Simulation of Energy Dispersive Mode for RITA-type Cold Neutron Triple Axis Spectrometer SIKA

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SIKA, a high flux cold triple axis spectrometer at OPAL reactor, is equipped with a 13-blade analyser and position sensitive detector. This multiplexing design endows SIKA with high flexibility to run in either traditional or dispersive modes. In this study, the energy dispersive mode for two different energy transfers is simulated using the Monte Carlo ray-trace package SIMRES. The results show that SIKA could work effectively in this mode at low and intermediate energy transfers with reasonable energy and Q resolution. The simulated energy resolution is about 0.23 meV for an energy transfer of $\hbar\omega$ = 5 meV and increases to 1.8 meV for $\hbar\omega$ = 15 meV. This work provides a valuable reference for future inelastic neutron scattering experiments on SIKA.

1. Introduction

A triple-axis spectrometer (TAS) is a powerful tool to investigate quasi-particle dynamics in condensed matter, such as phonon and magnon excitations [1]. Most of the TAS currently used are of traditional design with single detectors, allowing ($\boldsymbol{q}$, $\hbar\omega$) space to be detected only step by step. Since only a small fraction of the scattered beam is detected at one step, this design is inefficient in data acquisition, especially when the interesting ($\boldsymbol{q}$, $\hbar\omega$) space is large. In recent years, considerable effort has been directed at designing and building new types of TAS, capable of detecting series of points in ($\boldsymbol{q}$, $\hbar\omega$) space simultaneously. For example, RITA-1 at Risø, BT7 and SPINS at NIST are such unconventional TAS (they are also referred to as “RITA-type TAS”), which have been implemented and used for a variety of experimental tasks. Their common feature is that they have a multi-blade analyser and position sensitive detector (PSD). Each blade on the multi-blade analyser is able to rotate independently to any specific angle, which allows detectors to collect the scattered neutrons in a rather large range of reciprocal space (Q) or energy transfer ($\hbar\omega$) at the same time.

SIKA is a high flux RITA-type cold neutron TAS, mounted on the reactor face of the OPAL reactor of the Australian Nuclear Science and Technology Organization (ANSTO). The design of SIKA is based on BT7, the double focusing thermal neutron TAS at NIST. The secondary spectrometer of SIKA is composed of a multi-blade analyser, including 13 PG(002) blades, a linear PSD, and a separate single detector. It can operate in a traditional step-by-step mode by using the single detector or several multiplexing modes with the PSD (e.g. focusing analyser mode, q dispersive modes and energy-dispersive modes). Theoretically, the multiplexing operation modes can be realized in many different ways with various collimator-blade-detector configurations. The basic idea is to extend the Q or energy detecting range with one scattering configuration by driving the analyser blades to a series of specific angles and combining the efficiency of the PSD, to improve the data acquisition efficiency.

The energy-dispersive flat analyser mode (E1 mode [2]) is one of the most frequently used operation modes for RITA-type TAS. This operation mode can quickly survey a large ($\boldsymbol{q}$, $\hbar\omega$) space of the sample by mapping series of Q and energy transfers. We expect that half of the experiments on SIKA will be run with this mode in the future. Clausen *et al*. [3] demonstrated the excellent performance of RITA with a factor of approximately 2-5 intensity gain. In this study, we simulate the E1 mode for the configuration of SIKA by using the ray-tracing Monte Carlo method. At two different energy transfers (5 meV and 15 meV), the resolution functions have been calculated for each blade. The simulation presents detailed information about the resolution of each blade and overlapping (cross-talk) of different analyser-detector channels, very useful for future experiments on SIKA.

2. Simulation details

The simulations were conducted using the Monte Carlo ray-trace package SIMRES, which is a sister software of Restrax by J. Šaroun [4]. The simulation was done on a dummy sample of a cubic structure with a = 6.28 Å. The geometric configuration for the neutron source, guide and slits and collimators are from SIKA with some minor simplification. The pre-monochromator, pre-sample and after sample collimators are 40'/40'/40', respectively. The simulated experiment was done at the sample reciprocal lattice vector τ. SIKA will operate with two types of filters (Be and PG) for suppression of the second order signals. Therefore, two energy transfers (5 and 15 meV) close to the limits of Be- and PG-filtering , repectively, are used for the simulations. Table 1 details the simulation parameters employed.

Table 1. Parameters for the simulations for energy transfers of 5 meV and 15 meV.

$\hbar\omega$	Mosaicity		$K_i(Å^{-1})$	$K_f(Å^{-1})$	$\tau(Å^{-1})$
	Monochromator	Analyser			
5 meV	30'	30'	2.04	1.32	1.55
15 meV	30'	30'	3.78	2.66	1.55

3. Results and discussions

The instrumental configuration of the so-called energy dispersive mode is shown in Fig. 1(a). The analyzer blades keep flat like a traditional unfocused single analyzer, sitting at a cut-off angle A_2. The most important difference between the traditional mode and the E1 operation mode is the radial collimator between sample and analyser. In E1 mode (Fig. 1(b)), the radial collimator differentiates the energy of neutrons impinging on different analyser blades, which reflect the neutron beam to different sections of the PSD. Here we adopted linear post-sample collimation (40') for simulation since each blade is simulated independently. In Fig. 1(c), the scattering triangle in reciprocal space for E1 mode clearly shows that K_f slightly rotates when considering each blade as the analyser. The modulus of K_f changes as well in order to close the scattering triangle. Thus, both energy transfer $\hbar\omega$ and Q will change from one blade to its neighbours. Finally, we should see a series of resolution functions as shown in Fig. 1(d). Such results are not straightforward for a single point because they are dispersive in both energy and Q. However, when mapping a ($\boldsymbol{q}$, $\hbar\omega$) space of samples, the advantage of this operation mode becomes obvious due to its time efficiency.

In the E1 mode, the divergence angle, δ_i, which is the angle between beam to the *i*th blade and the central blade from the sample, is given by

$$\delta_i = \arctan\left(d_i * \sin(\frac{A_2}{2}) / \left(L_{SA} - d_i * \cos(\frac{A_2}{2}) \right) \right) \quad (1)$$

where L_{SA} is the distance between sample and analyser, d_i is the distance of the *i*th blade from the centre, A_2 is the take-off angle of the analyser. The diffraction angle for the *i*th analyser blade is $A_2/2+ \delta_i$, which defines K_f of the outcoming beam for this blade. The angle between K_i and K_f are defined by $S_2 + \delta_i$, where S_2 is the sample take-off angle.

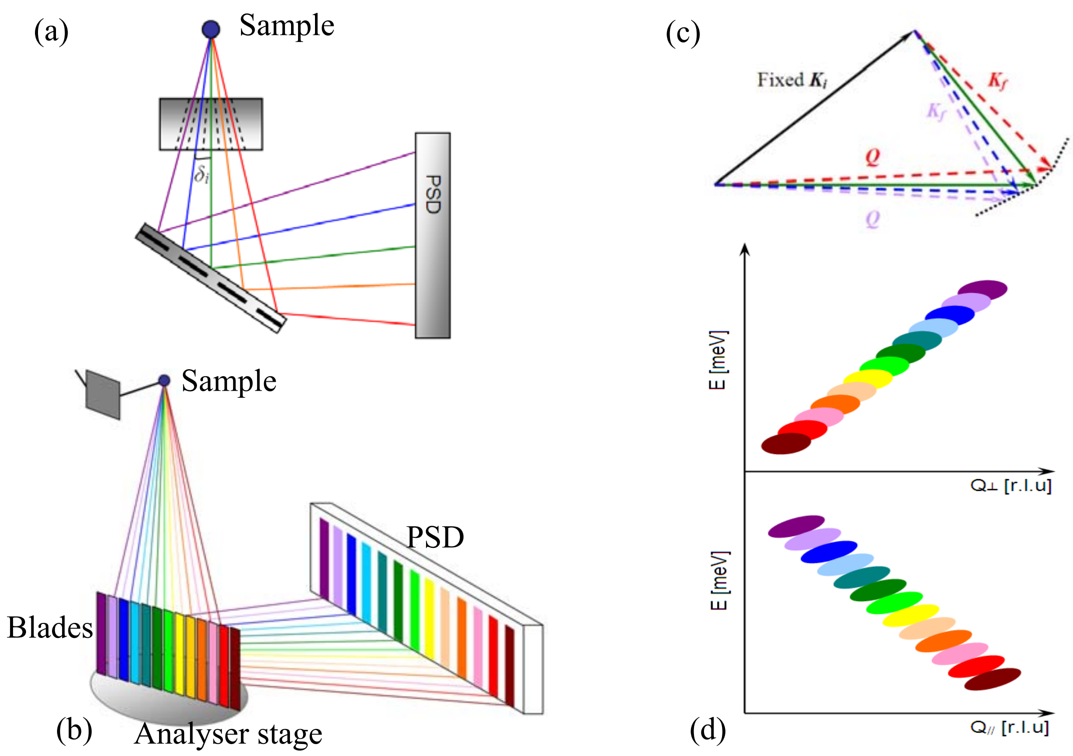

Fig. 1 (a) Configuration of analyzer and detector for E1 mode; (b) Schematics of scattering and detection system in E1 mode; (c) Scattering triangle; (d) Schematic resolution function projected on $\hbar\omega$-$Q_\perp$ and $\hbar\omega$-$Q_{//}$ planes.

3.1 Simulation for an energy transfer of 5 meV

Fig. 2 shows the simulated results for the energy transfer of 5 meV, which is most widely used for cold neutron TAS experiments. Fig. 2(a) and (b) are the resolution functions projected on the $\hbar\omega$-Q_X and $\hbar\omega$-Q_Y planes, where Q_X and Q_Y are the Q components perpendicular and parallel to τ, respectively. For SIKA, there are 13 blades on the analyser stage. We selected each second blade to be shown in these figures to avoid overlapping each other. As we can see from these figures, the resolution function from each blade has a quite similar ellipsoid shape. The dispersion in energy and Q can be clearly seen in these results. From lower to higher Q_X, the resolution function gradually shifts to the higher energy. For Q_Y, the trend is reversed, but with more elongated ellipsoids. And those ellipsoids are nearly separated from one another for the seven blades. In the case of 13 blades, the signal on the PSD will have cross talk between neighbouring blades. A further linear collimator between the analyser and the detector may be adopted to reduce the cross talk. The full width at half maximum (FWHM) in the energy scale is around 0.23 meV (see Fig. 2(c)) for the central blade, which means ≈ 4.5% of the energy transfer at this configuration, comparable with other instruments [5]. The simulated results show that the design of SIKA theoretically provides an applicable high resolution and time efficiency for experiments under the energy dispersive operation mode due to the multiple parallel data collecting channel.

3.2. Simulation for an energy transfer of 15 meV

Fig. 3 shows the simulated results for the energy transfer at 15 meV, which is the high energy end of the cold neutron TAS instrument. The results are presented in the same way as for Fig. 2. The elongated resolution ellipsoids in Fig. 3 (a) and (b) dispersed in a larger energy range. The resolution function deteriorates in the $\hbar\omega$-$Q_\perp$ space and shows obvious overlapping because of the increase of the energy transfer (correspondingly, both E_i and E_f increase). Provided that there exists software to directly handle arrays of 2D data from PSD, the E1 operation mode for reciprocal space mapping is still applicable for this relatively high energy range, keeping the time efficiency. The FWHM in the energy scale is around 1.77 meV (see Fig. 2(c)) for the central blade, around 12% of the energy transfer. [5]

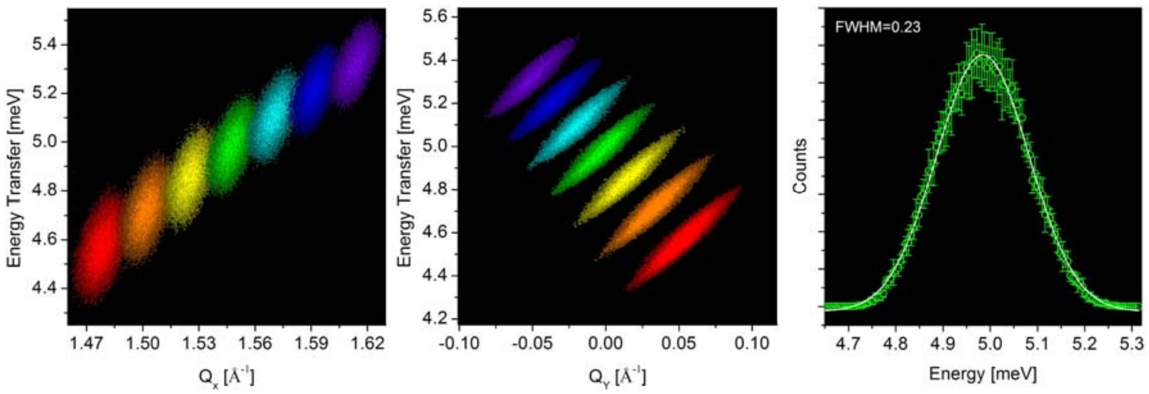

Fig. 2 Resolution maps in the (a) $\hbar\omega$-$Q_\perp$ and (b) $\hbar\omega$-$Q_{//}$ planes and (c) the resolution profile at low energy transfer of 5 meV

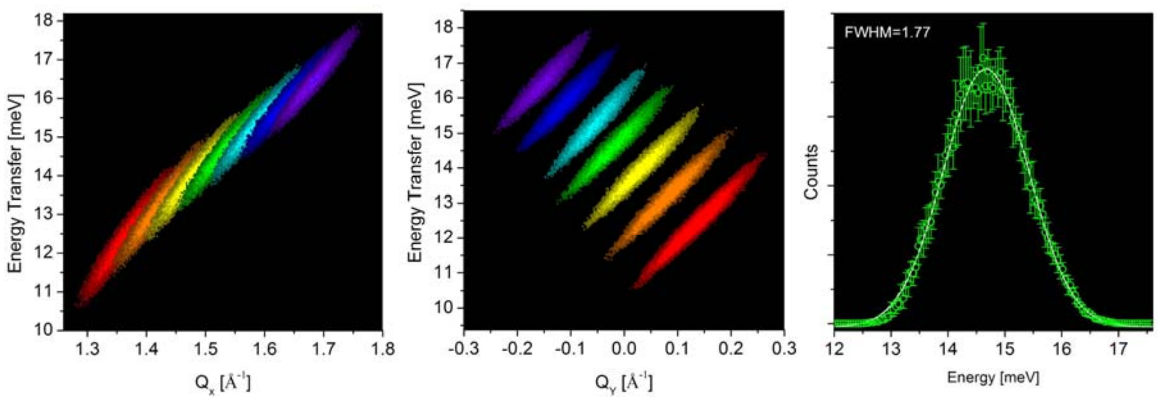

Fig. 3 Resolution maps in the (a) $\hbar\omega$-$Q_\perp$ and (b) $\hbar\omega$-$Q_{//}$ planes and (c) the resolution profile at higher energy transfer of 15 meV

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