispersive) double-bent-crystal settings with the second FAD crystal as an analyzer. It is clear that in practice, the FAD geometry can be effectively studied in the case of Si-BPC slabs, because the attenuation factor for thermal neutrons in Si is very low [11]. The first recent experimental investigations [12] have shown that thanks to the possibility of the variation of the curvature of both BPC crystals, one can easily manipulate with the width of the obtained monochromatic beam in the range from few to tens of millimetres. As the double crystal setting Si(111)+Si(311) is dispersive, the monochromatic beam is naturally highly collimated.
without the use of any collimators and the FAD crystal can work as one dimensional magnifying element. It should be mentioned that two possibilities of the FAD diffraction geometry are possible: with the output beam compression (FAD-OBC) or with the output beam expansion (FAD-OBE). In the case of the FAD-OBC geometry a wide incident beam (several centimetres) is incident on the FAD crystal and a condensed output monochromatized beam of the width of a few millimetres is diffracted. In the present case of the opposite FAD-OBE geometry (see figures 1 and 2) a narrow beam enters the bent FAD crystal slab (of the width of several millimetres) through its end face and after passing along the longest edge of the slab, depending on its curvature, the diffracted monochromatized beam is expanded to a rather large cross-section. In this paper the comparison of these two (+n,-m) and (+n,+m) settings is carried out. Dimensions of all Si crystal slabs used in the diffractometer performances were: 200x40x4 mm$^3$ (length x width x thickness).

2. Reflecting properties of the bent FAD perfect crystal

Bent perfect crystals (BPC) are usually employed in symmetric or slightly asymmetric diffraction geometry. They are well known, namely, for their focusing properties in real as well as momentum space with respect to a sample. Generally, the BPC elements are attractive for an employment from the following reasons: predictability and reproducibility of the effective mosaicity, predictability and reproducibility of a rather high peak reflectivity and its uniformity over large areas of the crystal, a rather high peak reflectivity for asymmetric or transmission geometry and predictability of the integrated reflectivity. In the transmission geometry one can also benefit from natural wavelength focusing. In the limiting case of the FAD-OBE geometry which was used in the present case, some more properties can be studied which could be possibly used for the application in neutron diffractometry. As can be seen from figure 1, depending on the curvature of the crystal slab a narrow incident beam can be spatially enlarged. In such a way, it is possible to manipulate not only with focusing in real and momentum space but also with a spatial distribution (width) of the diffracted beam. Even though one can expect some focusing in real space in the diffracted beam, due to the output beam expansion, it has not to be so pronounced. On the other hand, the expansion of the diffracted beam directly influences the separation of the wavelengths of individual neutron rays within the $\Delta x$ distribution (see figure 2) which is, of course, strongly correlated. It is well known that in the case of BPC symmetric and asymmetric diffraction, Bragg law introduces a correlation between the direction and the wave-vector of neutrons, but in the case of FAD geometry there is a new correlation.
between the position within the $\Delta t$ range and the wave-vector of neutrons. In some experiments this can be successfully exploited in combination with a position sensitive detector [6-10].

The general formula for the peak reflectivity (reflection probability) of neutron passing through a homogeneously deformed perfect crystal (see figure 3) has been derived in the form [1,13]

$$r(R) = \{1 - \exp(-Q_{\text{hkl}}(\partial\Delta\theta\partial\Delta s))\},$$

(1)

where $(\partial\Delta\theta\partial\Delta s)$ is the rate of the change of the Bragg angle $\theta$ on the flight path $\Delta s$ in the crystal in the incident beam direction and $Q_{\text{hkl}} = (F_{\text{hkl}})^2\cdot\lambda^4/(\Omega^2\sin 2\theta)$ is the kinematical reflectivity of the crystal unit volume. $F_{\text{hkl}}$, $\lambda$ and $\Omega$ are the structure factor, neutron wavelength and the unit-cell volume, respectively [14]. The effective mosaicity $\delta\theta = \delta\theta - \delta\theta_1$ (see figure 3) and the integrated reflectivity $\rho^h(R)$ can be for homogeneous bending defined as $\delta\theta = s/(\partial\Delta\theta\partial\Delta s)$ and $\rho^h(R) = \delta\theta(R)\cdot r(R)\cdot A(\mu)$, respectively [1]. $s$ is the distance between the points A and B (see figure 3), $t$ is the thickness of the crystal slab, $\psi$ is the angle of asymmetry and $A(\mu)$ is the attenuation factor. Then, for FAD geometry we can derive simple expressions for the effective mosaicity and the peak reflectivity [1]

$$\delta\theta(R) = s/R,$$

(2)

$$r(R) = 1 - \exp(-Q_{\text{hkl}}R).$$

(3)

Due to the difference in the path length $s$ in the crystal, the value of the effective mosaicity is different in the incident and diffracted beam direction. In the present FAD case, for the incident beam $\delta\theta(R) = L/R$, where $L$ is the length of the crystal. Figure 4 shows the calculated dependences of the peak reflectivities $r(R)$ for Si(311) FAD diffraction geometry and also for Si(220) slab set in symmetric diffraction geometry (for the sake of comparison) on the crystal curvature $(1/R)$. It can be seen from figure 4 that the peak reflectivity corresponding to Si(311) FAD geometry is smaller than the one corresponding to the symmetric Si(220) diffraction geometry, namely, due to the difference in $(F_{\text{hkl}})^2$ and thus in $Q_{\text{hkl}}$. As for the attenuation factor $A(\mu)$, then in our case of low attenuating Si crystal ($\mu=1.9\cdot10^{-2}$ cm$^{-1}$) and a rather short width of the diffracted beam (less than 3 cm, see figures 5 and 8), we can simply use for calculations the approximation expression $A(\mu) = \exp(-\mu/L/2)$.

3. Experimental results

The experimental studies of the $(+n,-m)$ and $(+n,+m)$ double-crystal settings with the FAD-OBE geometry of the second crystal-analyzer were carried out on the dedicated neutron optics diffractometer installed at the reactor LWR-15 in Rež. It operates at the fixed neutron wavelength of 0.162 nm provided by a bent Si(111) premonochromator (the radius of curvature - 10 m). No Soller collimators are used on the beam path from the reactor to the detector. Due to a small Bragg angle for Si(111) crystal ($15^\circ$), the premonochromatic beam of a rather large divergence and $\Delta\lambda/\lambda$ spread of
about $4.4 \times 10^{-2}$ [14] can be considered from the point of view of the resolution properties of (+n,-m) and (+n,+m) settings as quasi-polychromatic. Thus, it was used for the following studies. The distance between the Si(111) and Si(220) crystals was 1.7 m and the distance between the Si(220) and Si(311) FAD crystal was 0.5 m. As the curvature of both BPC slabs Si(220) and Si(311) were changeable, the properties of the beam profiles as registered by the scintillation camera (SC) or imaging plate (IP) could be studied for different combination of the individual curvatures. The width of the incident beam entering the FAD crystal was limited by a 3 mm slit.

3.1. Parallel (+n,-m) double-crystal arrangement

Figure 5 shows the experimental results of the width (represented by FWHM) of the output expanded beam as a function of curvature of FAD crystal for different curvatures of the Si(220) crystal slab. It can be seen from figure 5 that for small curvatures $1/R_{2,FAD}^2$, the length $\Delta L$ of the area inside the FAD crystal where the Bragg condition for neutrons coming from the bent Si(220) crystal takes place is less than 30 mm ($\Delta L = \text{FWHM} / \sin 2\theta$). In all cases of the fixed curvatures of the BPC Si(220) crystal, FWHM of the double diffracted beam decreases when the curvature of the FAD crystal increases. It achieves values of several millimeters at the place of the camera. As the corresponding peak intensity of the profiles does not change considerably for large curvatures of the FAD crystal, it means that the change of FWHM is not given directly by focusing in real space but by overlapping the phase space elements of individual crystals. It means that the length $\Delta L$ of the volume element where the diffraction process in the FAD crystal takes place and which then transforms to $\Delta x$, decreases with the curvature. It also means that the dispersity between the Si(220) and FAD-Si(311) crystals becomes more pronounced. Therefore, one can easily manipulate with the width of the double diffracted beam. When considering cylindrical bending of the FAD crystal, it could be expected that the deviation from the mean Bragg angle linearly changes along its longest edge. Figure 6 experimentally proves this

![Figure 5](image-url)
property of the linear change of the Bragg angle for different values of the bending radii when rocking the FAD crystal with respect to the bent Si(220) one. The shift of the diffraction profile on the scintillation camera can be expressed by a formula
\[ \Delta x = \Delta \theta \cdot (R_{\text{FAD}} \sin(2\theta)) \]
(see the insert in figure 2). Similarly to the exploitation of FAD crystal in the nondispersive (+n,-n) setting [6-8], this property can be successfully used for analyzing some effects related to scattering to small angles. The imaged refraction edge profiles obtained on Si samples (IP was at the distance of 35 cm from the sample) which are shown in figure 7 document that the obtained output monochromatic beam is of a high spatial coherence. For imaging a similar experimental arrangement as shown in figure 9 was used.

### 3.2. Antiparallel (+n,+m) double-crystal arrangement

Similarly to the quasi-parallel (+n,-m) setting, the properties of the output expanded beam in the

![Figure 6. Calibration of the rocking angle of the FAD crystal versus the peak position of the diffraction profile on the scintillation camera.](image1)

![Figure 7. Edge profiles obtained on the two sides of a Si prism of the 10 mm thickness and on the one side of a 3 mm thick Si slab.](image2)

![Figure 8. The dependences of the peak intensity and FWHM of the diffraction profile on the FAD crystal curvature as registered by the scintillation camera (at 56 cm from the FAD crystal) for fixed curvatures of the Si(220) one: (a) - 0.11 m⁻¹, (b) - 0.083 m⁻¹, (c) - 0.056 m⁻¹ and (d) - 0.028 m⁻¹.](image3)
(+n,+m) setting as a function of curvature of FAD crystal for different curvatures of the Si(220) crystal slab were investigated. The obtained results are summarized in figure 8. The comparison of the results from figures 5 and 8 reveals that in the (+n,-m) setting the FWHMs of the output beam diffraction profiles registered by the scintillation camera are slightly smaller than in the (+n,+m) one. However, in both cases FWHMs have a decreasing tendency with the increase of the curvature of the FAD crystal slab. It means that also in this setting the natural dispersity between the Si(220) and FAD-Si(311) crystals strengthens with the curvature of the FAD crystal slab. Similarly, the peak intensities of the profiles registered by SC are higher in the case of (+n,-m) setting. The different variations of the peak intensities vs crystal curvature (see figures 8c and 8d) can be explained by different focusing conditions of the BPC-FAD Si(311) crystal with respect to the BPC Si(220) one, namely, in momentum space. It should be pointed out that the peak reflectivity \( r(R) \) is not directly related to the peak intensity of the diffraction profile which is dependent e.g. on focusing in real and momentum space. The theoretical dependence of the peak reflectivity \( r(R) \) on the crystal curvature was experimentally verified in the past [1,2]. However, the peak intensities of the individual diffraction profiles can be theoretically hard to describe. Moreover, the diffraction profiles registered by SC were taken in one angular position (peak position) of the Si(311) crystal rocking curve with respect to the Si(220) one. Thus, the values of FWHM presented in figures 5 and 8 are not related to the rocking curve profiles but just to the profiles of the diffracted beam at the peak position of the rocking curves. The peak position of the rocking curve of the FAD crystal also means that the volume element where neutrons are diffracted is situated in the middle \((L/2)\) of the crystal slab. Even though the FAD crystal is illuminated along the whole length, due to a large homogeneous effective mosaicity \((\delta \theta(R) = L/R)\), monochromatic neutrons coming from the bent Si(220) crystal are diffracted in a rather short volume element inside the FAD Si-slab. However, by rocking it, the diffraction volume element moves along the longest edge of the crystal slab and then the diffracted neutrons step by step fall outside the acceptance window of SC. The resolution demonstrating a high spatial coherence of the (+n,+m) setting was also tested on the imaging of the edge refraction effects on three different samples (two Si plates of the width of the edges of 5 mm and 10 mm, respectively and a rectangular Fe prism of the width of the edge of 9 mm) The results are shown in figure 9. As expected, the calibration of the rocking angle of the FAD crystal versus the peak position of the diffraction profile imaged by SC was found the same as in the case of the (+n,-m) setting.

![Image](image.png)

**Figure 9.** Photo of the irradiated samples of different edge widths with the marked window for the beam and experimental edge profiles obtained for \( R_{2,FAD} = 36 \) m. Imaging plate was at the distance of 35 cm from the samples.

4. Summary

Diffraction properties of the FAD geometry of the BPC Si(311) slab as a second crystal in the (+n,-m) and (+n,+m) double-crystal settings with respect to the BPC Si(220) one were investigated and
mutually compared. In both cases, the output monochromatic beam provided by such a flexible double-crystal setting is highly collimated and FWHM of the profile could be easily manipulated by the curvature of the FAD crystal. Contrary to common opinion, though, it is the double diffraction process, the output monochromatic beam current can be sufficiently high and useful for employment in some special diffraction experiments. Thanks to a high peak reflectivity of the FAD Si(311) and Si(220) crystals (see figure 4), the obtained monochromatic neutron current after double diffraction process corresponds to the resulting phase-space element given by the overlapping of phase-space elements of the individual BPC Si(220) and FAD BPC Si(311) crystals in the (+n,-m) or (+n,+m) settings. Of course, the common peak reflectivity \( r = r_2 \cdot r_3 \) should be considered. The estimation of the reflectivity of the double crystal setting expressed by the product of the peak intensity and the corresponding value of FWHM (see figures 5 and 8) shows that both settings are from this point of view roughly equivalent. It should be also pointed out that due to the fact that the two step diffraction is carried out on crystals with different lattice spacings, the double diffracted beam has a narrow \( \Delta \lambda / \lambda \) spread \( \Delta \lambda / \lambda = \Delta \theta \cdot \cot \theta \) of the order 10\(^{-3}\) or less. It is dependent on the curvatures of the individual crystals (see figure 12 and the related text in another paper of ours in this proceedings where the beam divergence for less dispersive setting was of about 1x10\(^{-3}\) rad). It should be said that both (+n,-m) and (+n,+m) settings as presented in this paper can be used, namely, at high-flux neutron sources for experiments of neutron imaging when using the output beam of a large cross-section [15] or for high resolution (in scattering angle as well as \( \Delta \lambda / \lambda \)) diffraction experiments when using the output beam of small cross-section.

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