DOUBLE AXIS MODE OF BATAN'S TRIPLE AXIS SPECTROMETER

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ABSTRACT

DOUBLE AXIS MODE OF BATAN'S TRIPLE AXIS SPECTROMETER. Triple Axis Spectrometer (TAS), which is an indispensible tool to microscopically probe inelastic scattering processes in condensed matter, has been installed at the Neutron scattering Laboratory of the R & D Center for Materials Science & Technology, BATAN, since 1992. However, the control and data acquisition system have been nonfunctional since 1996. Following an in-house development of the alternative control and data acquisition hardware last year, TAS started to show the capability and reliability of handling the measurement in the double axis mode. This paper reports a double axis mode control and data acquisition software development which benefits from the hardware development.

Key words : Spectrometer, inelastic, neutron

ABSTRAK

DOUBLE AXIS MODE OF BATAN'S TRIPLE AXIS SPECTROMETER. Spektrometer Tiga Sumbu (TAS), yang penting untuk pengukuran hamburan neutron *inelastic*, telah dipasang di laboratorium hamburan neutron di P3IB, BATAN sejak 1992. Namun demikian, sistem kontrol dan pengumpul data tidak berfungsi sejak tahun 1996. Sesudah pengembangan perangkat keras untuk kontrol dan pengumpul data pada tahun lalu, TAS mulai menunjukkan kemampuan dan kehandalan untuk pengukuran mode dua-sumbu. Makalah ini melaporkan pengembangan perangkat lunak untuk kontrol dan pengumpul data mode dua-sumbu dengan memanfaatkan pengembangan perangkat keras tersebut.

Kata kunci : Spektrometer, *inelastic*, neutron

INTRODUCTION

The interest in the utilization of a neutron beam as a probe for the investigation of the dynamical behavior of condensed system is justified by the fact that thermal neutrons coming out from a research reactor and thermal motions of the atoms in the matter have associated momentum and energies lying in the same ranges of values. Easily observable change of the dynamical state of the neutron may then result from a scattering process. The measurement of the momentum and energy transferred by the neutron to the crystal or vice versa, directly leads to the knowledge of the corresponding quantities associated with the elementary excitations of matter. Such knowledge, when analyzed in conjunction with the techniques of the Fourier transforms, may conduct to a detailed space-time description of the scatterer on a microscopic scale [1-5].

Triple Axis Spectrometer (TAS), which is suitable for the inelastic scattering mentioned above, has been installed at the Neutron Scattering Laboratory of the R & D Center for Materials Science & Technology, BATAN, since 1992. However, the control and data acquisition system have been nonfunctional since 1996. It was difficult to fix the problem due to insufficient service manuals for such a complex instrument. TAS has 18 stepper motors to move the monochromator, the sample table and the analyzer axes equipped with the air compressor system to facilitate the movements of the massive axes.

Recently, as a part of in-house development of the neutron scattering facilities, an alternative control and data acquisition hardware have been developed by using local electronic parts. All motors can now be moved to specified positions as before but now with the know-how added value. The knowledge would ease further development and/or maintenance when necessary. This paper reports the software development which benefits from the in-house hardware development. The report is limited to the measurement in a double axis mode which is a prerequisite of the measurements in a triple axis mode.

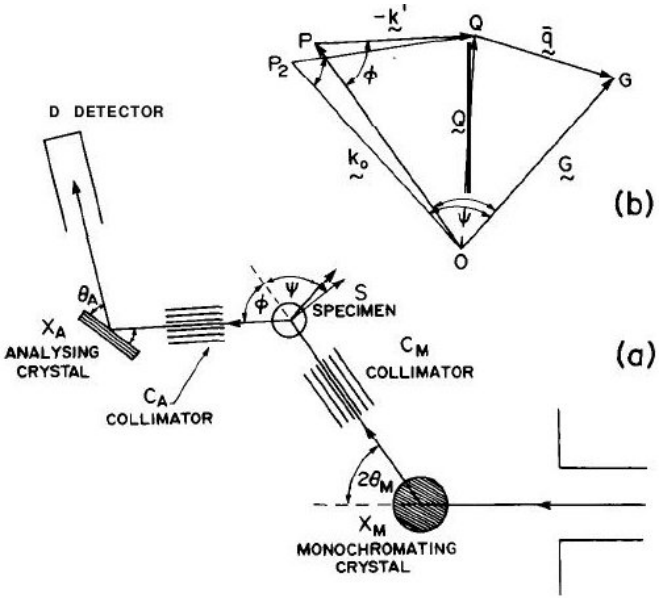

Figure 1. (a) A Schematic configuration of TAS together with (b) momentum space diagram in the same coordinate system. P2 indicates a second point on a constant-Q curve at fixed incoming energy. The massive shielding required, particularly around the monochromator, is not shown.

EXPERIMENTAL METHOD

TAS consists of the monochromator, the sample table and the analyzer axes as shown in Figure 1. It is possible to operate with a very flexible unit allowing automatic changes of the scattering angle ϕ, the crystal direction ψ, the magnitude of the incident wave vector $k0$ related to the monochromator scattering angle $2\theta_M$ and the magnitude of the scattered wave vector k' related to the analyzer scattering angle $2\theta_A$. Those changes can be triggered, at the end of any counting period (defined by the monitor), according with suitable pieces if information coming in general, from a computer. The control and data acquisition program code have been developed using GNU C++ programming language with visual capabilities provided by wxWidgets [6]. The GNU C++ and wxWidgets are available freely from the internet.

For the case of isotropic systems such as liquids, the triple axis spectrometer allows intensity measurements to be made at constant magnitude of the wave vector transfer Q. In such a case, the rotation ψ is evidently not essential and the most suitable arrangement is that of varying ϕ and $k0$ (or k') with k'(or $k0$) fixed. For the case of crystalline powder, in the vicinity of Q=0, the intensity is dominated by the elastic scattering as the Bragg peaks are much higher than the inelastic contribution. Hence, the analyzer can be taken out for the double axis mode measurement. The remaining axes are then the monochromator and the sample table axes with the scattering angle ϕ and the magnitude of the incident wave vector $k0$ as the relevant parameters.

Ni powder [7] was used as a sample with fixed structural parameters. The measurement was conducted at room temperature with Cu monochromator and preset count of 255 corresponding to 1.5 minutes per data point on average. The sample slit width and height are 10 mm and 20 mm, respectively. The analyzer crystal was taken out and the axes was set to zero. The important parameters to be refined using GSAS [8] were λ which was related to $k0$ and the zero of the instrument. Other refined parameters were the background, profile and thermal parameters.

RESULTS AND DISCUSSION

Figure 2 shows the refined diffraction patterns. The data is of good quality as judged by the difference curve between the calculated and the observed intensity with the weighted residual factor, residual factor and reduced χ of 13.74%, 10.12 and 1.115 respectively, for 9 variables (see Table 1). The input parameters were Ni powder standard which crystallizes in the F*m*3*m* space group with Ni atoms at (0, 0, 0) and the lattice parameter of 3.5238Å [7]. The diffractometer constants resulted from the analysis are λ=1.4542(3) Å and *zero*=-61.2(11) centidegrees. λ is used not only in the double axis mode, but also in the triple axis mode for unchanged value of incident energy and momentum. *Zero* is important in order to get the correct location of peak, which is then successively used for other peak determination in the single crystal sample for the inelastic scattering measurement later on.

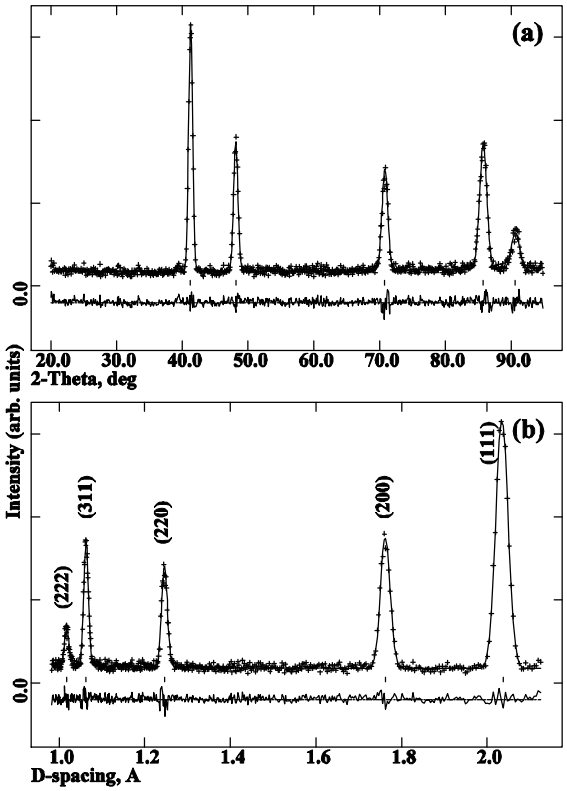

Figure 2. Ni standard sample [7] in (a) intensity versus 2θ and (b) intensity versus d-spacing. The numbers inside the parenthesis in (b) indicate the Miller indices in the cubic symmetry. In each figure, the upper solid curve and the plusses indicate the calculated and observed patterns, respectively. The lower curve indicates the difference between the calculated and observed patterns. Clearly, the difference curve fluctuates insignificantly around horizontal lines, indicating that the fits are of good quality, as detailed in Table 1.

Table 1 details the refined parameters corresponding to Figure 2. The number of the refined parameters is kept to be minima without lowering the fit quality. Probability theory tells us to choose the description with the least number of unknown which is consistent with the experimental measurements (i.e., the 'simplest' explanation). Although the parameters of interest are only λ and *zero*, other parameters, which are basically nuisance, with varying values remain to be switched on. The estimate of the error-bars can be misleadingly small if one holds the nuisance fixed at their optimal value.

CONCLUSION

After a long nonfunctional period, TAS started to show the capability and reliability of handling the measurement in the double axis mode with a user friendly control and data acquisition system. This enables further development towards a triple mode option, which is much more demanding and prone to errors.

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Table 1. Refined Parameters showing λ and *zero*, as well as the nuisance parameters and the fit qualities (see refined patterns in Figure 2).

Parameter	Value		
λ(Å)	1.4542(3)		
Zero(centidegrees)	-61.2(11)		
Thermal parameter	65.8(89)		
Histogram scale factor	3828.5(793)		
Profile	*U*=3527(136)	*V*=-7.60(fixed)	*W*=753.5(367)
Cosine background	47.2(21)	-17.9(32)	5.2(16)
Fit Quality	wR_p=13.74%	R_p=10.12	Reduced χ^2= 1.115

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