Appl. Phys. A 74 [Suppl.], S224–S225 (2002) / Digital Object Identifier (DOI) 10.1007/s003390201740

Applied Physics A
Materials
Science & Processing

Monte Carlo simulation of single-crystal spectroscopy and diffraction at spallation sources

G. Zsigmond[1,*], **K. Lieutenant**[1], **F. Mezei**[1,2]

[1] Hahn-Meitner-Institut Berlin 14109, Berlin, Germany
[2] Los Alamos National Laboratory, Los Alamos, NM 87545, USA

Received: 19 July 2001/Accepted: 12 March 2002 – © Springer-Verlag 2002

Abstract. The simulation package VITESS offers an advanced Monte Carlo technique for the numerical calculation of flux, count rates and resolution functions for single-crystal neutron spectrometers and diffractometers. The comparison of various moderator (decoupled-poisoned, decoupled and coupled) and target (short and long pulse) options for backscattering spectrometers and single-crystal diffractometers at the future European Spallation Source (ESS) is one of the main applications of VITESS. Single crystal instrument components highly determine both the wavelength selection and the intensities measured at the detectors. Both intensity and beam divergence are highly influenced by the focussing geometry of the monochromators or analysers. Detailed resolution calculations are presented. Crystal-sample modules were implemented to analyse the options mentioned above for single-crystal diffraction at the ESS. We made a detailed line-shape analysis of the detector signals.

PACS: 29.30.Hs; 29.85. +c; 29.25.Dz

Monte Carlo simulations are used for detailed resolution calculations of time-of-flight backscattering (TOF-BS) spectrometers in a wide dynamic range where experimental methods are not possible and also implemented in neutron scattering instrument design and development [1]. The resolution performance of the Backscattering Spectrometer at SNS has been analysed by MC using VITESS as reported in [2]. We report here on simulation results for a similar TOF-BS instrument at the European Spallation Source (ESS) (For BS at ESS see also [3]). The very high flux of short wavelength neutrons of the short pulse target of ESS will give the opportunity for very high resolution single crystal applications [4]. First results of MC simulations are here presented. More about the MC code can be found on the VITESS-website at HMI [5].

*Corresponding author.
(Fax: +49-30/8062-2523. E-mail: zsigmond@hmi.de)

1 TOF backscattering

A primary flight path (L_1) of 84 m and a large spherical Si(111) analyser ($L_2 = 4.679$ m) were used [2]. Two types of ESS pulse-shapes [6]: a) a decoupled poisoned and b) a coupled LH2 moderator combined with two 250 Hz counter-rotating modulating choppers at the distance 6 m from moderator were simulated. The FWHM-s are 60 µs for the decoupled and 240 µs for the un-modulated coupled moderator. The modulating chopper window width was 10 cm, larger than the 3.5 cm guide exit width in order to gain transmitted intensity within 70 µs FWHM of the resulting signal. The time pulses corresponding to 6.267 Å analyser wavelength are shown in Fig. 1. The intensity ratio is 1.6 (see values in brackets). The silicon crystal analyser used in the MC simulation was a 2° scattering angle interval section, consisting of $19 \times 240 = 4560$ horizontal and vertical flat elements (0.5×0.5 cm^2) oriented (111). The energy resolution of the used spherical analyser depends on the d-spacing spread as shown in Fig. 2. The main Bragg angle was set to 88.0° and the d-spacing spread to 0.01%. The resulting elastic en-

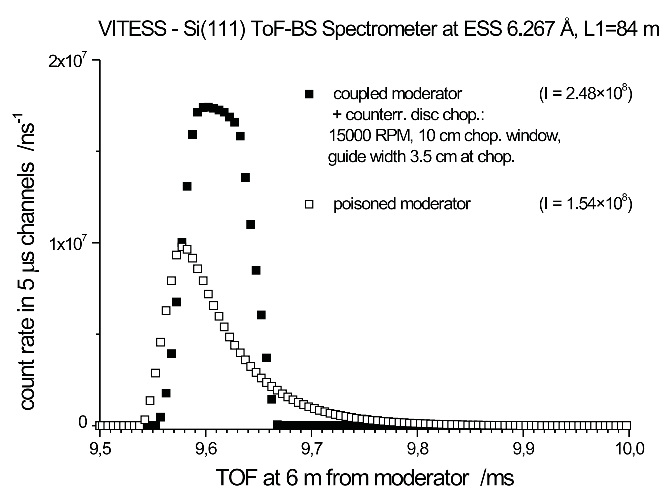

Fig. 1. Pulses at 6 m from moderator on the TOF-BS instrument

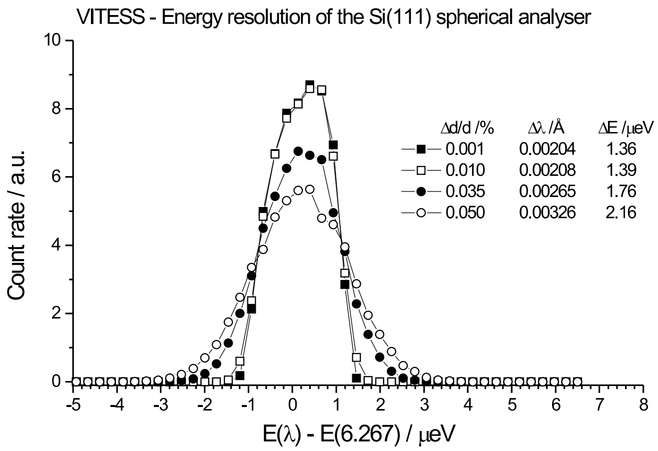

Fig. 2. Secondary energy resolution (spherical analyser) as function of $\Delta d/d$

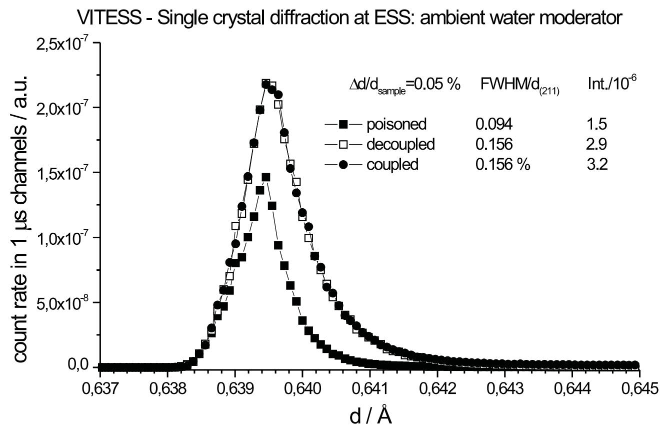

Fig. 4. Performance of single crystal diffractometers at ESS as function of moderators

ergy resolutions for small scattering angles can be read in Fig. 3.

In conclusion, the coupled moderator-modulating chopper combination (70 μs) provides the same resolution as the decoupled moderator (60 μs) due to the absence of the late neutron tail. The integral intensities of the detector signals give 85.2 and 54.1 n/s i.e. the same ratio as in Fig. 1.

2 Single-crystal diffraction

Single crystal diffraction at spallation sources uses the time-of-flight Laue technique to access large 3-D volumes of reciprocal space in a single measurement. In order to make a detailed analysis of the signal shape/asymetry, MC simulations were done using VITESS for decoupled poisoned, decoupled unpoisoned and coupled ambient water moderators at the ESS. The moderator-sample distance was 50 m, the secondary flight path was 1.575 m and the beam beam divergence was reduced only to illuminate the sample. The single crystal sample was *bcc* type, $a = 3$ Å, with one edge oriented in beam direction. The resolution of the PSD was 3×3 mm^2. In Fig. 4 the TOF has been converted to d-spacing corresponding to $2\theta = 50.57°$ scattering angle. The shown (211) reflection corresponds to 0.546 Å wavelength. It can be concluded from Fig. 4 that this technique combined with the ESS short pulses makes possible to achieve very high d-spacing resolutions of 0.09%–0.16%. In addition we demonstrated that, by using ESS coupled moderators, the intensity gets 2.13 times larger then in the poisoned case – at 1.66 times resolution FWHM – and only 9% larger as in the decoupled case at the same resolution (the difference being mainly in the tails at the reflected wavelength). This yields a figure of merit ($I/\Delta E^2$) ratio: $Q_p/Q_c = 1.3$. The intensity ratio supports the use of a coupled moderator.

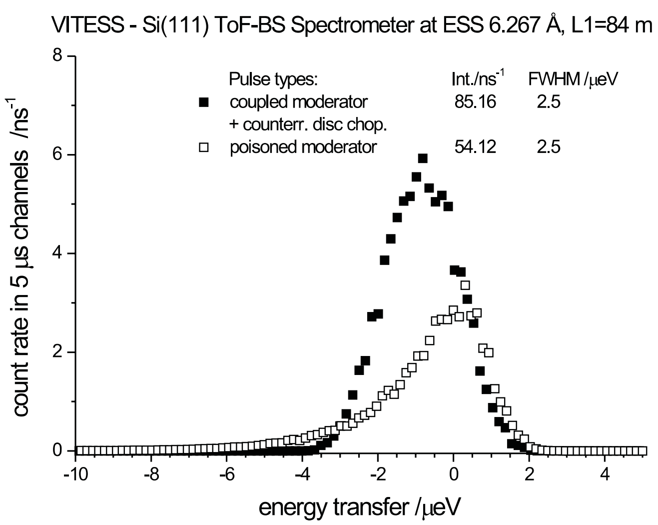

Fig. 3. Comparison of the energy resolutions for the two time pulse options

References

1. G. Zsigmond et al.: Nucl. Instrum. Methods Phys. Res., Sect. A **457**, 299 (2001)
2. G. Zsigmond et al.: Proceedings of ICANS-XV ed. by J. Suzuki, S. Itoh (JAERI, Tsukuba, 2001) Vol. I, p. 354
3. K. Andersen et al.: Performance of a Suite of Generic Instruments on ESS, SAC Workshop, ed. by F. Mezei, R. Eccleston (ESS, 2001) p. 11
4. C. Wilson et al.: Performance of a Suite of Generic Instruments on ESS, SAC Workshop, ed. by F. Mezei, R. Eccleston (ESS, 2001) p. 33
5. see website: http://www.hmi.de/projects/ess/vitess/
6. F. Mezei: http://www.hmi.de/bereiche/SF/ess/ Moderator parameters II