POWTEX — updated design of the high-intensity TOF diffractometer

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During the BMBF funding period since 2007, POWTEX has undergone many changes and improvements. The optimized chopper system and the increase of solid angle detector coverage were reported last year. This year, we want to address the dramatic changes to the detector system, unavoidably caused by the $^3$He shortfall, as well as our improvements to the neutron guide design and our contribution to the open source Monte Carlo instrument simulation program VITESS. The proposal for the follow-up funding of POWTEX by the BMBF from 2010—2013 has been recently submitted.

$^3$He: At present, the so called $^3$He crisis is becoming aware to a broader public, and it is not mere coincidence that this crisis is the central theme in Schätzling’s last novel called “Limit”. While maybe interesting to read in a novel, for POWTEX and many other parts of science the shortage of $^3$He is a sad reality that came true long before attracting public attention.

Because the reasons have been elaborately discussed already in all kinds of literature [1, 2], we want to address herein how the POWTEX project plans to deal with this shortage. It is obvious not possible to buy the demanded 3700 l $^3$He within the next years. Currently, many alternative neutron detector concepts are under investigation by different groups worldwide. For POWTEX, because using thermal neutrons with a wavelength down to $\lambda = 1.0$ Å and the huge coverage in detector solid angle (large detector surface) of 10 sr the $^3$He-PSD tubes were an ideal choice because of their high detection efficiency for such wavelengths and the formerly low price/area. Thus, the search for alternative concepts will meet the same conditions. Gas based detectors using BF$_3$ suffer from a low detection efficiency and there is no prospect of an improvement to this. Semiconducting detectors are in very early design states and do not match POWTEX’s short time scale for finding a proper solution. The remaining methods are scintillation detectors using $^6$Li or $^{10}$B. While the concept of the CASCADE detector is far too expensive for our huge detector coverage, two promising concepts can be found, namely the Wavelength-Shifting-Fibre (WSF) concept and the Blade concept. In order to investigate and proof the applicability of both concepts to the POWTEX requirements a prototype will be build of each method. Only by this, a decision for the future POWTEX detector concept can be made. The WSF-concept uses $^6$Li/ZnS to convert neutrons to photons which can be captured by a wavelength shifting fibre and transported to a photo-multiplier. This type of detectors is currently installed at two instruments, namely POWGEN, which has similar requirements to POWTEX, and VULCAN, both located at the SNS. The Blade concept uses a $^{10}$B converter under grazing incidence in order to yield a higher neutron detection efficiency.

Neutron guide: A detailed description of the initial instrument design, including the neutron guide system, has been published in [3]. In general, the highest neutron flux can be achieved using a double elliptic neutron guide geometry. In the case of POWTEX, the neutron guide system will be intersected by the pulse chopper (opening of 1x1 cm$^2$), such that it is a needles eye between two separate elliptic guides.

Next to the choice of the best geometry the super-mirror reflectivity is of crucial importance while optimizing the neutron beam properties. These are namely, a high and equally distributed flux and in contradiction to this, a homogeneous and gaussian-like divergency distribution at the sample position of 1x1 cm$^2$. The neutron guide geometry, as shown in FIG. 1 (left), has been chosen to have a maximal transported divergency (FWHM) of 0.5$^\circ$ for neutrons with a wavelength of $\lambda = 1.0$ Å. By this, the ratio of both elliptic half-axes is already fixed.

The super-mirror reflectivity can be characterized by its total reflection properties up to a critical momentum transfer perpendicular to the surface ($Q_c = 4\pi\lambda^{-1}\sin(\theta)$). This is usually expressed by the index $m = Q_c/Q_{c}(^{58}Ni)$ that is relative to $^{58}$Ni. In FIG. 1 (left) this index is represented by the color and along the flight path x it changes symmetrically to the pulse chopper. The higher the index, the higher is the super-mirror’s maximal angle of total reflection for a given wavelength. Due to the symmetric arrangement of the two ellipses (the second one is shrunk by a constant factor in all dimensions, leaving the optical properties unaltered), the focal points are coinciding in the center of the pulse chopper. The following considerations are characteristic for such coupled elliptic systems with an even number of guides and a needles eye (pulse chopper) in between. Assuming an
ideal point source, neutrons with a small divergency are reflected for the first time in the half-ellipse near the chopper. Hereby, owing to the elliptic shape, the divergency is increased. After passing the chopper, the neutron is scattered gain in the half-ellipse near the chopper, but this time the divergency is (almost) reduced to the initial value. Such neutrons reach the sample position with the maximal divergency as defined by the geometry of the ellipses for the lowest wavelength (1.0 Å). In accordance to this, neutrons starting with a high divergency are always reflected on the half-ellipse far away to the chopper. In order to avoid such neutrons with a high divergency the areas far away from the chopper are absorbers while neutrons with a small initial divergency are transported using high m-values near the chopper.

Owing to this, a minimum divergency can be achieved by applying the super-mirror coating only to both half-ellipses near the chopper. Of course, this leads to a dramatic loss in neutron flux. Therefore, and also due to the fact, that the FRM II is not a point source, one needs to apply further corrections, e.g. the choice of the other two focal points. While the second ellipse will be focused on the sample position, the focus of the first ellipse will lie behind the area with the highest neutron flux inside the reactor in order to transport neutrons coming from any position of the source. Furthermore, the super-mirror m-values have to be adjusted with regard to this. In order to simulate and optimize the neutron guide system, the open source software VITESS (Virtual Instrumentation Tool for Neutron Scattering at Pulsed and Continuous Sources) working with the Monte Carlo technique is used. FIG. 1 (right) compares two simulations with similar neutron flux (1x1 cm² sample; \( \lambda = 1.0 - 2.4 \) Å). The optimized profile is more homogeneous and has a smaller FWHM.

VITESS Instrument Simulations: In last year’s report we presented a diffractogram simulation based on the analytical description of the instrument parameters of POWTEX. By this, we gained experience on simulating such diffractograms which will also help to do the data analysis of the experimental diffraction data once POWTEX is in operation. In early summer 2009 we started to focus our work on numerical simulations of such diffractograms. Of course, an excellent choice for this is the open source project VITESS that is already used for the simulation of the neutron guide system and that also has support for the simulation of a diffraction process. Thus, the final goal is to simulate the complete instrument. In contrast to conventional neutron diffractometers at research reactors being monochromatic instruments, POWTEX will be the first pulsed instrument located at a continuous source and used for diffraction experiments by using a wide wavelength spectrum combined with time-of-flight analysis and a huge detector coverage. For this reason, one of our contributions was to implemented the evaluation of the diffraction process as a function of the two parameters scattering angle and wavelength in [4] (module eval_elast2). The preliminary results can be seen in FIG. 2.

Funding: The RWTH Aachen and the Forschungszentrum Jülich submitted a proposal for a BMBF funding from 2010 to 2013 in order to build the POWTEX instrument, while our colleagues at the University of Göttingen proposed to build the sample environments for the geo-sciences.

FIG. 2: Simulation of a POWTEX diffractogram using VITESS (\( \text{RhFe}_3\text{N}, \) perovskite-like, space-group \( \text{Pm}3\text{m} \)).