High Throughput Inelastic Spectrometer

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1 Introduction

The "High Throughput Inelastic Spectrometer" is intended to provide the neutron scattering equivalent of infra-red spectroscopy for studying molecular vibrations. It is expected to find applications in vibrational spectroscopy of the solid phase, adsorbed species, and hydrogen in metals and alloys. It will be installed initially at the Harwell linac as soon as possible and eventually moved to the SNS. Most of the specification given below apply equally to installation on either neutron source but a few apply specifically to installation at the Harwell linac. In particular, it will be noted in Figure 1 that there is space for two energy analysers (either side of the sample). On the linac, the beryllium filter will occupy one side while the other is used for developing a high resolution analyser system which will be incorporated into the machine when it is moved to SNS. Only the beryllium filter analyser will be discussed here.

2 Principle

A wide range of observable energy transfers can be obtained by detecting down scattered neutrons with a band pass filter-detector. If the energy of the detected neutrons is low compared with the incident energy, their scattering vector Q is practically independent of scattering angle. A high count rate can therefore be obtained by detecting neutrons over a large solid angle without losing the Q resoltuion.

$$Q = 0.7 \sqrt{E_o + E - 2\sqrt{E_o E}\cos 2\theta}\ \text{Å}^{-1} \qquad 0.7\sqrt{E_o}\ \text{Å}^{-1} \text{ for } E \ll E_o$$

where E_o (E) is the incident (final neutron energy in meV and 2θ is the scattering angle. The main limitation of this technique is that there is no possibility of varying Q independently of the energy transfer ($\hbar\omega = E_o - E$) but this is unimportant for many applications.

3 Construction

The primary spectrometer consists of a 12 m initial flight path with associated collimation, supports and vacuum system. A special sample cryostat would allow cooling of the sample to 10K to minimise the loss of intensity from the Debye-Waller factor and multiphonon effects but would permit rapid sample changes if required. The sample would typically be a cylinder 25 mm x 100 mm.

The analyser will consist of a nitrogen cooled beryllium filter which only transmits neutrons with less than 5 meV energy to an array of 25 mm 2 atm boron trifluoride counters. The filter will be 0.15 m thick and cover a solid angle of 1.1 str and will be divided into 24 sections separated by 1 mm thick B_4C loaded resin sheets. This arrangement provides adequate fast neutron discrimination without degrading the time resolution. The output from 3 groups of 4 detectors will be separately time sorted to allow for different background conditions and the spectral distribution of the incident beam will be obtained by time-of-flight analysis on the output of a U^{235} monitor before the sample.

A 0.025 mm gadolinium foil will be placed before the monitor in order to absorb neutrons of 5 meV and less which would be elastically scattered by the sample and cause a high background. Figure 3 shows a spectrum with (solid line) and without (dashed lines) the gadolinium. For a source with a pulse repetition period of 6.7 ms, it is clear that the gadolinium must be used.

4 Resolution

The energy transfer resolution of the instrument is dominated by the effect of the pass band (ΔE_2) of the filter with smaller contribution from the pulse width (Δt) from the ambient temperature moderator and the distribution of secondary flight-paths (ΔL_2). The three terms are:

$$T_1 = \frac{\Delta E_2}{\hbar\omega}\left[\left(\frac{E_1}{E_2}\right)^{3/2}\frac{L_2}{L_1} + 1\right]$$

$$T_2 = \frac{\Delta t}{\hbar\omega} \cdot \frac{2E_1^{3/2}}{2286\, L_1}$$

$$T_3 = \frac{\Delta L_2}{\hbar\omega} \cdot \frac{2E_1^{3/2}}{L_1 E_2^{1/2}}$$

where $\hbar\omega = E_2 - E_1$ meV is the energy transfer. The contribution from the distribution in initial flight-paths is negligibly small. The total energy transfer resolution is

$$\frac{\Delta\hbar\omega}{\hbar\omega} = \sqrt{T_1^2 + T_2^2 + T_3^2}$$

Using the design parameters (L_1 = 12.0 m L_2 = 0.24 m) the above expression has been evaluated for various values of $\hbar\omega$ and shown in Figure 2. It should be noted that ΔE_2 is not 5 meV but typically 1.7 meV FWHM because the long time side of the peak (eg in Figure 3) decays rapidly (approximately τ^{-4}).

5 Intensity

Figure 2 also shows the total counts in an inelastic peak from a 10% scattering sample. The inelastic peak is assumed to result from down scattering from the fundamental mode of an isotropic Einstein oscillator with unit effective mass (eg hydrogen in a metal). Figure 3 shows the time-of-flight spectrum that would be expected from such a sample with a fundamental frequency equivalent to 100 meV. The shape of the spectrum has been determined by the pass band of the filter only. Incorporating the effect of the moderator pulse width and the distribution of secondary flight paths would round the corners of the peaks considerably but would not change the total intensities.

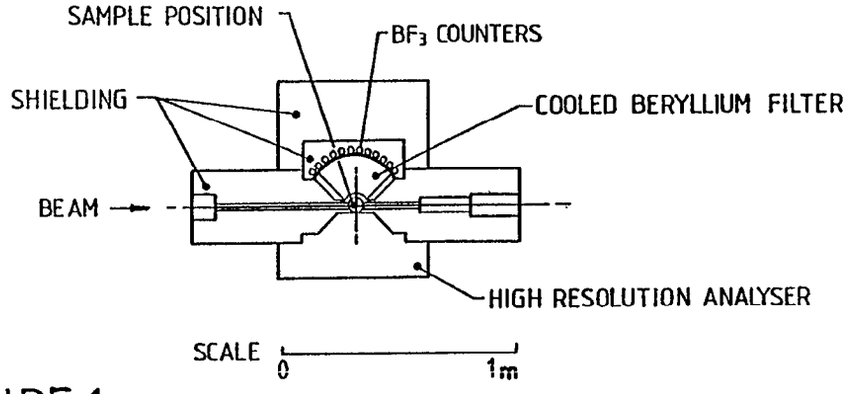

FIGURE 1

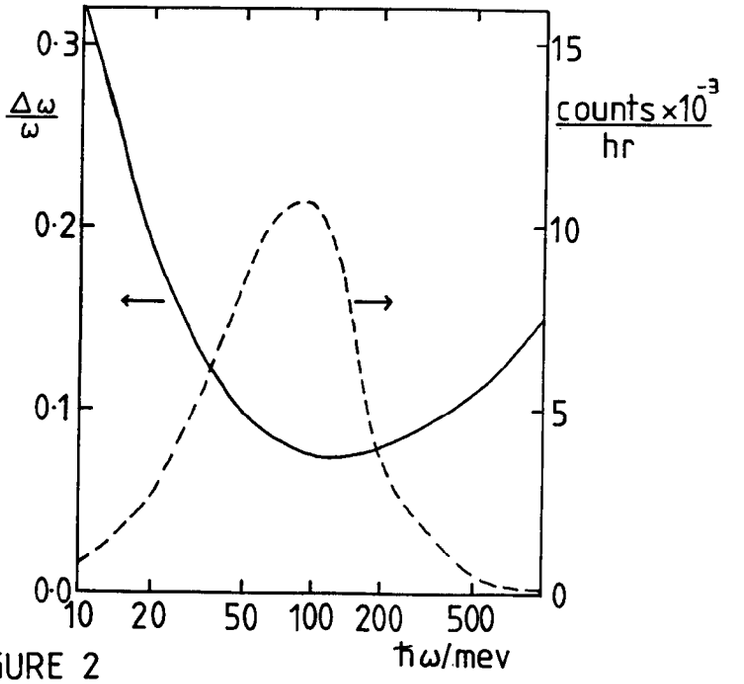

FIGURE 2

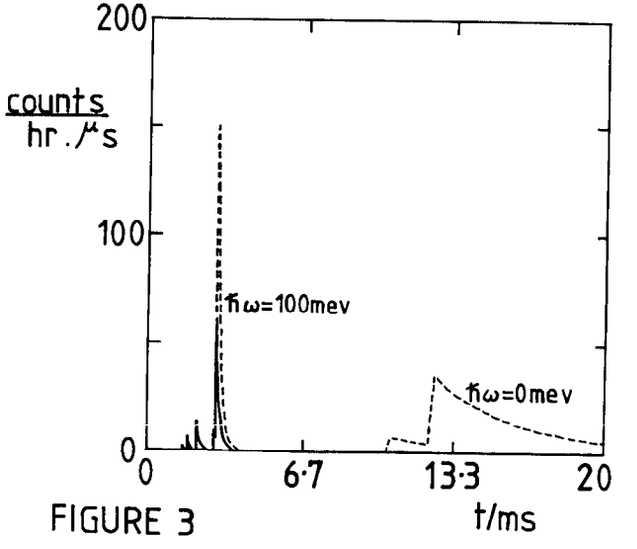

FIGURE 3