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Recent progress on MAX

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Introduction

Crystal analyser spectrometer MAX at KENS can observe collective excitations such as phonons and magnons in single crystals by means of TOF method. Excitation spectrum along a desired direction of the sample crystal can be measured using fifteen independent analyser-detector systems[1-5]. In practical use, the energy transfer range is 1meV to 150meV depending on the Q region to be covered. The energy resolution $\delta E/E_f$ is about 0.1 and can be adjusted by inserting Sollar collimators before and/or after the analyser. MAX exhibits its better performance in several tens meV energy transfer region. This energy region is not so easy to observe using a triple-axis spectrometer at a medium power steady reactor. MAX is now being used mainly to investigate magnetic excitations. Dispersion relations of the magnetic excitations in various magnetic materials have been determined. Advantages in the application of MAX to the low-dimensional systems should be noted[4,5]. All the scans made by the detectors of MAX are constant-q when the incoming neutron beam is set parallel to the direction in which the system has no correlation, i.e. the direction perpendicular to the plane (chain) of the two- (one-) dimensional material. Furthermore, better experimental condition is found in the case of low-dimensional systems because the strong restriction on the TOF scan due to the periodicity of the $S(Q,\omega)$ is relaxed.

Improvements

In order to improve the signal-to-noise ratio (S/N), the counting rate and the flexibility of the spectrometer, several modifications have been made. During the past few years S/N of the spectrometer has been improved significantly. Furthermore, new inpile collimator with sintered B_4C arrays has been inserted in order to eliminate the fast neutron background. We have improved the counting rate by focusing the neutron beam reflected by the analyser crystals. Small pieces of pyloritic graphite (5 cm x 0.6 cm) are aligned on a holder which has appropriate vertical curvature so as to focus the reflected beam to the small area on the ^3He counter. Note that we can obtain a better counting rate without sacrificing S/N because it is not necessary to enlarge the aperture of the counter shielding box. Moreover, the vertical slit Sollar collimators are still useful for these vertically curved analyser mirrors. The size of the analyser mirrors is enlarged to 7 cm (height) x 10 cm (length) from 5 cm x 10 cm. Consequently, without increasing the background or sacrificing the resolution, we have obtained more than 2 times higher counting rate than the previous flat ones. In order to obtain more flexibility, the direction of the rotation of the detector arms has been changed from counterclockwise to clockwise. (Analyser arms are rotated clockwise.)

Resolution of spectrometer

Resolution characteristics of MAX have been investigated in detail. Analytical resolution function was derived and examined experimentally. The derivation is based on the formalism of Cooper and Nathans [6], Komura and Cooper [7] and Windsor and Heenan [8]. Since, as is usual, Gaussian distributions were assumed for all the broadenings which occur due to the finite angular collimations, the mosaic of the analyser crystal, the time distribution of the neutron pulse and the time broadenings due to the finite sample size or gate width, the resolution function can be expressed analytically in terms of a Gaussian form in the 4-dimensional (Q, ω) space. Derivation of the resolution function of MAX and

the so-called resolution matrix is shown in reference 9. Here we only give a useful expression for the energy width which can be derived from the resolution function:

$$(\Delta\hbar\omega)^2 = 4E_I^2\left[\left(\frac{\tau}{T_I}\right)^2 + \left(\frac{E_F}{E_I} + \frac{L_F}{L_I}\sqrt{\frac{E_I}{E_F}}\right)^2 \cot^2\theta_A\,(\Delta\Theta_A)^2\right]$$

where

$$\tau^2 = \tau_m^2 + \tau_s^2 + \tau_c^2$$

and

$$(\Delta\Theta_A)^2 = \frac{\alpha_2^2\alpha_3^2 + \alpha_3^2\eta_A^2 + \eta_A^2\alpha_2^2}{\alpha_2^2 + \alpha_3^2 + 4\eta_A^2}$$

α_2 and α_3 corresponds to the divergence angle of the collimator placed between sample to analyser and analyser to detector respectively and η_A is the mosaicness of the analyser crystal. The time distribution (width τ_m) of incident neutron pulse is a function of wavelength. τ_s gives the time broadening due to the finite sample size. τ_c is chosen so that the corresponding Gaussian has the same standard deviation as the actual distribution caused by the finite time channel width. Usually τ_m is the largest compared with τ_s and τ_c. Parameters α_2, α_3 and η_A in the analyser part were determined so as to reproduce the observed energy width. We have plotted in Fig. 1(a) the observed energy width of incoherent elastic scattering from Vanadium for various collimations. The calculated widths using eq.(1) are indicated by solid lines in the figure. Figure 1(b) is a graph of calculated energy width as a function of E_F and $\hbar\omega = E_I - E_F$. In the figures the nominal aperture angles of the Sollar collimators are denoted as 20', 30', ... ("B" : without the Sollar collimator).

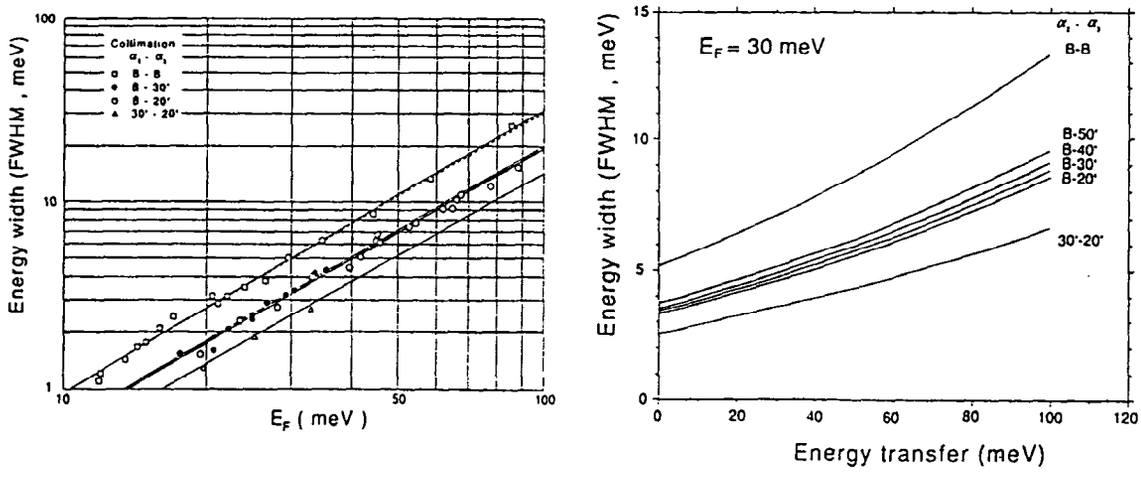

Fig. 1 Energy resolution of MAX for various collimations. (a) shows the observed energy widths as a function of E_F at $\hbar\omega = 0$. The solid lines are the corresponding calculations described in the text and the dotted line expresses the $E_F^{3/2}$ dependence[9]. (b) is calculated as a function of $h\omega$ in the case of E_F =30meV.

We have also measured the spatial shape of the resolution at the elastic position by using Bragg scattering from a small perfect Ge single crystal. A spatial map of the intensity was drawn by rocking the sample and the analyser. Good agreement was obtained in both volume and spatial orientation of the resolution ellipsoid. By using the resolution function the effect of the spectrometer configuration on the resolution can be estimated. The volume of the resolution ellipsoid for the configuration of clockwise rotation of the detector arms (present configuration of MAX) is larger than the previous counterclockwise rotation or "W-configuration". However, present configuration has more flexibility. Note that the direction of the longer axis of the ellipse projected on to the scattering plane is always close to the direction of k_F in the present configuration as shown in Fig. 2(b).

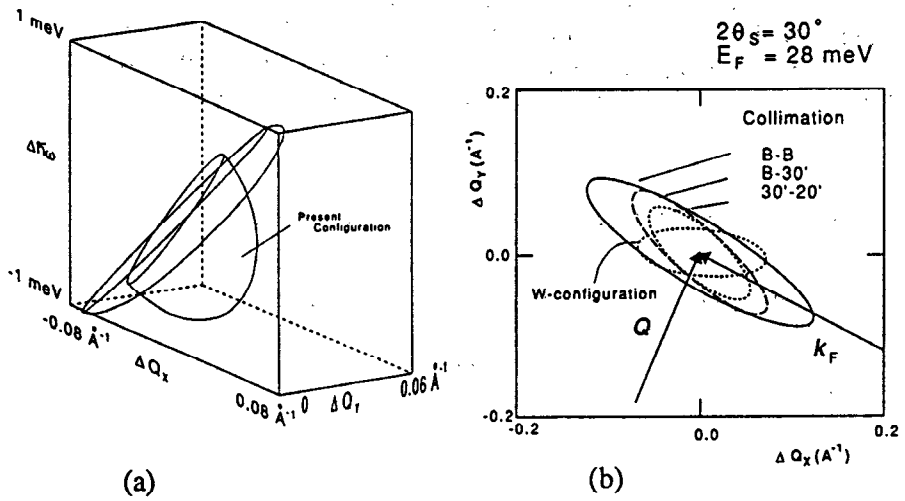

Fig. 2 Calculated resolution ellipsoids. (b) is the projected ellipses on to the scattering plane, where ΔQ_X is parallel to $-k_I$.

The resolution function derived analytically is useful for qualitative discussion of the instrumental resolution characteristics. Occasionally, however, observed peak shapes do not have the symmetric Gaussian form because the incident neutron pulse has a highly asymmetric time distribution. The resolution function derived above cannot reproduce this asymmetry. Employing the neutron pulse shape function proposed by Ikeda and Carpenter[10], numerical calculation of the resolution function was performed. It has been found that ,without any other adjustable parameters, observed incoherent elastic profile is well reproduced by a Monte Carlo calculation as shown in Fig.3. We are now extending this calculation to the inelastic scattering.

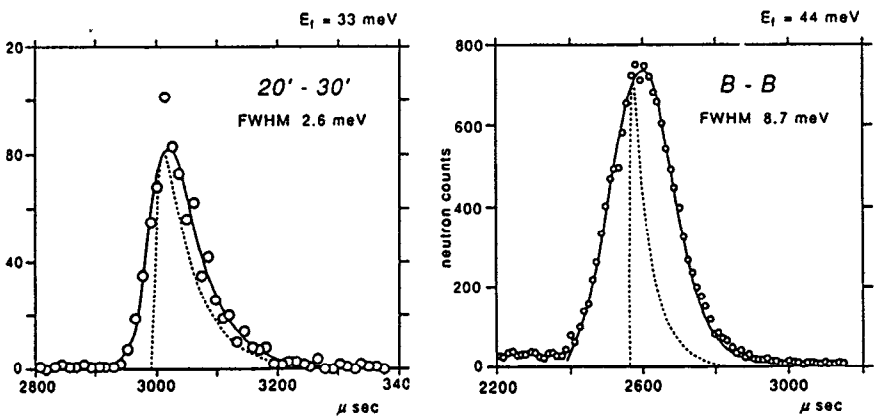

Fig. 3 Observed and calculated incoherent elastic peak profiles. Dotted lines represent the incident neutron pulse.

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Q(U.Steigenberger): Which improvements do you plan to increase the flexibility of MAX.
A(Y.Todate): N/A

Q(H.Tietze): Did you try to factorize the influence of the sample, i.e. its size, mosaicity etc., on the resolution function of MAX?
A(Y.Todate): The sample size effect is included in the resolution function, but the mosaicity is not.
Q(H.Tietze): What about the Q-resolution of MAX?
A(Y.Todate): ΔQ is about $0.1 Å^{-1}$ at $Q = 2 Å^{-1}$.