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Estimation of Pulse Shape Functions for High Resolution Chopper Spectrometers by means of the Simulation Calculation Program, McStas

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Abstract

To optimise parameters for very high resolution chopper spectrometers, we have estimated the resolution functions by means of the simulation calculation program McStas. Results of simulation indicate that a chopper spectrometer with L_1 of 15 m and L_2 of 4 m gives an energy resolution, $\Delta\varepsilon/E_i$, of 1% when it is installed at a decoupled liquid H_2 moderator in the Joint Project. Moreover, even very high resolution chopper spectrometers with $\Delta\varepsilon/E_i$ of 0.1% must be feasible by using a double Fermi chopper system. Because of its quite wide $Q-\omega$ space, high resolution chopper spectrometers become important and powerful tool for investigation in wide scientific fields.

Introduction

For design of high resolution Fermi chopper spectrometers in the Joint Project, we have performed simulation calculation of the performance, in particular, its energy resolution which determines the lowest energy of measurable $Q-\omega$ space using Monte Carlo simulation technique. This work was based on discussion in the chopper spectrometer group (group leader : S. Itoh of KEK) in the Joint Project in Japan.

Important performance of general purpose spectrometers is that the instruments can measure in wide $Q-\omega$ space at once so that users can select the best condition for their purposes. Figure 1 shows $Q-\omega$ space which is covered by a direct geometry spectrometers with an energy resolution, $\Delta\varepsilon/E_i$, of 1% and 0.1%. As shown in the left figure of Fig. 1, the spectrometer with $\Delta\varepsilon/E_i$ of 1% can measure in $Q-\omega$ space of 10^{-2} meV $\leq \varepsilon \leq 10^3$ meV and $0.06\text{Å}^{-1} \leq Q \leq 30\text{Å}^{-1}$ by changing incident neutron energy. Moreover, when $\Delta\varepsilon/E_i$=0.1% will be realised, the $Q-\omega$ space becomes much wider to low energy regions: 10^{-3} meV $\leq \varepsilon \leq 10^3$ meV. Since the wide $Q-\omega$ space embraces many kinds of dynamic and spacial properties, this type of chopper spectrometers are definitely

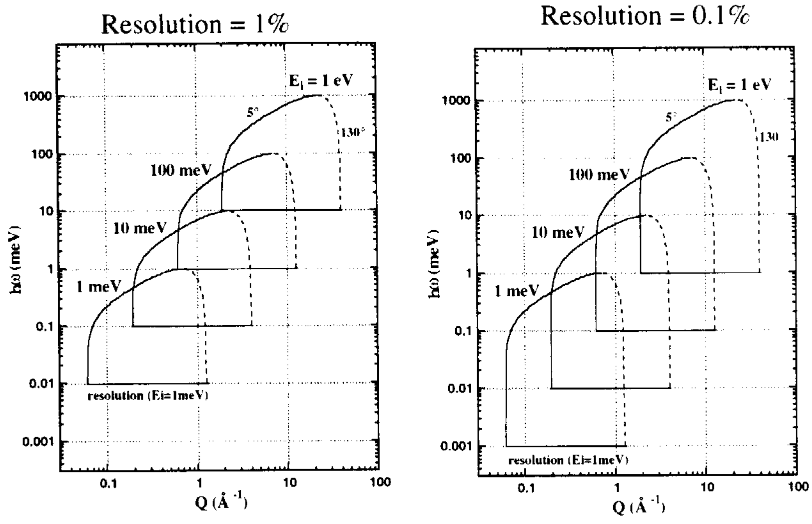

Figure 1: $Q-\omega$ space of a chopper spectrometer with an energy resolution, $\Delta\varepsilon/E_i$, of 1% (left) and 0.1% (right) with different incident neutron energy. 2θ range is from 5 deg. to 130 deg.

important and powerful for investigation in wide scientific fields: condensed matter, soft matter, biology, material science, for instance. Since the lowest energy of the measurable $Q-\omega$ space is determined from the energy resolution at the elastic condition because of strong elastic scattering from samples, high resolution is indispensable performance for chopper spectrometers, even for measurements of broad excitations.

Monte Carlo simulation by means of McStas

To confirm feasibility of high resolution of 1%, and even 0.1%, we have performed simulations of resolution functions of chopper spectrometers in the Joint Project using the Monte Carlo ray-tracing simulation software, McStas (ver. 1.2), written by K. Nielsen and K. Lefmann of Risϕ[1,2]. Though McStas aims basically at designing triple axis spectrometers, it includes time-of-flight components for pulse neutron sources as well. For the simulations of chopper spectrometers in this paper, a decoupled liquid H_2 moderator was selected because of the sharp pulse shape. To represent the time structure of the neutron pulse at the moderator surface, Ikeda Carpenter function was used[3]. The complete set of parameters of Ikeda-Carpenter function for the pulse shape of the decoupled liquid H_2

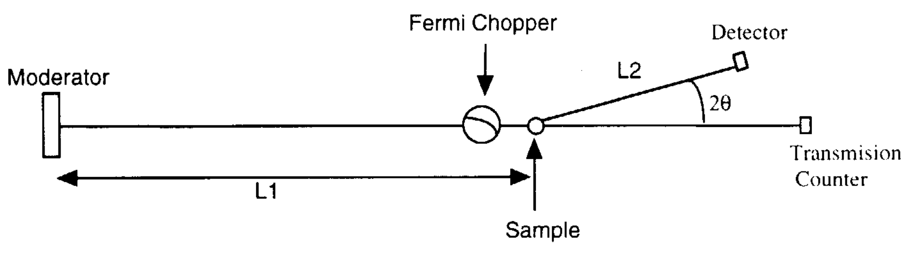

Figure 2: Arrangement of a chopper spectrometer with a Fermi chopper. The moderator is a decoupled liquid H_2 moderator.

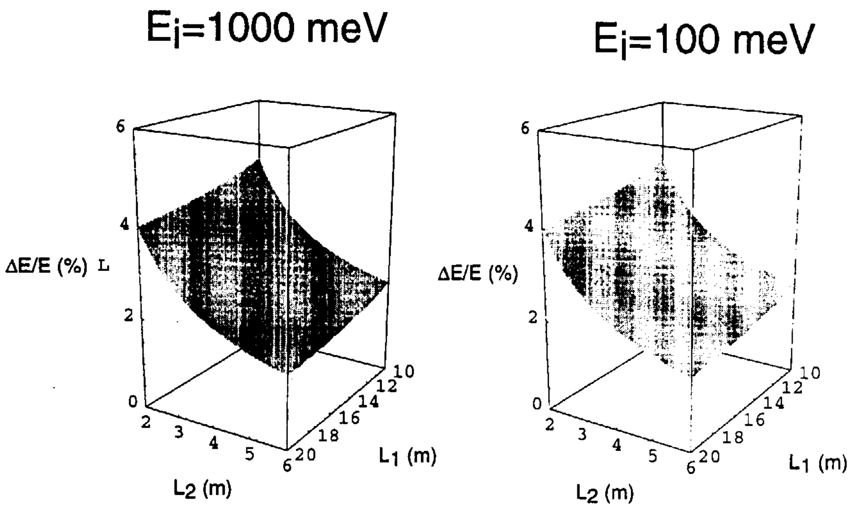

Figure 3: Flight pass dependence of energy resolution at the elastic condition (ε=0 meV with incident energy of 100 meV and 1000 meV

moderator in the Joint Project has been already given by the Neutron Source group and Simulation group of the Joint Project. Figure 2 shows the arrangement of a chopper spectrometer: L_1 is the flight length between the moderator and the sample, and L_2 is that between the sample and the detectors. 2θ is scattering angle of a detector. Conventional Fermi choppers which are used in ISIS and KENS were used in the calculations.

First of all, to find optimised flight length, we have calculated flight length dependence of energy resolution. Figure 3 shows flight length dependence of energy resolution at the elastic condition (ϵ=0) with E_i=100 meV and 1000 meV calculated with an analytic formula[4]. An important result of the calculation is that energy resolution at a detector is almost independent of L_1. Therefore, since we need enough room between the shield of the moderator house and the sample for a back ground chopper, pre-chopper or so on, we have determined L_1 as 15 m. On the other hand, as shown in Fig. 3, energy resolution shows obvious L_2 dependence; resolution becomes better with increasing L_2, while the intensity obtained at a detector decreases. Since results of the calculation indicate that the difference of energy resolution at L_2=4 m and L_2=6 m is small though resolution becomes worse below L_2=4 m, we think that L_2=4 m is the best choice to avoid losing intensity and worsening resolution.

Using the determined flight length (L_1=15 m and L_2=4 m), we tried to estimate resolution function of chopper spectrometers. At first, we confirmed the accuracy of calculation by means of McStas using spectra obtained on the chopper spectrometer.INC, installed at KENS, KEK; calculated results by McStas with Ikeda Carpenter function were well coincide with observed pulse shapes at the transmission counter of INC, and observed elastic incoherent scattering spectra at detectors as well, without any fitting parameters except scaling factors. This means that simulation calculation by McStas is reliable for estimation of performance of chopper spectrometers in the Joint Project.

Figure 4 indicates calculated elastic incoherent scattering spectra around ε=0 meV obtained by a chopper spectrometer installed at a decoupled liquid H_2 moderator of the Joint Project with E_i= 50 meV, 100 meV, 200 meV and 500 meV. Horizontal axes indicate the energy transfer and the centre of the axis is the position of ε=0. The sample in the simulation calculation was a vanadium rod with a diameter of 1 cm which has real

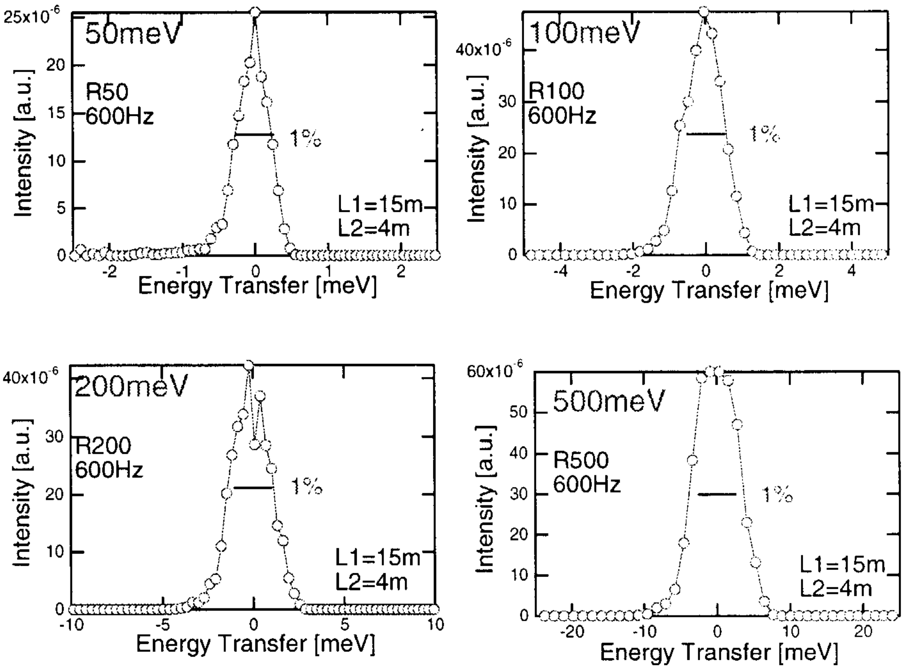

Figure 4: Elastic incoherent scattering spectra from a vanadium rod with E_i=50, 100, 200 and 500 meV by means of McStas. In the calculation, the chopper spectrometer with a conventional Fermi chopper is installed at a decoupled H_2 moderator in the Joint Project. Horizontal lines in the figures indicate an energy resolution, $\Delta\epsilon/E_i$, of 1% under each condition.

scattering and absorption cross sections. The horizontal lines in the figures show an energy resolution, $\Delta\epsilon/E_i$, of 1% under each condition, where $\Delta\epsilon$ is full width of half maximum. As shown in the figures, the peak shapes are almost symmetric and an resolution of about 1% is already realised, though slight tails exist in the negative energy sides which are due to tail structures of the pulse shapes at the moderator, and the peak with E_i=500 meV has a flat top structure. When the pulse shape at the moderator becomes slightly sharp, the tails in the negative energy transfer region disappear. On the other hand, the origin of the flat-top structure in the peak with E_i=500 meV is unknown yet. The results mean that a conventional chopper spectrometer with L_1=15 m and L_2=4 m installed at the decoupled H_2 moderator has an energy resolution of 1% at the elastic condition in wide E_i range without particular effort.

Nextly, we calculated resolution at inelastic regions. For the simulation, the sample was a virtual material which causes incoherent inelastic scattering with negligibly narrow energy width. Fig. 5 indicates inelastic spectra at ε=100 meV and 150 meV with E_i=200 meV obtained from calculations by McStas. Note that the scattering intensity in Fig. 5 can not be compared with the spectra from a vanadium rod shown in Fig. 4, because the cross section of the virtual sample is not real. As shown in Fig. 5, the energy resolution are 0.32% at ε=100 meV (=0.5 E_i) and 0.15% ε=150 meV (=0.75 E_i). The lower figure in Fig. 5 indicates energy transfer dependence of energy resolution which were determined as the full width of half maximum of inelastic peaks calculated by McStas. The energy resolution becomes better with increasing energy transfer, ε. Note that, in most of experiments, important excitations exist in the middle of the energy transfer

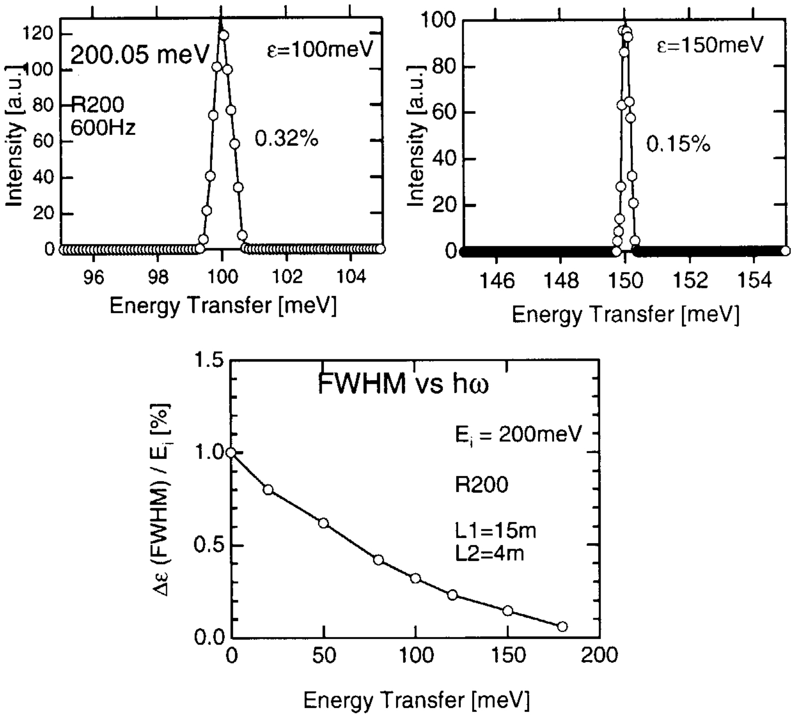

Figure 5: Peak shapes of inelastic scattering at ε=100 meV and 150 meV with E_i=200 meV calculated by McStas. The lower figure shows energy transfer dependence of energy resolution (FWHM) with E_i=200 meV.

range. Thus, the results in Fig. 5 mean that one can obtain high quality data with about 0.5% or better resolution using this type of chopper spectrometers
In other word, when this type of chopper spectrometers are constructed in the Joint Project, information in the wide $Q-\omega$ space shown in Fig. 1 with satisfactorily high resolution can be obtained by only one spectrometer. In this meaning, this type of chopper spectrometers is an effective and indispensable instrument which should be constructed at the first step of the schedule in the Joint Project.

Double Chopper spectrometer

As mentioned above, we have confirmed that a conventional chopper spectrometer with an energy resolution of 1% is feasible in the Joint Project. As a next step, the chopper spectrometer group has discussed possibility of a novel chopper spectrometer with very high energy resolution, $\Delta\varepsilon/E_i$=0.1%. From the discussion, we propose a chopper spectrometer with a double chopper system. Vertical and Horizontal axes in Fig. 6 indicate the position of each equipment and Time-of-Flight. The slant lines in Fig. 6 indicate the relation between Time-of-Flight and flight length of neutron with a particular energy. The left figure of Fig. 6 shows a case with a conventional chopper spectrometer with a single Fermi chopper. As well known, since conventional single chopper spectrometers detect an opposite image of the pulse shape at moderator owing to the "pin-hole effect", if the pulse at the moderator has a tail, it is impossible to avoid asymmetry of the pulse shape at detectors even though the chopper window is extremely narrow. Thus, to obtain sharp and symmetric peak shape, it is essentially important that single chopper spectrometers

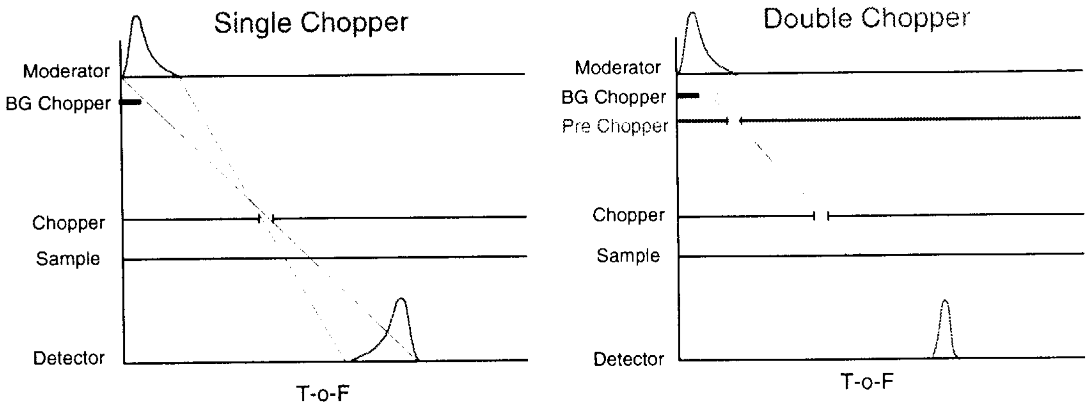

Figure 6: Time-of-Flight relation of a conventional single chopper spectrometer (left) and a chopper spectrometer with the double chopper system(right)

are installed at a moderator with a very sharp pulse shape.

On the other hand, when another pre-chopper is installed above the chopper (the right figure of Fig. 6), the permitted flight pass is quite limited when the distance between the pre-chopper and the main chopper is large enough. Therefore, only controlling the open timing of the pre-chopper, one can select any part of the pulse at the moderator. Thus, using this double chopper system (pre chopper + main chopper), users can obtain symmetric resolution function at detector positions even though the pulse shape at the moderator has a long tail.

We have confirmed effects of the double chopper system using McStas. Figure 7 shows some results of simulation calculations of the resolution function on a double chopper spectrometer installed at a decoupled H_2 moderator. The distance from the moderator and the pre-chopper is 7.5 m in the calculations. The left figure of Fig. 7 indicates the resolution function of a single chopper spectrometer at the elastic condition (ε=0 meV) with E_i=200 meV. The resolution is 1% as mentioned above. On the other hand, the right figures show elastic spectra obtained by a spectrometer with the double chopper system. As shown in the upper figure of Fig. 7, when the slit width of the main Fermi chopper is 0.5 mm, $\Delta\varepsilon/E_i$ at the elastic condition is about 0.5%. Moreover, even $\Delta\varepsilon/E_i$=0.3% are realised with a slit width of 0.25 mm (the lower figure in Fig. 7. Thus, by choosing a rotor carefully, one can obtain higher resolution than 0.5%, though The intensity becomes ten times weaker than that of the single chopper spectrometer. Therefore, we think that 0.1% resolution must be feasible by optimising parameters of the double chopper system, although we have to overcome some engineering problems, in particular, accurate control and phasing of the rotors.

In the calculations here, spectrometers installed at a decoupled liquid H_2 moderator in the Joint Project were considered because the discussion in the chopper spectrometer group of the Joint Project was based on a conventional single chopper spectrometer, and we thought the double chopper system as an option for the single chopper spectrometer. The results of simulation indicate, however, that the spectrometer with the double chopper system should be installed at a coupled moderator because the long tail of the pulse shape of the coupled moderator does not affect the peak shape obtained by the spectrometer with the double chopper system, and the flux is much stronger than that of the decoupled moderator.

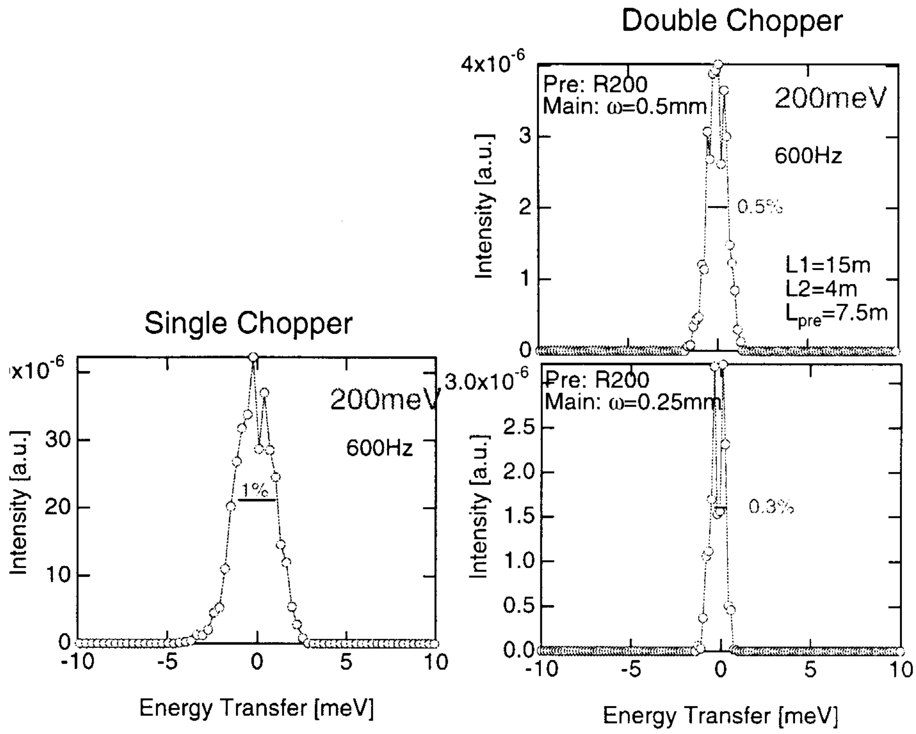

Figure 7: Effect of the double chopper system with E_i=200 meV. The left figure shows a pulse shape at the elastic condition (ε=0 meV) of a conventional single chopper spectrometer. The right figures show pulse shapes of a chopper spectrometer with the double chopper system. FWHM of the elastic peaks are 0.5% and 0.3%, when slit width, ω, of the main chopper is 0.5 mm and 0.25 mm, respectively.

Summary

We have performed simulation calculation to estimate performance of chopper spectrometers in the Joint Project in Japan by means of a Monte Carlo program, McStas of Risϕ. We have confirmed that McStas is a powerful and reliable tool for estimation of performance of chopper spectrometers. The results of the simulations indicate that a conventional chopper spectrometer with L_1=15 m and L_2=4 m has an energy resolution of 1% or better when it is installed at a decoupled liquid H_2 moderator of the Joint Project. Moreover, when double chopper spectrometers are realised, experiments with an energy resolution of 0.1% must be possible. Therefore, chopper spectrometers in the Joint Project can measure dynamic and spatial properties in materials in very wide $Q-\omega$ space with satisfactorily high resolution.

References

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