Development of a NRSE spectrometer with the help of McStas - Application to the design of present and future instruments

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Abstract

The flux is still a major limiting factor in neutron research. For instruments being supplied by cold neutrons using neutron guides, both at present steady-state and at new spallation neutron sources, it is therefore important to optimize the instrumental setup and the neutron guidance. Optimization of neutron guide geometry and of the instrument itself can be performed by numerical ray-tracing simulations using existing open-access codes. In this paper, we discuss how such Monte Carlo simulations have been employed in order to plan improvements of the Neutron Resonant Spin Echo spectrometer RESEDA (FRM II, Germany) as well as the neutron guides before and within the instrument. The essential components have been represented with the help of the McStas ray-tracing package. The expected intensity has been tested by means of several virtual detectors, implemented in the simulation code. Comparison between simulations and preliminary measurements results shows good agreement and demonstrates the reliability of the numerical approach. These results will be taken into account in the planning of new components installed in the guide system.

Keywords: Virtual experiments, Neutron optics, Neutron Resonance Spin Echo

1. Introduction

One of the main issues of neutron-based science is the limited brilliance of the source. Research reactors and steady-state sources have a maximum flux of about $10^{15}$ neutrons cm$^{-2}$ s$^{-1}$ in the moderator region. The time integrated flux at new spallation sources like the SNS (Spallation Neutron Source, USA) and the planned ESS (European Spallation Source, Sweden) will be of the same order of magnitude with a peak flux being approximately 30 times higher. Instruments using cold neutrons are typically located several tens of meters apart from the source, which naturally causes a reduction of the intensity.

A major improvement of usable neutron intensities at the instruments was achieved by the invention of neutron guides. However, even with modern optics, angles of total reflection are limited to a few degrees and further losses appear due to finite surfaces roughness and imperfect joints between guide segments. It is therefore important to design the instrumental setup and the neutron guidance in an optimized way, so
that as many neutrons as possible actually reach sample position while losses and background radiation are minimized. Nowadays, improvements of instruments can be planned by numerical ray-tracing simulations, for example by making use of the McStas package [1].

In the following we show, using the example of the quasi-elastic Neutron Resonance Spin Echo (NRSE) spectrometer RESEDA ([2]) at FRM-II (Munich), how Monte Carlo simulations can be used to reveal weak spots of the setup and how, based on this information, improvements of the instrument can be efficiently performed.

2. McStas simulations of a NRSE/MIEZE instrument on the example of RESEDA

Neutron Spin Echo (NSE) is a Larmor precession technique, which means that the energy change of the neutron is not determined directly by measuring its velocity but by evaluating the phase difference $\varphi$ of the neutrons spin in well defined magnetic fields, placed before and after the sample. As $\varphi$ is independent at first order of the velocity of the single neutrons, spin echo techniques allow the use of moderately polychromatic beams, thus enabling higher intensity at the sample position while achieving high energy resolution [3]. This makes NSE an efficient time-of-flight method but constraints the tolerable flight path deviations.

NRSE is similar to NSE. The main difference is that the static magnetic field is replaced by two radio-frequency spin flippers (the so-called NRSE coils), which are separated from one another by a zero field region [4]. At the NRSE-spectrometer RESEDA a neutron guide is placed in the zero field region.

The CASCADe detector ([5]), available at RESEDA, is a large scale Position Sensitive Detector (PSD) with a resolution of $128 \times 128$ (pixel size: $1.5 \times 1.5$ mm$^2$). Its high dynamics makes it also perfectly suitable for Modulation of Intensity Emerging with Zero Effort (MIEZE, see e.g. [6]) applications [7]. Our simulations are especially focused on the investigation of the intensity in order to maximize the neutron flux at the sample position. Therefore spin manipulating devices, like the NSE/NRSE coils and static spin flippers are just considered as slits according to their dimensions.

The principle design of the first arm of RESEDA is shown in Fig. 1. The simulations aim to analyze the following parts of the setup:

- The gap after the velocity selector (1)
- The following neutron guide (2)

Fig. 1. Instrumental setup of RESEDA considered in our studies. The red labels give the McStas components which have been used to represent each individual device. All of them belong to the basic software distribution besides Transmission_polarisatorABSnT which is derived from Guide_gravity and emulates the instrument V-cavity mirror polarizer [8]. The secondary arm is not depicted here, because it is not part of our simulations.
The free flight path in between the RF flippers

The neutron guide between the two NRSE-coils

McStas offers a variety of virtual detectors, the so-called monitors, to survey the properties of the neutron beam. In order to evaluate the beam intensity at relevant positions, a stack of several monitors is installed, which contains wavelength-, divergence- and PSD-monitors with different dimensions.

Furthermore, to get a more universal solution, the selector is not considered as a component in the simulation. The adjustment to the modified wavelength spectrum is rather done by convolving the full spectrum with a triangular distribution as generated by a selector (see Fig. 2). This allows us performing the simulations at arbitrary wavelengths.

To see if the results of the simulations are representative, we compare the simulated intensity values to a gold foil measurement performed at two different positions within the instrument. In a second step, we compare the virtual PSD-monitors with a measurement performed with the CASCADE detector.

3. Results and discussion

The comparison between the measurements and the simulations shows a good qualitative and reasonable quantitative agreement (Tab. 1). Among others, this verifies that the numerical computation, in its very principle, but also the convolution used for simulating the velocity selector deliver applicable results.

| Position   | Experimental $[10^8 \text{ cm}^{-2}\cdot\text{s}^{-1}]$ | Simulated $[10^8 \text{ cm}^{-2}\cdot\text{s}^{-1}]$ | Deviation [%] |
|------------|---------------------------------------------------|------------------------------------------------|---------------|
| Before selector | 46.7 | 45.3 | 3.0 |
| After selector | 3.56 | 3.69 | 3.7 |

Table 1. Results for the measured and simulated intensities, respectively before and after the velocity selector, for a neutron wavelength $\lambda = 4.8 \text{ Å}$.

Moreover, the simulation of the CASCADE detector (Fig. 3 a) shows that the beam geometry is also in good accordance with the actual measurement (Fig. 3 b). The measurement of the direct beam was performed with a slit of size $10 \times 20 \text{ mm}^2$ at the sample position. The evaluation was only done in a section of $25 \times 25 \text{ pixels}$ of the detector, where the events appeared with sufficient statistics.

By comparing the simulations with the count rate of the CASCADE detector, we can make a good guess of the detection efficiency. In our case, for neutrons with a wavelength of $\lambda_0 = 4.8 \text{ Å}$ and $\Delta \lambda/\lambda_0$ (FWHM)
= 0.13, we obtain an efficiency of 25%. This value is within our expectations.

Fig. 3. Image section (25 × 25 pixels) of the PSD placed 1m behind the sample position (a) measurement with CASCADE (b) simulation. The apparent inhomogeneity between the two datasets is due to a slight optical misalignment of the slit system during the experiment. This vertical shift can not be ascribed to gravity as this would only lead to a displacement of the intensity in −y direction by less than 500 μm.

Furthermore, we were able to show that installing a neutron guide in the zero field region between the two NRSE coils increases the intensity at the sample position by ∼ 30%. This order of magnitude has also been confirmed by test measurements. Interestingly, this new optical element has no effect on the divergence of the beam with respect to a classical setup without guide, as revealed by the simulation (see Fig. 4) and by the conservation of the beam polarization when working in the spin-echo mode, which would be altered otherwise. Based on this information, we decided to adopt this configuration and will run further simulations in order to find an optimal neutron guide for such a purpose.

Fig. 4. Simulated intensity distribution for the CASCADE detector placed in the direct beam 1m behind the sample position, (a) with neutron guide between the NRSE coils and (b) without.

4. Conclusions

We have shown that the quality of the simulations provides us with a very powerful tool to investigate the performance of the RESEDA beam line, especially the intensity distributions at the critical parts of the instrument. The successful simulations will allow us to improve the various components of RESEDA. In the near future we intend to introduce guide geometries with various supermirror coatings and tapering in order to improve the performance of RESEDA. In addition several concepts for focusing the neutron beam will be considered. The latter will play an important role for the use of smaller samples. It is worth noting that
such an approach, validated by its application to the case of an existing spectrometer, already offers a solid ground for designing future instruments ([9]) and determining applicability ranges of existing techniques.

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