EXED – the new Extreme Environment Diffractometer at the Hahn-Meitner-Institut Berlin

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Abstract. The Extreme Environment Diffractometer EXED, which is currently under construction at the Hahn-Meitner-Institut (HMI) Berlin and shall become operational in 2006, is presented here. The general ideas of the design are given and a special attention is addressed to resolution excellence including first simulation results.

Introduction

The EXED instrument is a very high resolution time-of-flight powder diffractometer, which has been optimised for diffraction in extreme environments. A special focus is on high magnetic fields and thus the instrument will be equipped with a dedicated 25 T cryomagnet. The instrument is being built at the steady state reactor BERII of the HMI, but its sophisticated chopper system allows the application of the time-of-flight (TOF) principle and, compared to a common crystal monochromator instrument, EXED offers a number of advantages on a continuous source: a) it can provide higher resolution, comparable to what is now achieved at synchrotron radiation sources; b) it makes small *d*-spacing readily accessible; c) it is more efficient in terms of neutron intensity for conventionally high resolution neutron diffraction work and d) it facilitates the use of extreme sample environment equipment by providing a full coverage of the relevant *Q* domain at very limited angular access in scattering angles. The physical reason for these advantages is that at high scattering angles good resolution can be achieved without collimators.

Instrument description

A schematic view of the EXED instrument is given in figure 1. It uses the TOF technique at a continuous neutron source originally proposed by Buras [1] in the 1960's, which was further developed and tested in HMI-Budapest Neutron Scattering Centre collaboration [2] in the 1990's.

The main advantages of the TOF methods are that a) high resolution can be achieved in backscattering geometry without the need to use collimators (i.e. at an enhanced detector solid angle and incoming beam divergence) and b) the full relevant *Q*-range can be covered by limited angular access allowed by extreme sample environment equipments.
The chopper system allows a very flexible use of the instrument: As the repetition rate is not defined by the source, bands of arbitrary width of *d*-spacing can be achieved in the forward as well as the backward scattering direction. In addition, a slewing of the chopper phases permits a continuous variation of the wavelength band. In the backward direction it can be combined with a very high resolution. The EXED beam line is unique in the sense that it has access to both the cold and the thermal moderator and takes advantage of a large wavelength band ranging from 0.7 - 20 Å with local maxima at 1.4 and 3.8 Å.

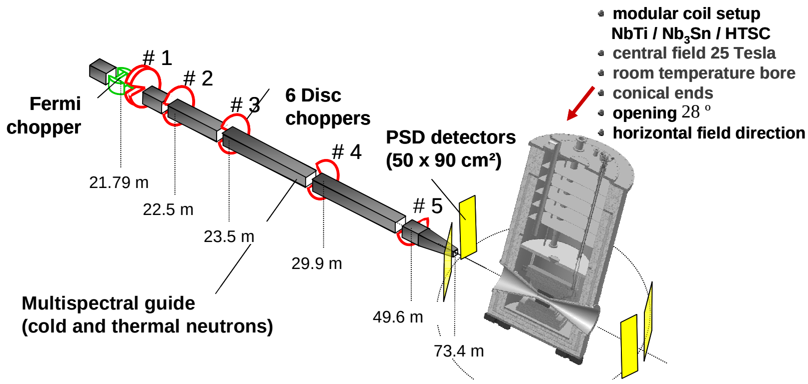

Figure 1. Schematic view of the EXED instrument. The grey tubes correspond to a ballistic neutron guide (straight guide and the compressor [3,4]). The neutron pulses are produced alternatively by a Fermi chopper or by a counter rotating double disk chopper (# 1). The other disk choppers (# 2-4) are frame overlap choppers and a wavelength band chopper (# 5). The position sensitive gas detectors can be moved around the sample and the magnet.

As the magnet has an angular aperture of maximum ± 14°, it can be used in a symmetric as well as in asymmetric neutron beam configuration, which leads to a maximum scattering angle of 28° at one side of the neutron beam (see figures 2a,b).
In the day-one configuration, the instrument will essentially have two purposes: High resolution diffraction and neutron diffraction in highest magnetic fields.

High resolution (powder or single crystal) diffraction

It will be the task of the Fermi chopper to create pulses in the highest resolution domain. The curved Fermi chopper package will allow time resolutions of $\Delta t \approx 6$ µs. In the backward direction (150 – 178°) a total resolution of 0.07 % > $\Delta d/d$ > 0.027 % can thus be achieved at $d \approx 1$ Å with a secondary flight path of 6 m and pin hole collimation (see figure 2a). With a secondary flight path of 2 m, a total resolution of 0.13 % > $\Delta d/d$ > 0.03 % is obtained in backward direction at the same *d*-spacing (see figure 2b). A typical resolution function in backscattering configuration is shown in figure 3a for both secondary flight paths. Using the converging exit of the guide, a flux of about 4 x 10^5 n/cm²/s has been calculated at the sample (2 x 2 cm²) by Monte Carlo simulations [5] of the instrument, taking a wavelength range of 0.7 Å < λ < 1.8 Å and a repetition rate of 60 Hz.

The detector banks are planned to be equipped with tubes with a diameter of 1 cm and an effective length of 90 cm, which are filled with ^3He gas. They shall be position sensitive with a resolution of 1 cm and will cover an effective surface of 50 x 90 cm² (W x H). It will be possible to move them around the sample position or to translate them. In the 2 m position, the two detector banks will cover a 28° scattering angle range, while in the 6 m position only 10° are covered. In the latter configuration, a movable vacuum tank between the sample and the detectors will be used to reduce air scattering.

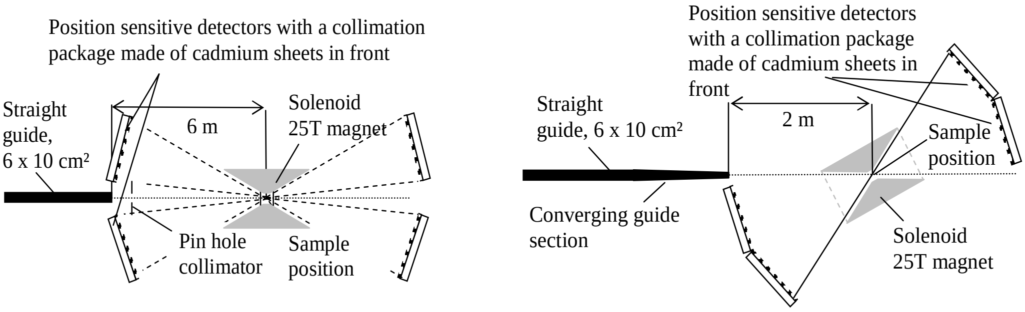

Figure 2. a) Schematic layout of the symmetrical scattering configuration, which can achieve highest resolutions with a secondary flight path of 6 m and a pin hole collimator. b) Schematic layout of the asymmetrical scattering configuration, which can achieve high resolutions with a secondary flight path of 2 - 6 m.

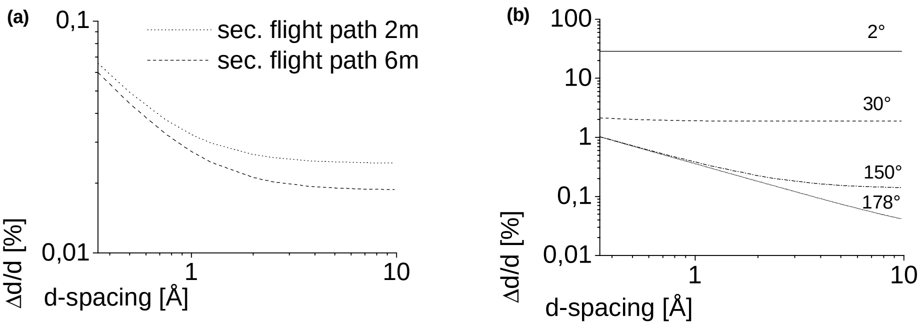

Figure 3. a) Resolution function in backscattering configuration with Fermi chopper for the angle of 2θ = 176° and a horizontal divergence of the incoming beam of 0.15° at 6 m and 0.2° at 2m. b) Resolution function for the case of the double disc chopper used to produce pulses (full line at 2°, dashed line at 30°, dotted line at 150°, dashed-dotted line at 178°). The horizontal divergence of the incoming beam is 0.25°. The secondary flight path is 2 m, sample size 2x2 cm², beam cross section 6x10 cm², ΔL = 1 cm.

Different collimation modules can be applied to further optimise the resolution: the final removable converging guide section significantly increases the flux on the sample. Or, alternatively, a pin hole collimator (see figure 2a) permits the fine tuning of the horizontal and vertical divergences. The *d*-spacings and momentum transfers *Q* accessible with the various detector bank configurations are listed in table 1. The instrument is designed for both narrow-bandwidth and broad-bandwidth operations, the latter achieved by repetition-rate reduction and/or chopper slewing.

Table 1. Various detector bank configurations. For the two first columns the symmetrical arrangement of the detector is supposed with the corresponding angular coverage of 14° on each side of the neutron beam axis, the two last columns correspond to an asymmetrical arrangement with an angular coverage of 28° on one side of the neutron beam axis.

Bank	(171 ± 7)°	(9 ± 7)°	(164 ± 14)°	(16 ± 14)°
d-spacing	(0.35 – 10.1) Å	(2.52 – 571) Å	(0.35 – 10.4) Å	(1.35 – 573) Å
Q	(0.62 – 17.9) $Å^{-1}$	(0.011 – 2.49) $Å^{-1}$	(0.6 – 17.9) $Å^{-1}$	(0.011 – 4.64) $Å^{-1}$

Higher intensity diffraction
For applications that need higher intensity the pulses are created by the double disc chopper with a typical time resolution of $\Delta t \approx 100$ µs, which results in an average total resolution of $\Delta d/d \approx 0.36$ % at $d = 1$ Å in backscattering configuration (see figure 3b). The corresponding flux at the sample is estimated by Monte Carlo simulations to be 3 x 10^6 n/cm²/s with a repetition rate of 60 Hz and a wavelength band range of $0.7 < \lambda < 1.8$ Å. In the backscattering geometry the effect of magnetic fields can be studied on the overall (chemical) crystal structure. Magnetic Bragg peaks need to be studied in the forward scattering direction (*B* approximately perpendicular to *Q*).

The multispectral extraction system
Both cold and thermal neutrons are delivered by a supermirror beam extraction system [6] placed behind the moderators. The guide has various coatings on all sides ($1.5 < m < 2.4$). This new extraction concept is based on a ballistic guide [3,4]: by enhancing the guide cross section by a factor of two in both dimensions, the number of reflections is reduced by about four and thus, an enhanced beam can be delivered over large distances (≈ 80 m). A 17 m long kink section, made of 4 parts that are each offset by 0.1° with respect to the initial beam direction, removes high-energy neutrons ($\lambda < 0.7$ Å). It is important to remember that the choppers become transparent for lower λ values. Apart from the kink section, the guide is essentially straight (60 m) and has a cross section of 60 x 100 mm² (W x H). The guide has four 30 mm gaps that accommodate the single disc choppers (# 2 – 5) and approximately a 300 mm gap for both the double disc chopper (# 1) and the Fermi chopper. At the end of the guide, a 7.5 m long converging exit [7] allows a good focussing on the sample. As an alternative the converging section can be completely removed. This last option allows for a longer secondary flight path of 6 m and small divergences.

The chopper system
The guide system and five disc chopper housings share a common vacuum, only the Fermi chopper, with two different slit packages, has a separate housing and a separate vacuum. The curved Fermi chopper slit package can achieve the highest time resolution with a pulse length of 6 µs FWHM at wavelengths between 0.7 and 5.6 Å. The resolution can be adjusted to the requirements of the specific experiment by extending the pulse length to up to 4000 µs with the help of alternate choppers (lower resolution straight Fermi chopper and the first double disc chopper with variable slit width). The intermediate single disc choppers # 2, 3

and 4 remove higher orders and the last single disc chopper defines the wavelength band (see figure 4).

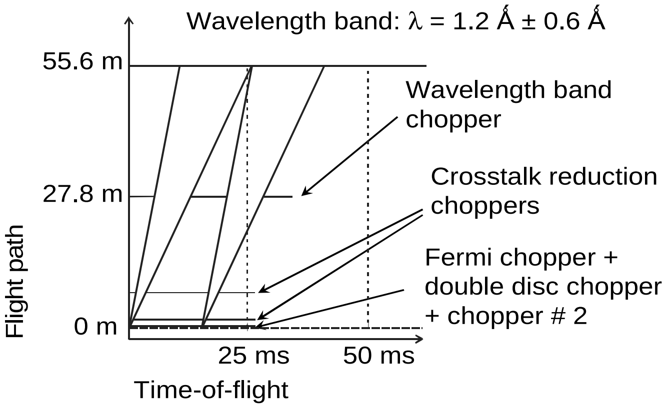

Figure 4. Time-of-flight diagram for the EXED diffractometer using the Fermi chopper to produce the pulses. The double disc chopper runs simultaneously to avoid that two consecutive pulses of the Fermi chopper are transmitted at highest repetition rate. In this example, a wavelength band of $\Delta\lambda$ = 1.2 Å is obtained at a repetition rate of 60 Hz.

Furthermore, the wavelength band can be varied continuously by a so-called slewing of the chopper phases. In fact, the chopper phase can be calculated through

$$\phi[°] = f[Hz]\frac{L[m]\lambda_0[A]}{3.956}\frac{360}{1000}, \qquad (1)$$

where ϕ is the chopper phase, f the chopper frequency, L the distance between the aforesaid chopper and the first chopper and λ_0 the averaged wavelength.

The double discs have two windows – one of the same width as the cross section of the guide and the second one three times that wide. The angular arrangement of the windows on a given pair of discs allows us to select a single pair of windows of identical width, one on each disc, that transmit neutrons by choosing an appropriate relative phase of the two choppers.

Sample environments and further possible extensions

The most important feature is the high field steady state magnet which can create a magnetic field of up to 25 T (later on possibly 40 T). Depending on the range of scattering angle required, the magnet can either be used in a symmetric or an asymmetric neutron beam configuration (see figure 2) or it can be removed from the experiment to allow for usual diffraction work. Additionally to the magnet or separately, further sample environment elements like cryostats creating low or high temperatures ranging from 1.5 – 700 K and pressure cells of up to 20 kbar can be employed. In a medium-term perspective possible extensions are a small angle scattering (SANS) option with a collimator length of up to 6 m and an inelastic neutron scattering option combined with high magnetic fields.

Simulation results

First Monte Carlo simulations using the VITESS package [5] show typical powder pattern diagrams for an Al sample and confirm the theoretically calculated resolution in backscattering direction of $\Delta d/d \approx 3 \times 10^{-4}$ (see figure 5) for the wavelength range of 0.7 Å < λ < 1.8 Å and at scattering angles 156° < 2θ < 179°.

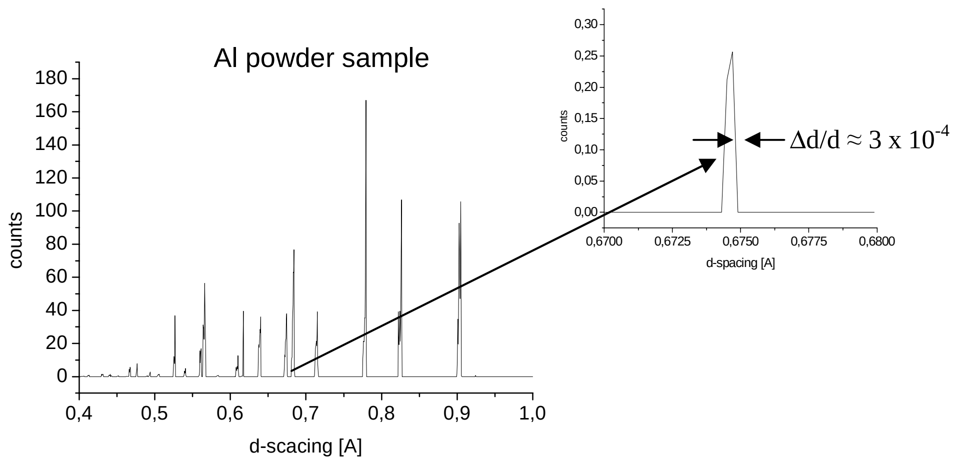

Figure 5. Powder pattern MC simulation results for 0.7 Å < λ < 1.8 Å and 156° < 2θ < 179° as a function of the d-spacing. At $2\theta \approx 176°$ and λ = 1.34 Å (right hand side figure), nearly the highest total resolution of $\delta d/d \sim 3\times10^{-4}$ is obtained.

Concluding remarks

The EXED instrument will be an all-purpose powder and single crystal diffractometer with a main emphasis on extreme environment conditions, primarily very high magnetic fields. It can satisfy high resolution as well as higher flux requirements. The proposed wavelength range is suited to cover crystal and magnetic structure needs. The instrument shall become operational in 2006 and will then be integrated into the BENSC user service instruments of the HMI Berlin.

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