ICANS-XV
15th Meeting of the International Collaboration on Advanced
Neutron Sources
November 6-9,2000
Tsukuba, Japan

14.10

Possible implementation of focusing based on Bragg diffraction optics for TOF neutron scattering devices

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Abstract

Neutron Bragg diffraction optics (NBDO) employing cylindrically bent perfect crystals (BPC) as neutron monochromators/analyzers has been proved as a powerful way how to increase luminosity and angular/energy resolution of some dedicated scattering devices installed at steady state neutron sources, namely when samples of small dimensions have to be investigated. However, in the case of scattering devices working in the TOF regime, the use of NBDO based on the BPC elements is far from a large exploitation. In this paper we introduce some new practical applications of NBDO arrangements which can be used for time and spatial focusing and can be implemented on the TOF instruments.

1. Introduction

It is a frequent intensity problem when small sample volumes must be probed. When also a high resolution is required one has to perform experiments with highest possible neutron fluxes on the sample position. In case of convetional diffractometers (or spectrometers) installed at steady state sources and equipped with flat mosaic crystals and a system of Soller collimators one has to work with a correspondingly reduced phase space volume leading often to unnecessary detector-signal losses. Focusing techniques with BPC elements can help to overcome these limitations. In many cases implementation of the BPC elements permits one to benefit from focusing in real and momentum space simultaneously (resulting in a high resolution and a high luminosity) and to work efficiently with open beams without Soller collimators [1-5]. In such cases the BPC-elements can be considerably superior to flat mosaic crystals, though, it is usually in a smaller range of momentum transfer ΔQ [6-11] or energy range ΔE [12-15]. However, as far as we know, besides focusing mosaic crystals (e.g. [16]) NBDO using BPC elements have not been employed at the pulsed sources.

2. Focusing properties of bent perfect crystals

For imaging in the scattering plane by a thin cylindrically bent perfect crystal the general lens formula ($f_a/a + f_b/b = 1$) can be used, where $f_{a,b}$= ($R\sin(\theta_B \pm \psi)$)/2 is the focal length dependent on the asymmetry cut (ψ is the angle of the reflection planes with respect to the crystal surface)[3]. According to Fig. 1 a parallel beam diffracted by the BPC element is focused to

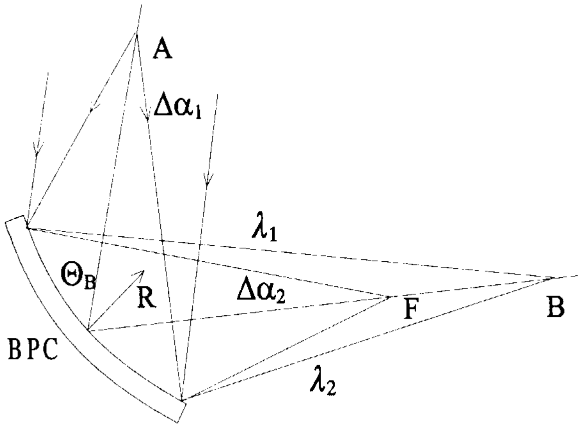

Fig. 1. Schematic sketch of focusing by a bent perfect crystal slab

the focus F being at the distance f_b and the object A situated at the distance a before the BPC element is imaged at the distance b behind it as the image B. Then for a given Bragg angle θ_B and the bending radius R, we arrive at the relation

$$a(R) = f_a/(1 - f_b/b), \qquad (1)$$

The divergency $\Delta\alpha_1$ and convergency $\Delta\alpha_2$ of the rays before and behind the curved crystal, respectively, are related as

$$\Delta\alpha_2 = 2\varepsilon(R) - \Delta\alpha_1, \qquad (2)$$

where $\varepsilon(R)=(a\Delta\alpha_1/R)\sin\theta_B$ is the total change of the angle of incidence (exit) over illuminated crystal length.

3. Focusing analyzers

A typical example of focusing in real space can be e.g. the analysis of divergent neutron beam of $\Delta\lambda = \lambda_2 - \lambda_1$ spread by a BPC analyzer after diffraction by a slit-like polycrystalline sample situated at the point A. The situation when $\Delta\lambda = 0$ ($\lambda_2 = \lambda_1$) is called monochromatic focusing providing a high energy resolution (see Fig. 2). Such BPC analyzers have been successfully used at the steady state neutron sources in high resolution powder diffractometry, namely, for residual strain measurements [17] and for inelastic scattering studies by three axis spectrometer [18,19]. However, it is clear, that they can similarly be employed in the TOF spectrometers.

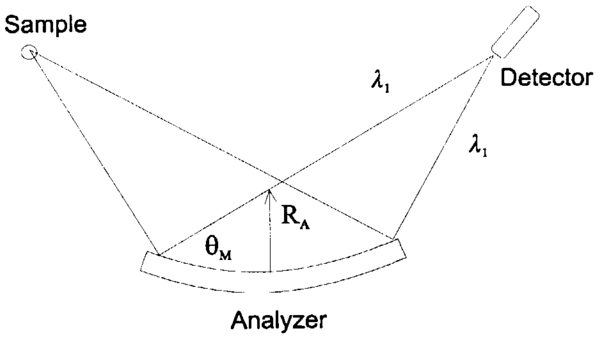

Fig. 2. Schematic sketch of the BPC analyzer set for monochromatic focusing analysis.

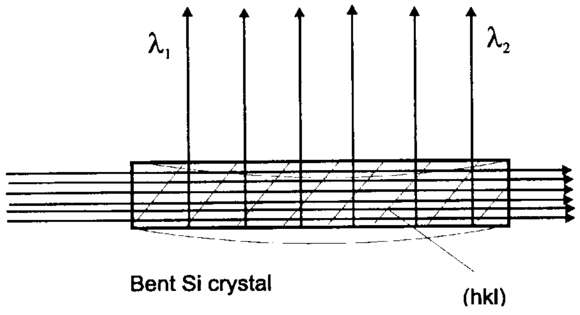

Fig. 3. Schematic sketch of the fully asymmetric diffraction geometry of the analyzer.

Special attention deserves the fully asymmetric diffraction geometry of the BPC analyzer which due to a low attenuation can be used practically only with perfect Si crystals in the range of neutron wavelengths 0.15 nm – 0.4 nm (see Fig. 3) [20]. The analysis of the beam is performed in momentum space. Transformation of angular/energy scale on the spatial scale can be advantageously used in combination with a position sensitive detector. Analyzer of this type can provide an extremely high angular/energy resolution because its uncertainty contribution coming from the effective mosaicity can be usually neglected. This type of the analyzers have been succesfully used at the steady state sources in powder diffractometry for residual strain measurements [21,22], high resolution small-angle neutron scattering [6-8,23] and Bragg edge investigations [12,13]. However, in the case of the pulsed sources, as can be seen from Fig. 3, in correlation with a linear deviation from the Bragg angle $\delta\theta=\delta x/R$ (δx is the coordinate parallel to the longest edge of the cylindrically curved slab of the length l), a fine spatial separation of the individual wavelengths, though it is only in a limited range of $\Delta\lambda$, can be achieved independently of the pulse length. In practice, the total angular range $\Delta\theta = l/R$ is usually not larger than 5×10^{-2} and the FAD analyzer can provide as good resolution $\delta\lambda/\lambda$ as about 10^{-4}.

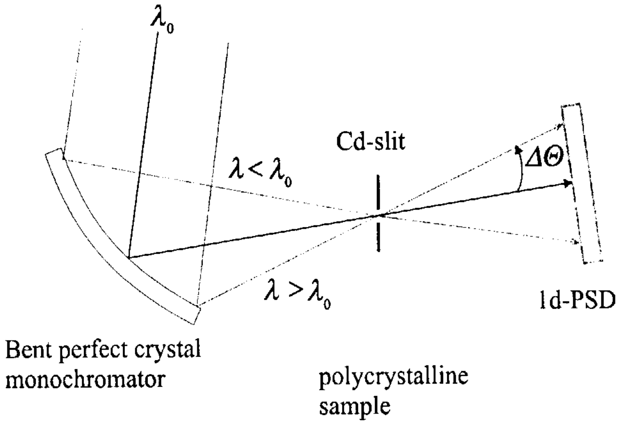

Fig. 4. Sketch of the simplest focusing set-up for Energy Dispersive Neutron Transmission Diffractometry

Recently, several focusing techniques have been tested at the steady state sources for high resolution energy-dispersive neutron transmission diffraction (EDNTD) for investigation of an influence of strains on Bragg diffraction edge positioned at $\lambda_0=2d_0$ [12-15]. The simplest EDNTD setting strongly distributing the neutron wavelengths within $2\Delta\theta$ divergence represents the one displayed on Fig. 4 [14-15]. Also in this case, as good resolution $\delta\lambda/\lambda$ as about 10^{-4} can be achieved independently of the pulse length.

4. Double-crystal arrangements

As can be seen from Figs. 5 and 6, the introduced double-crystal arrangements are based on FAD geometry of the BPC crystals which easily permits to transform a chosen $\Delta\lambda$ range on a spatial range simply determined by the length of the curved crystal slab. Double BPC settings profit from a high peak reflectivity of individual elements and have already been tested for neutron monochromatization [24-26]. The inspection of Fig. 5 reveals that the arrangement with both BPC elements in FAD geometry can be employed as a static selector of well defined $\Delta\lambda$ range of neutrons. On the other hand, the arrangement introduced in Fig. 6 can be used for time focusing thanks to an easy adjustment of the mutual nondispersive setting of the BPC elements though, they are set for different diffraction geometries [27,28].

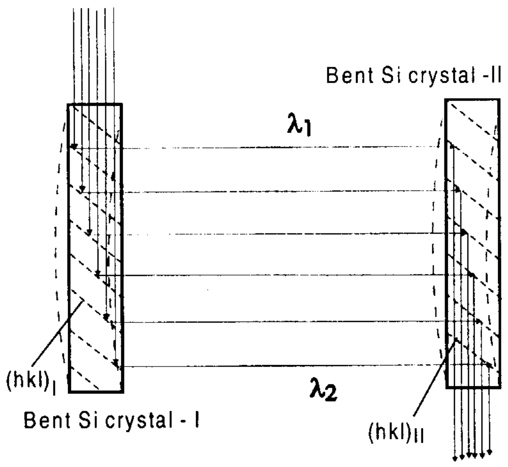

Fig. 5. Schematic sketch of the double bent crystal setting of two BPC elements both in the FAD geometry.

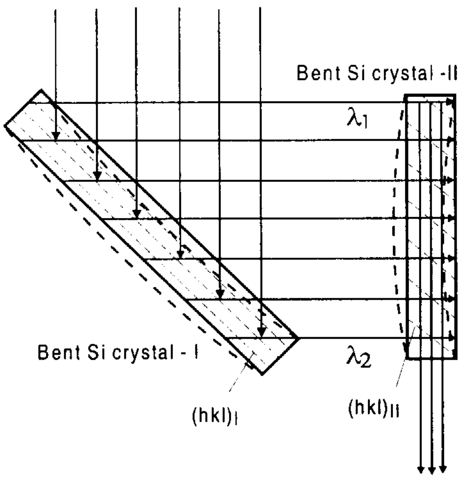

Fig. 6. Schematic sketch of the double bent crystal setting of two BPC elements with one of them in the FAD geometry.

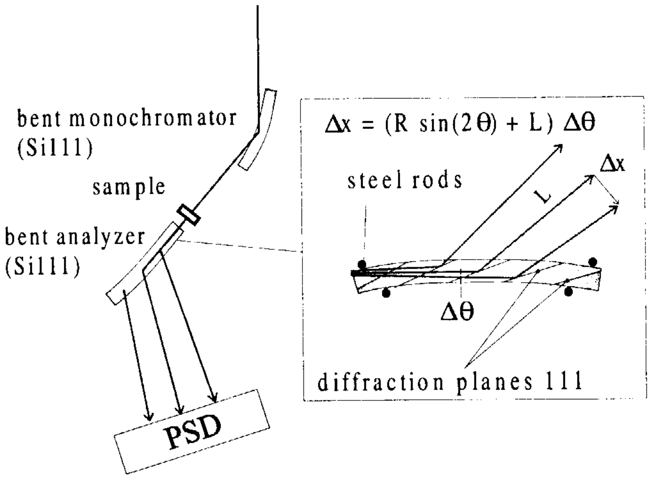

Fig. 7. Sketch of the double bent crystal diffractometer for high-resolution SANS operating in NPI Řež.

Concerning the high-resolution small angle neutron scattering, double crystal arrangements employing slightly bent perfect crystals or channel cut perfect crystals are already routinely used at the steady state neutron sources [8,23,29,30]. However, up to now their alternative have not been developed for exploitation of the pulse structure. Therefore, one can expect that these arrangements will be also used at the pulsed sources.

5. Conclusion

Neutron diffraction instruments employing the BPC elements may optimally use an available neutron flux and achieve higher detector signal with an excellent resolution in comparison with the instruments employing flat mosaic crystals. Besides the *d*-spacing, the other parameters, namely cutting angle ψ, curvature $1/R$ and possibly constant lattice gradient, bring three more degrees of freedom. However, it makes the problem of optimization of the focusing experiment more difficult. The resolution is determined by the sharpness of the θ–λ correlation, and the sample dimension (thickness in the plane-like samples). Therefore, all focusing tricks promise a gain for small samples and usually in a smaller range of ΔQ or $\Delta\lambda$. The absence of secondary extinction opens possibility of using a FAD geometry of the curved analyzer in combination with a position sensitive detector which can be effectively used for excellent high-resolution nondispersive as well as dispersive measurements. Usual problem of the BPC elements is their brittleness. The choice of the asymmetric diffraction geometry can help to avoid this problem as it requires a smaller focal length with a larger bending radius. Smaller bending radii with thicker crystals can be reached in some cases by using sandwiches consisting of two or more thinner and mutually well oriented individual lamellae. However, sandwich of two or three curved BPC slabs of different cuts which monochromatize/analyze two or three neutron wavelengths simultaneously, can in some cases correspondingly increase an efficiency of scattering instruments [31-33]. A big challenge for a further implementation of Bragg diffraction optics is expected after growing single crystals with the interplanar distance linearily varying along the monochromator/analyzer surface which permits one to use a monochromatic *superfocusing* [34].

Acknowledgement

Investigations of Bragg diffraction optics and its implementation in neutron diffractometry are supported by the Grant Agency of the Czech Republic No. 202/97/K038, Grant Agency of Czech Academy of Sciences No. A1048003 and the TMR-Network ERB FMR XCT 96-0057.

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