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A new gradient monochromator for the IN13 back-scattering spectrometer

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Abstract

We present new McStas simulations of the back-scattering thermal neutron spectrometer IN13 to evaluate the advantages of a new temperature gradient monochromator relative to a conventional one. The simulations show that a flux gain up to a factor 7 can be obtained with just a 10% loss in energy resolution and a 20% increase in beam spot size at the sample. The results also indicate that a moderate applied temperature gradient ($\Delta T \simeq 16\,\mathrm{K}$) is sufficient to obtain this significant flux gain.

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Keywords: Monte Carlo simulations; Neutron instruments; Imperfect crystals

1. Introduction

The main peculiarity of the neutron back-scattering (BS) spectrometer IN13, installed at the Institut Laue Langevin (Grenoble), is the possibility to access a large window of momentum transfers (0.2–4.9 Å^{-1}) with a high and almost Q-independent energy resolution (~8 μeV). This makes the instrument particularly attractive for soft-matter dynamics investigations [1–3]. However, the low neutron flux at the sample requires long acquisition times and large amounts of

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sample in order to achieve adequate statistics. Originally, the instrument was designed mainly for tunneling studies in crystals [4], and for this kind of application a very high intensity was not a strong prerequisite. On the contrary, when dealing with complex macromolecular systems as polymers and biomolecules [5], the small amount of sample usually available imposes some stringent constraints on the flux requirements. Furthermore, due to the appreciable amount of quasielastic scattering observed in these systems, a high neutron flux at the sample with no significant degradation in energy resolution is needed to discriminate with sufficient accuracy between the elastic and quasielastic scattering contributions. A possible way of increasing the flux, and at the same time keeping the high-energy resolution of IN13, is to modulate the *d*-spacing of the monochromator along its thickness. This can be obtained by applying a temperature gradient [6] to the monochromator crystals. Indeed, experimental tests performed years ago by Barthelemy et al. [7] indicated that some gain in neutron flux could be achieved with this method. We decided to perform a detailed simulation of IN13 with a temperature gradient monochromator, with the goal of a quantitative estimate of the flux gain.

The increasing complexity of modern neutron scattering instruments nowadays requires the use of powerful simulation tools, in particular, ray-tracing methods, to optimize the overall performances by numerical prediction of the different relevant parameters (flux, resolution, divergence, etc.) [8,9]. Indeed, the effects encountered in the last generation instrumentation are so subtle that the validity limits of purely analytical descriptions can be soon reached. Furthermore, numerical analysis is also becoming a common tool during the conception and design of neutron optical components and in instrument development, due to the high cost of such projects, both in terms of money and time. The upgrade of a full spectrometer can be speeded up by carrying out simulations to optimize the various instrument development steps. The most accurate way to simulate the profile of complex configurations is the Monte Carlo (MC) technique. Amongst recent MC codes for neutron simulation, the freely available scientific software McStas package [10] has proven to be reliable and, at the same time, rather flexible. It can be used in many different configurations [11], since it is relatively simple to build up new specific components, or even a whole instrument, from a standard McStas one.

In this work, MC simulations have been carried out to investigate the effects of the insertion of a temperature gradient monochromator on both flux and resolution. Results with the gradient monochromator are compared to those obtained in the current configuration. The work is structured as follows: we describe the essential components of the current configuration of IN13, followed by the simulation model for this configuration. We introduce a new McStas code for the temperature gradient monochromator, and present the gain in intensity and the effects on resolution that can be obtained by applying different temperature gradients.

2. Main technical characteristics of the IN13 spectrometer

Fig. 1 shows the general layout of the BS spectrometer IN13. The instrument is based on the combination of a (4 2 2) CaF_2 crystal monochromator oriented in near BS geometry with similar (4 2 2) CaF_2 crystal analyzers placed in exact BS geometry. The monochromator has a size $4.95 \times 13.5\,cm^2$ and is composed of three high-quality crystals 1-cm thick and with mosaicity $\eta_M = 2.5'$. The analyzers are composed of crystals of individual size $2 \times 2\,cm^2$, thickness 0.16 cm and mosaicity $\eta_A = 2.5'$, organized in seven spherical segments, each covering a solid angle of 0.18 sr, and a spherical cap covering the small scattering angles.

A vertically curved pyrolytic graphite deflector, composed of nine crystals of size $1.5 \times 5\,cm^2$ and average mosaicity $\eta_D = 45'$, focuses the beam diffracted by the monochromator onto the sample. Typical values of monochromator–deflector, deflector–sample and sample–analyzer distances are 1.48, 2.76 and 1 m, respectively.