ICANS-XV
15th Meeting of the International Collaboration on Advanced Neutron Sources
November 6-9, 2000
Tsukuba, Japan

9.2

Monte Carlo simulation of crystal monochromators/analysers - Applications for time-of-flight backscattering spectroscopy with high resolution

G. Zsigmond[1,*], F. Streffer[1], D. Wechsler[1], F. Mezei[1,2]
[1]Hahn-Meitner-Institut Berlin, Glienickerstr. 100, D-14109, Berlin, Germany
[2]Los Alamos National Laboratory, Los Alamos, NM 87545, USA
*E-mail: zsigmond@hmi.de

Abstract

It is shown that Monte Carlo simulations of a crystal monochromator/analyser by means of the Virtual Instrumentation Tool for ESS (VITESS) offer a correct basis for the computation of the resolution function of crystal analyser backscattering spectrometers. It was demonstrated that Monte Carlo simulations can be used to explore a wide range of properties inaccessible to experimental observation. Relying on comparisons of MC computed and measured data of vanadium and superfluid helium, a bench marking of the programme codes was performed practically limited only by the statistics of the experimental calibration data. The comparison of moderator performances was an important application of instrument design by means of the computer simulations. The energy resolution can be improved by combining a Si(111) crystal analyser system and a fast-chopper modulated moderator pulse. The analysed intensity can be increased by large high precision focussing geometries.

1. Introduction

The perspectives of new spallation sources (ESS, SNS, JSNS) give opportunity to build crystal analyser instruments with highly optimized geometry. Our example is the future Backscattering Spectrometer at SNS using 84 m primary flight path (L_1) and a large 7.5 m^2 analyser surface area in focussing geometry (L_2 = 4.679 m). The details on the geometry can be read in reference [1]. Three types of pulseshapes from I. a decoupled poisoned LH2 moderator, II. a coupled moderator, III. a coupled moderator with modulating choppers, were combined with two focussing options for the Si(111) analyser: a) constant λ focussing b) constant flight path length. We compared intensities and resolutions for the six cases.

2. Results and conclusions

The time pulses (see data of Iverson in [2]) corresponding to 6.267 Å analyser wavelength are shown in Fig. 1. The shapes and intensities of the decoupled and coupled moderator signals are conserved at 6 m from the LH2 moderator. The intensity ratio is 1:8 (see values in brackets). The FWHM-s are 70 μs for the decoupled and 240 μs for the coupled moderator. A third pulse option was analysed by using a 250 Hz counter-rotating fast disk chopper pair for the coupled moderator at the distance 6 m [3]. The chopper window width was 6 cm larger than the guide exit width in order to gain transmitted intensity within 70 μs FWHM of the

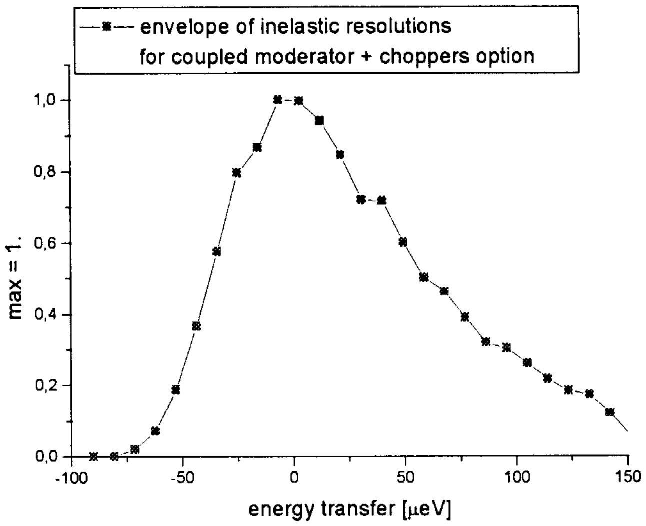

Fig.4.: Intensity versus energy range.

resulting signal. The intensity of the chopped pulse is 2× the intensity of the decoupled option. The silicon crystal analyser used in the MC simulation was a 2° scattering angle interval section, consisting of horizontal 19 and vertical 240 flat elements ($0.5\times0.5 cm^2$) oriented (111). The main Bragg angle was 88.0° and the *d*-spacing spread 3.5×10^{-4}. In Fig.2 the elastic energy resolutions for small scattering angles can be read for a constant λ focussing geometry. The integral intensities of the detector signals give the same ratio 8:2:1 as in Fig.1. However, the decoupled moderator provides poorer resolution than the coupled moderator–modulating chopper combination. (Two 70 μs FWHM pulses can yield different resolutions in MC due to the shape of the time distributions.) By setting the choppers to zero frequency, an additional option of 8 μeV elastic resolution can be obtained (IRIS 15 μeV) having 8 times larger intensity. There is an additional freedom to modulate the pulse with any frequency between 0 – 250 Hz. In the case shown in Fig.2, all 4560 crystal elements were exactly oriented to give 88.0° Bragg angles for trajectories emerging from the sample centre ($3\times3\times3 cm^3$). This arrangement yields constant 6.267 Å analysed wavelength with a spread 0.003 Å FWHM, to cost of changes in the secondary flight path length (in function of vertical angles). This last negative effect turned out to be important for the large analyser arrangement. Therefore a constant L_2 focussing geometry option was studied. The sample centre and detectors being close relative to the 2.50 m radius of the crystal analyser, an elliptical focussing can be effectively achieved by a spherical geometry (demonstrated by simulation with small vertical angles giving the same ideal resolution). The resolution could be improved to 2.9 μeV and 3.3 μeV, respectively, as can be seen in Fig.3. The analysed wavelength distribution computed was similar to that in the λ focussing case, consequently, a time focussing geometry was practically achieved by using a spherical analyser. The dynamic range for the coupled moderator–modulating chopper setup was found to be close to that of the decoupled case (Fig.4).

References

[1] K. W. Herwig, http://www.sns.anl.gov/ScatInst/Instrument/BaSp.htm
[2] E. B. Iverson, http://www.sns.anl.gov/RDProjects/project/moderator/moderator.htm
[3] G. Zsigmond et al, Nucl. Instr. and Meth. in Phys. Res. A, accepted

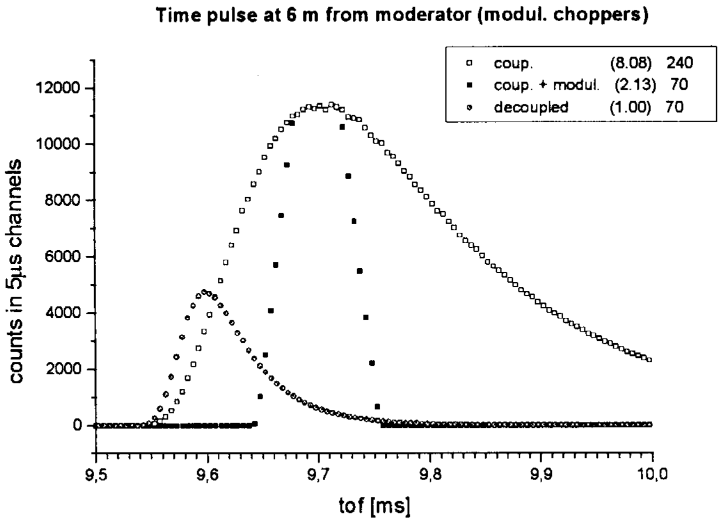
Time pulse at 6 m from moderator (modul. choppers)

Fig.1: Pulses at 6 m.

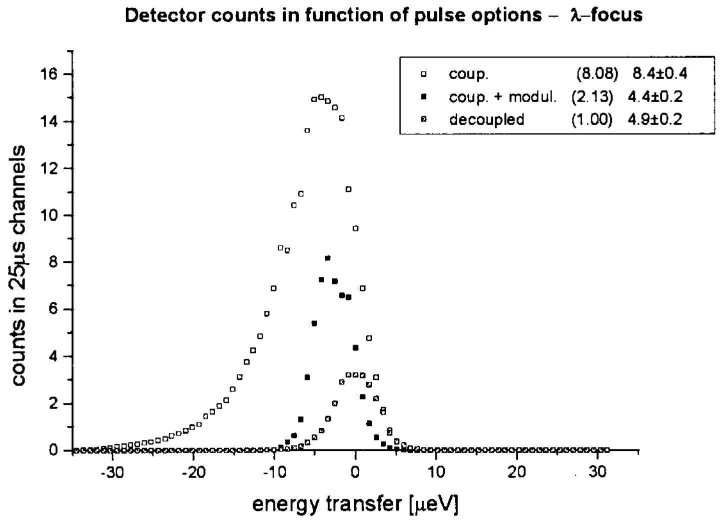
Detector counts in function of pulse options – λ-focus

Fig.2: λ focus (see text).

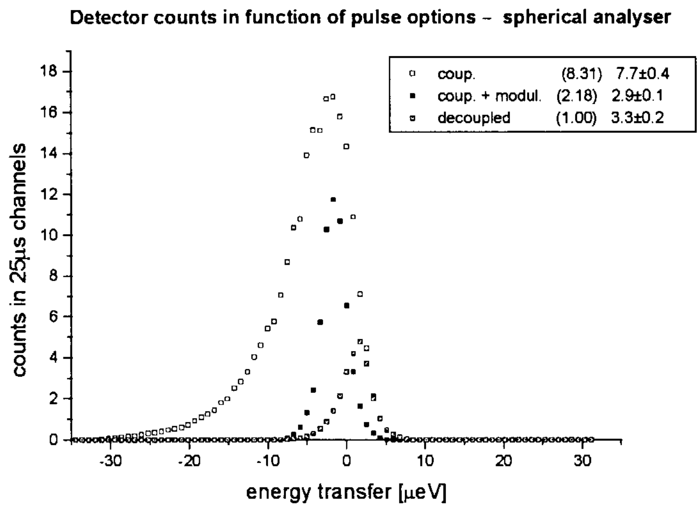
Detector counts in function of pulse options – spherical analyser

Fig.3: L_2 focus (see text).