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Wide-wavelength band powder diffraction at the long pulse source ESS

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Abstract

Within the ESS design update programme funded by the german Federal ministry of education and research we investigate the performance of an instrument concept for powder diffraction at the long pulse sourse of the ESS, which promises the best applicability to most general and standard needs from science.

Since time-of-flight (TOF) powder diffraction typically requests for better resolution than given by the natural long pulse of the ESS, it will be mandatory for many applications to produce shorter pulses by choppers. The position of a first chopper at a minimal distance of 6 m from the moderator requires a rather long instrument of 150 m, when using a single pulse with the given 14 Hz source frequency. Alternatively, more pulses can be generated filling the TOF frame of 71.4 ms with an accordingly wider wavelength spectrum and a shorter instrument. A wide wavelength spectrum is of interest to exploit the backscattering option with high resolution. Furthermore, a large Q-range is desirable in order to obtain pair distribution functions from total scattering. Using a bispectral moderator additional cold neutron flux can favorably extend the thermal flux spectrum [1]. In order to account for varying resolution requests, a most flexible solution for the pulse shaping chopper system can be set by counter rotating disks; with different sets of openings and relative change in phase the time of flight resolution can be varied from 10 μs to 1 ms. The aperture of the chopper system at 6 m from the moderator defines an image of 5 to 10 mm diameter with an initial divergence of +/- 0.6°, a phase space density, which can be transported by elliptic guides to the sample position of similar size with only little losses by current neutron guide qualities as shown by our VITESS Monte Carlo simulations. Moreover, the chopper's aperture represents an important eye of the needle for reducing background by more than two orders of magnitude and will also help to design more cost efficient shielding. While the final detector choice may depend on many currently ongoing developments, it is clear that there will be a request for large solid angle coverage with a high resolution adapted to typical small sample sizes. Thus the instrument will also be usable for single crystal TOF Laue diffraction. Based on this new and flexible instrument concept, the performance, particularly for powder diffraction looks very promising at the brightest future neutron source.

[1] G. Zsigmond, K. Lieutenant, F. Mezei, Neutron News 13.4 (2002) 11.