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Virtual experiments: Combining realistic neutron scattering instrument and sample simulations

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ABSTRACT

A new sample component is presented for the Monte Carlo, ray-tracing program, *McStas*, which is widely used to simulate neutron scattering instruments. The new component allows the sample to be described by its material dynamic structure factor, which is separated into coherent and incoherent contributions. The effects of absorption and multiple scattering are treated and results from simulations and previous experiments are compared.

The sample component can also be used to treat any scattering material which may be close to the sample and therefore contaminates the total, measured signal.

1. Introduction

Neutron scattering provides a large variety of instruments to probe structure and dynamics of condensed matter. However, the technique is flux limited, which motivates continuous efforts to improve both the flux and the overall efficiency of the instruments. Therefore both analytical and numerical methods are used in order to determine optimal instrument configurations.

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For simple neutron beam configurations, analytical models are available to describe the different neutron optics elements of the instruments, which modify the characteristics of the beam (e.g. divergence, wavelength spread, spatial and time distributions). This approach is valid for individual elements such as guides [1,2], choppers [3,4], Fermi choppers [5,6], velocity selectors [7], monochromators [8–11], and detectors [12–14]. In the case of a limited number of optical elements, the so-called acceptance diagram theory [2,15,16] may be used, within which the neutron beam distributions are considered to be homogeneous, triangular or Gaussian. However, real neutron instruments are composed of a large number of optical elements, and this brings additional complexity by introducing strong correlations between neutron beam parameters like divergence and position – which is the basis of the acceptance diagram method – but also wavelength and time. The usual analytical methods, such as phase-space theory, then reach their limit of validity in the description of the resulting effects.

In order to cope with this difficulty, the simulation of neutron spectrometers may be performed using Monte Carlo methods (for a general review, see Ref. [17]), which are commonly used for the description of microscopic physical processes such as absorption, scattering or reflection. Integrating these events over the neutron trajectories results in an estimation of measurable quantities characterizing the neutron instrument. Moreover, using importance sampling reduces the computation time and gives better accuracy. Early implementations of the Monte Carlo method for neutron instruments used *home-made* computer programs (see [18,19]) but, more recently, general packages have been designed, providing models for most optical components of neutron spectrometers. The most widely-used packages are NISP [20], ResTrax [21], McStas [22], Vitess [23], and IDEAS [24], which allow a wide range of neutron scattering instruments to be simulated. The neutron ray-tracing Monte Carlo method has been used widely for guide studies [15,25,26], instrument optimisation and design [27–29]. Since Monte Carlo ray-tracing gives accurate estimates for the flux and resolution, it enables optimum parameter sets for the instrument to be determined, which is not always possible with classical analytical methods. In addition, as for any instrument, in certain experiment configurations, the experimental signal may be contaminated due to various contributions to the total signal coming either from the instrument or from the sample such as background, coherent and incoherent scattering, self-shielding and multiple scattering.

Some of these questions may be tackled directly with Monte Carlo neutron scattering instrument simulations but others depend intrinsically on the sample. Indeed the experimental signal is the convolution of the instrument response and the signal due to the interaction between neutrons and the sample (structure and dynamics). Separating instrument and sample contributions requires both to be known in detail. As a consequence, the concept of virtual experiments [30], that is simulations including accurate models for both instruments and samples, has recently become a logical and important extension of Monte Carlo neutron scattering instrument simulations. For instance, for the multiple scattering contribution, no experimental method makes it possible to accurately measure this contribution, even though it can become significant at low q momentum transfers, for example, below the first diffraction maximum in liquids and glasses, where the single scattering coherent signal is weak in most materials. This is why attempts have been made to reduce the multiple scattering contribution by partitioning the sample with absorbing layers, as in [31]. However, this is not always applicable thus making the simulation approach very valuable.

Many methods and approximations have been developed to quantify these contributions and, for example, analytical formulae exist that can be applied for correcting multiple scattering [32]. However, these methods remain limited in their capability to handle strongly cross correlated neutron parameter states, which originate from, e.g. complex instrument and sample geometry descriptions. A number of previous Monte Carlo codes [33–36] have been designed to evaluate single and multiple scattering, absorption, self-absorption and transmission factors. However, they are often limited regarding, e.g. the instrument geometry, the sample environment and shape, or the type of experiment (diffraction, time-of-flight).

This paper presents the component *Isotropic_Sqw* in the *McStas* code [22]. It allows the sample scattering function $S(q,\omega)$, where q and ω are the wavevector and energy transfers, to be included in a Monte Carlo neutron scattering instrument simulation. This implies that both elastic and inelastic scattering are taken into account, for the coherent and incoherent processes. The object of the study is to demonstrate that complex instrument descriptions can be coupled to sample simulations in order to produce virtual experiment results that compare with real measurements.

In the next section, the general principle of sample simulations, dedicated to the global simulation of neutron scattering experiments, is explained. In Section 3 we compare a virtual experiment on liquid Rb with the direct analysis of the corresponding experimental data and we focus on the possibilities for handling multiple scattering in order to demonstrate the usefulness of such a numerical approach for the analysis of experimental data. While the rubidium work does not reveal a particular high level of multiple scattering, we regard the work of Copley [31] as a reference in this context. Finally we discuss the results and give some perspectives of the present work.

2. Sample simulation for virtual neutron scattering experiments

With a view to performing virtual neutron scattering experiments, a new sample component has been developed for the *McStas* package [22] in order to simulate neutron scattering from any isotropic material such as liquids, glasses (amorphous systems), polymers and powders (currently, mono-crystals cannot be handled by this component). The component *Isotropic_Sqw* treats coherent and incoherent neutron scattering and may be used to model most materials, including sample environments with concentric geometries. The method presented here for handling neutron interaction with isotropic materials is similar in many respects to the earlier MSC [33], Discus [34] and MSCAT [35] methods, but the implementation presented here is part of a more general treatment of a sample in an instrument.