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# Progress with the PRISMA spectrometer

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**Abstract**
The PRISMA spectrometer is an indirect geometry multi-analyser instrument at the ISIS spallation neutron source, which is intended for the measurement of coherent excitations in single crystal samples. A brief description of the present status of the instrument is given and in light of this description aspects of the current spectrometer design which limit its use are discussed. Possible developments which may overcome these limitations are outlined.

## I. Introduction

The development of the PRISMA spectrometer at ISIS is a joint project between the Italian Consiglio Nazionale delle Richerche and the United Kingdom Science and Engineering Research Council. The participating laboratories in this project are the ISIS Facility at the Rutherford Appleton Laboratory, U.K. and the Istituto di Struttura della Materia, Frascati, Italy. The name PRISMA is derived from the acronym Progetto dell'Istituto di Struttura della Materia. PRISMA is designed for the measurement of coherent excitations (phonons, spin waves etc. ) in single crystal samples. An original design for such a spectrometer at ISIS was given by Andreani et. al. [1] and a recent description of the actual spectrometer and its initial performance has been given by Steigenberger et. al. [2].

The installation and commissioning of PRISMA was started in 1987 and since the middle of 1989 the spectrometer has been available for scheduled experiments at ISIS. However it is not the intention of this paper to describe these experiments but instead to discuss areas of the spectrometer design where we have, during commissioning and the recent experiments, identified the need for improvement. In section II we give a brief description of PRISMA, which is required in order to facilitate the discussion of improvements. For a more detailed description the reader is referred to ref. [2]. The improvements described in section III have already been, at least in part, implemented and we include a discussion of their initial performance, while those described in section IV are still under consideration. Finally section V contains a brief conclusion.

## II. Spectrometer Description

PRISMA is an indirect geometry multianalyser spectrometer. The sample is exposed to a

polychromatic neutron beam and the final energies of the detected neutrons (after scattering from the sample) are determined by an array of analyser-detector arms. From the total time of flight of the detected neutrons and a knowledge of their final energy the incident energies can be calculated. On PRISMA we have an array of 16 analyser-detector arms which are very closely spaced (2° apart) mounted on a single scattering arm which can rotate by ±120°. A schematic diagram of this arrangement is shown in figure 1. All of the analyser and detector angles can

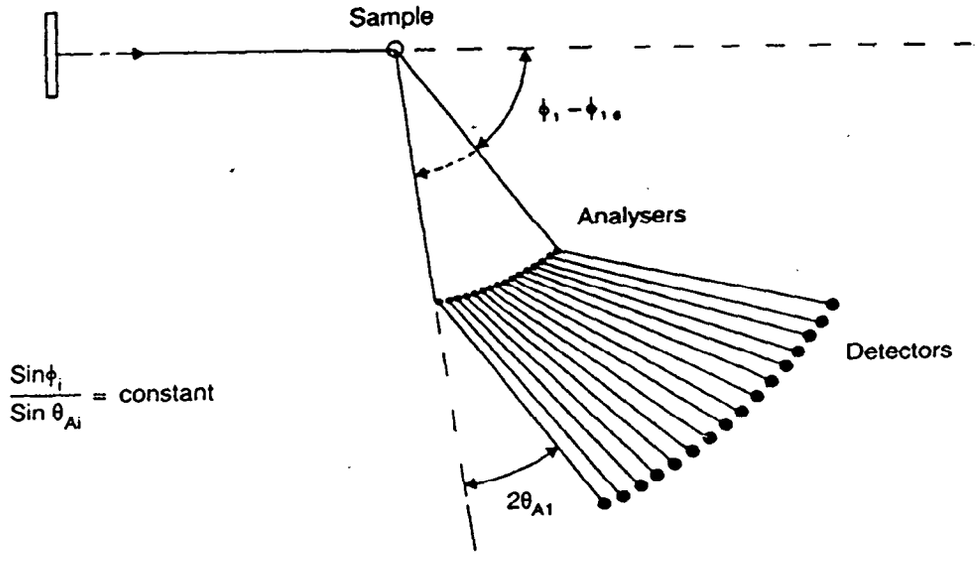


Figure 1: A schematic diagram of the PRISMA spectrometer.

be moved individually subject to the condition that the detector arms do not collide. In figure 2 we show how the wavevector transfer $\mathbf{Q} = \mathbf{k}_i - \mathbf{k}_f$ varies during a measurement on PRISMA. A high symmetry direction in the crystal is aligned parallel to $\mathbf{k}_i$. Since $\mathbf{k}_f$ is fixed in direction and length for a particular detector the wavevector transfer scans along the direction given by the dashed line in figure 2 as a function of the length of $\mathbf{k}_i$ (ie. time of flight). It is possible for all of the analyser detector systems to measure along this same direction (ie. the dashed line) if they have different values of $|\mathbf{k}_f|$. The condition for this situation is that the Bragg angle $\theta_A$ of the analyser crystal and the scattering angle $\phi$ for each analyser-detector system are related by the equation :

$$Q_\perp = \frac{\pi}{d_A} \frac{\sin\theta_A}{\sin\phi} \tag{1}$$

where $Q_\perp$ is the component of the wavevector transfer perpendicular to the direction of the incident neutron beam and $d_A$ is the d-spacing of the analyser crystal planes. The energy transfer measured in each analyser detector system is therefore given by :

$$E = \frac{\hbar^2}{2m}\left(Q_\parallel^2 - 2(Q_\perp \cot\phi)Q_\parallel - Q_\perp^2\right) \tag{2}$$

Since the scattering angles $\phi$ are different for each of the analyser detector systems the energy transfers measured at a given wavevector on the dashed line in figure 2 are different and the spectrometer performs a net of scans in the $(E, Q_\parallel)$ plane.

## III. Recent Developments

It is always desirable in a scattering experiment to have the background as small as is practical, and this is especially true for inelastic scattering where the cross-sections for phonons etc.

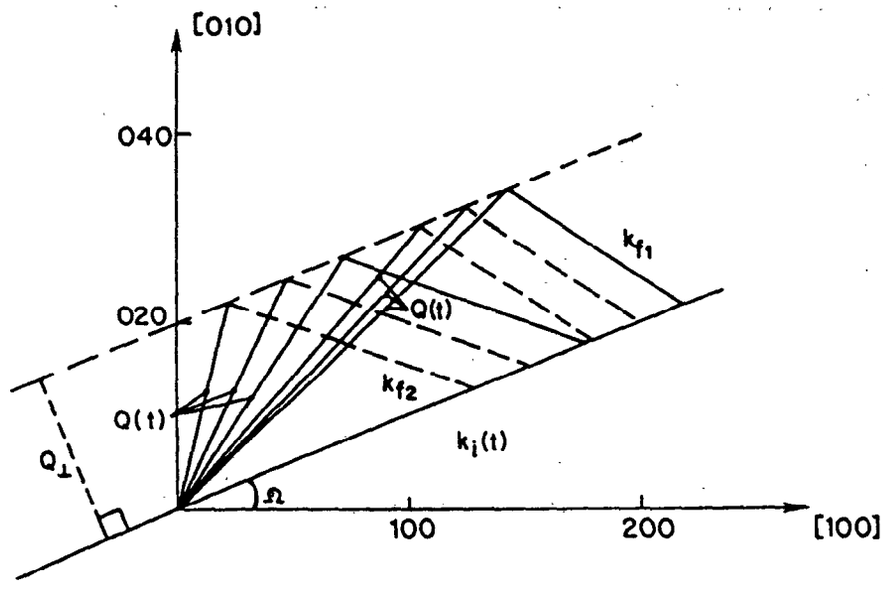


Figure 2: The vector triangles in reciprocal space representing the wavevector transfers in a scattering measurement on PRISMA.

are $\approx 10^{-5}$ those for Bragg scattering. On PRISMA we have found that the background (with a non-hydrogenous sample) for scattering angles $\phi \geq 40°$ is about 25 counts/meV transfer/day with ISIS running at $100\mu$A proton current and a $U^{238}$ target. This background originates from 3 approximately equal sources. There is an ambient background, with the beam on but no sample (or sample environment equipment) of $\approx 8$ counts. It should be noted that these counts are neutronic and that the electronic background is considerably less than this level. The remaining $\frac{2}{3}$ of the background is associated directly or indirectly from the sample. We have discovered that when the direct path from the sample to the detector via the analyser is blocked by absorber but the sample is in position then the background is increased by a further 8 counts above the ambient. This presumably arises from the effect of scattering (predominantly Bragg) by the sample into the surrounding shielding. The remaining 8 counts therefore arises from direct scattering from the sample via the analyser to the detector. This background is flat as a function of energy transfer. We presume it arises from elastic incoherent scattering both at the sample and at the analyser.

For scattering angles $\phi < 40°$ the background was found to increase rapidly with decreasing scattering angle. A significant part of this increase was discovered to be due to neutrons with energies $E > 270$ meV (which is the absorption edge of Cd). Much of the shielding around the detectors on the scattering arm is Cd since this shielding must be thin. This latter point will be discussed further in section IV. In order to reduce the background at low $\phi$ we have recently installed a background chopper in the incident beam line. This chopper limits the wavelength band which is seen by the sample. This is achieved by blocking the incident neutron beam at $t \approx 0$, i.e. the time when the proton pulse hits the target with a block of nimonic material. The size of the nimonic block is such that it covers completely the aperture of the beam for a time period of about $255\mu$s at a chopper frequency of 50Hz. The effect on the incident spectrum is shown in figure 3. Here the ratio of two normalised monitor spectra is plotted (monitor with chopper / monitor without chopper) as a function of incident energy. The reduction in the number of neutrons with energies greater than 500meV is clearly visible. The chopper is

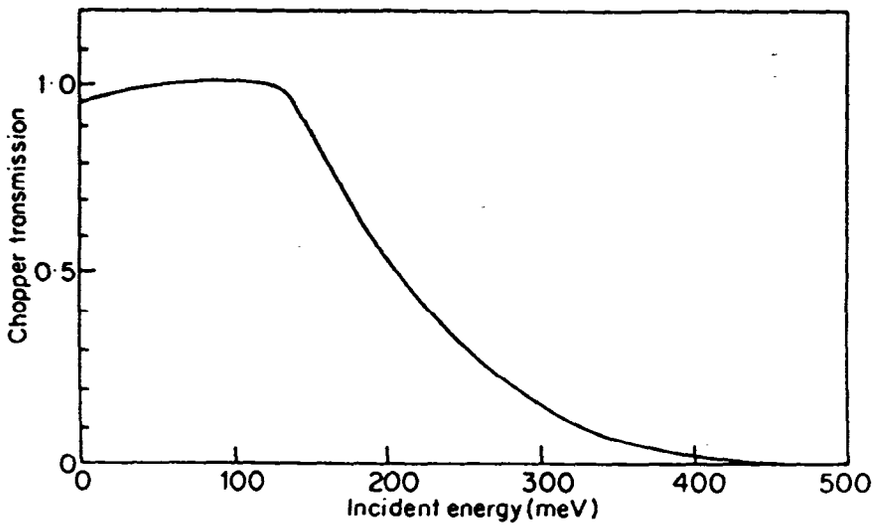


Figure 3: The chopper transmission spectrum.

additionally equipped with a tailcutter disk (12mm thick, 90% Mg, 10% Cd) which blocks the very low energy neutrons between 6667$\mu$s and 20000$\mu$s when running at 50 Hz. As the chopper has two nimonic blocks separated by 180°, an alternative option is to spin it at 25Hz. This doubles the time during which the nimonic part covers the beam, although such a mode would require the removal of the tailcutter disk.

As well as reducing the background, work is also being carried out on increasing the measured intensity for certain experiments by having the different analyser crystals available. At present on PRISMA we are using cylindrical Ge crystals with a $[1\bar{1}0]$ axis perpendicular to the scattering plane as analysers. This allows us to employ the (111), the (400) and the (220) reflections for analysis. The virtue of using the (111) reflection lies in the fact that second order contamination is absent due to the zero structure factor of the (222) reflection in the diamond crystal structure. The structure factors of the (220) and (400) reflections are twice that for the (111) reflection but have the disadvantage of second order contamination.

We are planning to have available a second set of analyser crystals of highly oriented pyrolytic graphite (HOPG). The high reflectivity of HOPG will allow us to gain a significant increase in measured intensity for experiments where the desired energy transfer range will not be contaminated by second order reflection from the analysers. HOPG is available from the Union Carbide corporation in two forms, one with mosaic spread 0.4° and one with mosaic spread 0.8° in various thicknesses. The choice of which form to use to maximise intensity without degrading resolution depends upon the effective collimation of the spectrometer after the sample. In order to be sure that we optimise our intensity we have performed test measurements on PRISMA using two samples provided by Union Carbide. Sample #A had a mosaic spread of 0.4° and was 2mm thick, and sample #B had a mosaic spread of 0.8° and was 4mm thick. We masked the samples to have identical surface area in the polychromatic beam on PRISMA and positioned one detector to view the sample at a scattering angle corresponding to a neutron energy of 15 meV. The results are shown in figure 4 for both sample #A and sample #B. Clearly the line width in energy is the same for both samples but the reflectivity of sample #A is higher by nearly 50%.

We have also compared the HOPG #A sample with a Mica analyser and one of the present Ge analyser crystals (c.f. figures 5a-c) for similar energies. The d-spacings of the Ge (111)

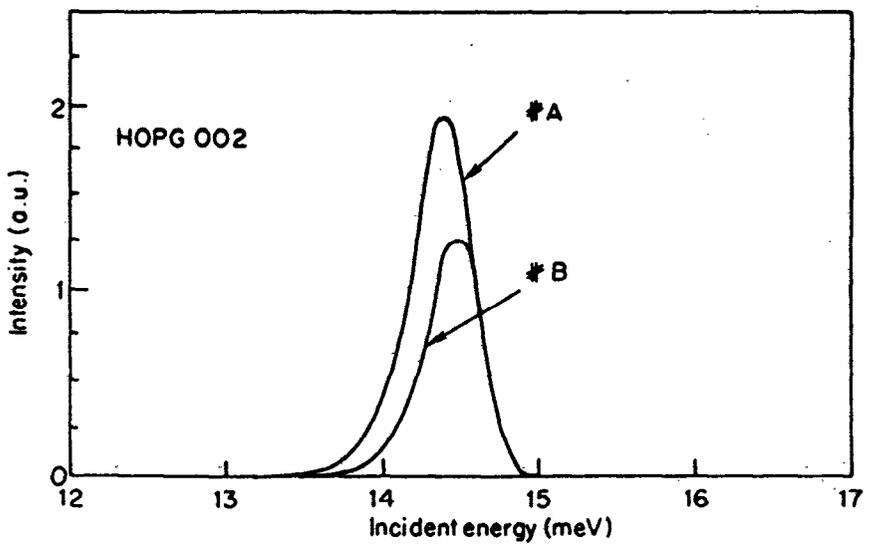


Figure 4: The relative reflectivity of two highly oriented pyrolitic graphite crystals is shown for neutrons with an energy of 15 meV. Sample #A had a mosaic spread of 0.4° and sample #B a mosaic spread of 0.8°.

reflection of 3.266 Å, the HOPG (002) reflection of 3.355 Å and the Mica (003) reflection of 3.334 Å are all quite similar (the possible usefulness of this similarity will become more apparent in the next section. Mica is a 2-dimensionally layered aluminia-silicate and the lattice constant perpendicular to the layers is around 10 Å depending on the exact chemical composition. We have used thin sheets of natural amber Mica, tightly packed to give an overall thickness of 3mm. As can be seen from figure 5b the resolution for the Mica (003) reflection at an analysing energy of 27 meV is about 1.29 meV and lies in between the values of 1.56 meV for the Ge (111) reflection and 1.0 meV for the HOPG (002) reflection. Although the measurements were performed for very similar settings of the spectrometer angles, it is not possible to make a comparison of the absolute reflectivities, because of the different sample geometries. However, the intensity difference between HOPG and Mica is too large to be explained by geometry alone hence Mica must have a lower reflectivity. Our interest is not therefore primarily in using the (003) reflection but the possibility of using the (001) reflection. At present the minimum analysing energy that can be used on PRISMA is 18 meV (again this point is discussed further in section IV). The use of Mica (001) would, for the same range of $2\theta_A$ angles available at the moment lower this minimum limit to 2 meV. Although correspondingly it will of course lower the upper limit as well. However the possibility of such low analysing energies is attractive for certain low energy transfer experiments. A careful evaluation of possible problems such as, the lower reflectivity, contamination from the (002) reflection or linewidth effects from using energies in the range of the Maxwellian of the methane moderator is required.

## IV. Possible Future Developments

In order to obtain a densely packed net of scans in the $(E, Q_{\|})$ plane the analyser-detector systems are close together at only 2° separation. This can be compared with the much wider angular separation on the very similar spectrometer MAX at the KENS spallation source [3]. However the small angular separation on PRISMA leads to two serious restrictions. Firstly, as was alluded to in section II, the measuring configuration described can only be used if the detector arms are in an arrangement where they do not collide. This depends upon the

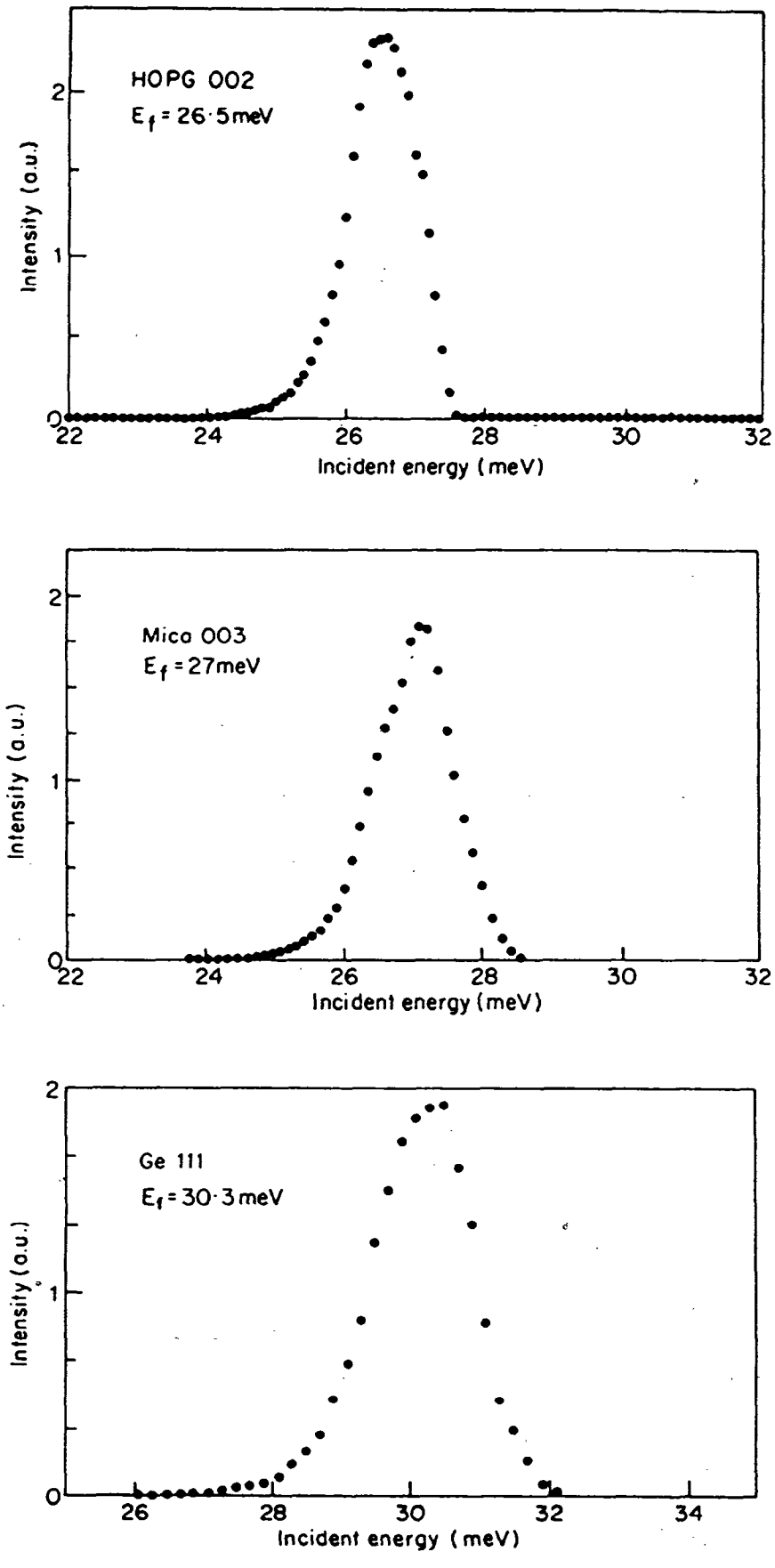


Figure 5: The measured scattering from analyser crystals of (a) HOPG (002), (b) Mica (003) and (c) Ge (111) at energies of 26.5, 27 and 30 meV respectively.

distances involved as well as the angular separation. On PRISMA the sample-analyser and analyser-detector distances are 573mm and 170mm respectively and each arm is 12mm across. Further to this there is an overall maximum $2\theta_A$ angle for any detector of 38° set by the shape of the frame supporting the arms. For the Ge (1,1,1) analysing planes this means a minimum analysing energy of 18 meV. These limitations impose severe restrictions on the E range accessible for small values of |Q|. In figure 6 we show the available range using Ge (1,1,1) analysers for two cases, (i) where only one detector is used and the remaining 15 are driven as far out of the way as possible and (ii) where all 16 detectors are used. It should be noted that

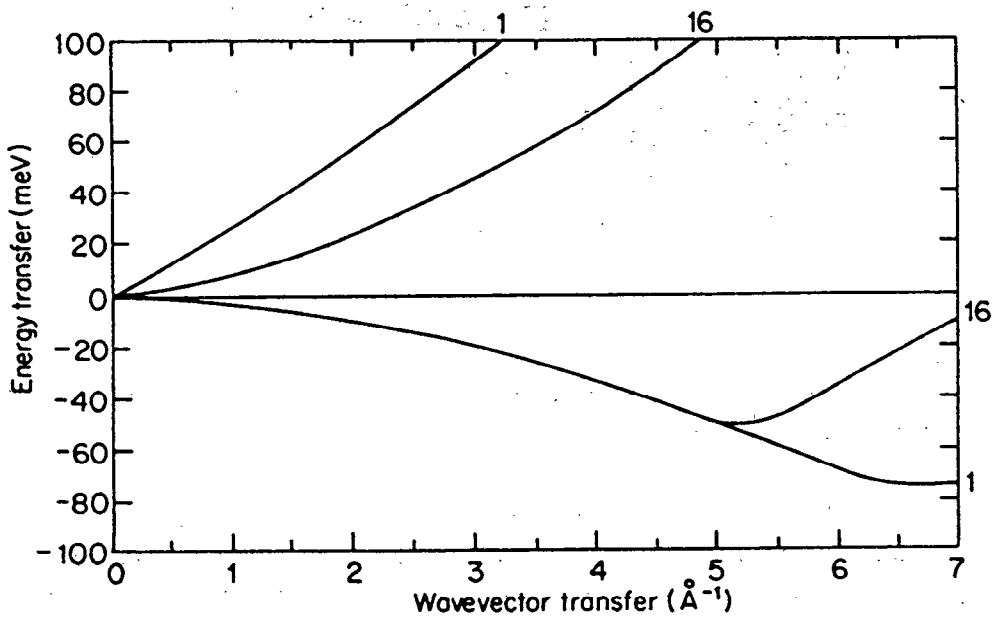


Figure 6: The possible minimum and maximum energy transfers are shown as a function of the magnitude of the wavevector transfer for the cases of 1 and 16 analyser-detector systems in use, as described in the text.

this figure applies to |Q| and that in a single crystal experiment where a particular direction as well as magnitude is required the situation may well be worse.

The second side effect of the small angular separation is that the shielding around each detector arm must be small in order to allow the arms to approach each other as close as posssible. On PRISMA we have 1mm of Cd around each detector arm. Around the whole array of arms there is a further "shielding box" of $B_4C$ and Cd but this is not as preferable as having a significant amount of shielding around each individual detector.

These constraints could be overcome by the use of a double-bounce analyser system as schematically indicated in figure 7. In such an arrangement a change of the analyser energy would not require the detector to move. Furthermore, increasing the angular separation between the detector arms would enable us also to improve substantially the shielding around the detectors. Of course, the double reflection will lead to loss of intensity. However, by a suitable choice of analyser material this can be minimized. Obviously these intensity considerations exclude the combination Ge/Ge and mean that an HOPG/HOPG combination would be best. However an alternative combination of Ge(111)/HOPG(002) which profits from the absence of second order contamination due to the first Ge crystal without the loss of reflectivity of a second Ge crystal may also be a possibility. Although the outcoming beam from such an analyser is not parallel to the incoming beam its deviation for analyser energies greater than

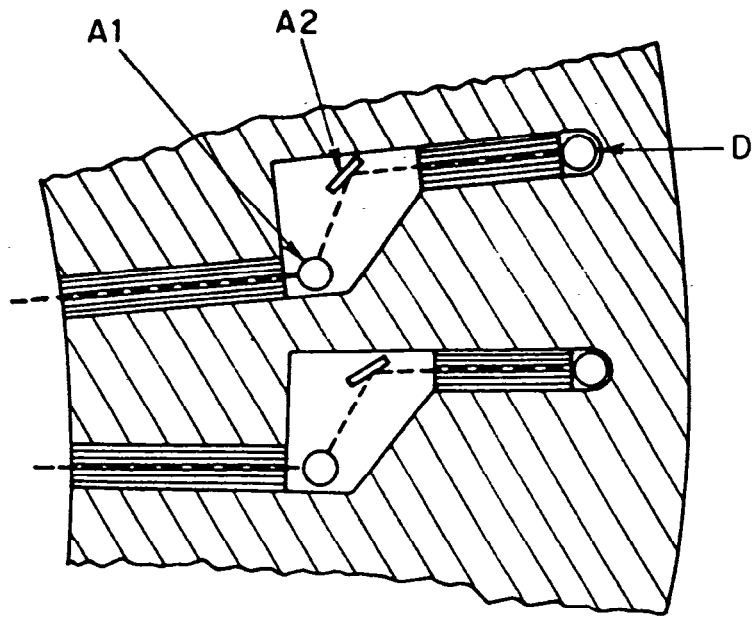


Figure 7: A schematic diagram of a double-bounce analyser system. A1 and A2 indicate the two analyser crystals and D the detector.

4 meV is less than 3°. We have started a research and development programme to study the feasibility of these ideas. The prototype of a double-bounce analyser should be ready by the end of next year and we plan to study a series of combinations of analyser crystals.

## V. Conclusion

The PRISMA and MAX spectrometers have both shown that measurements of phonon or spin wave dispersion relations are quite feasible at pulsed neutron sources. This does not mean, however, that these particular spectrometers necessarily represent the ultimate design for instruments to carry out such measurements. In this paper we have described a number of ideas for improving and expanding the capabilities of the PRISMA spectrometer. These ideas are at different stages of development and their effectiveness remains to be assessed. However such is the usefulness of the information from the measurement of coherent excitations that they are certainly worth pursuing.

## Acknowledgement

Our thanks go in particular to the ISIS chopper group for their support and to our colleagues at ISIS for many useful discussions.

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Q(H.Tietze): The 30meV phonon in $D_2O$ is only poorly separated from the elastic central line. Is that resolution of PRISMA dominated by the sample or by the instrument itself?

A(U.Steigenberger): In that case the resolution is limited by sample properties, because of disordering in the $D_2O$-sample.

Q(N.Watanabe): Is the $D_2O$ sample the single crystal?

Do you think the liquid $CH_4$ moderator has advantage than a room temperature moderator for typical PRISMA experiments? Is time structure of neutron pulse important?

A(U.Steigenberger): Yes, the $D_2O$ sample is a single crystal.

The time structure of the neutron pulse has certainly an influence on the resolution of the instrument. On the other side, resolution appears to vary so rapidly as a function of time of flight due to other effects that we are not too concerned about the contribution from the neutron pulse width.

Q(H.Tietze): Do you think of using a Si-multi-layer crystal as a tiny device for double analysers on PRISMA or would the intensity obtained from double-Si-analysers be too weak?

A(U.Steigenberger): It is thought of wing PG together with the existing Ge-analysers, which will them be moved independently.

Q(P.A.Egelstaff): Could you expand your statement that 1μeV resolution with 20Å neutrons is available on ISIS? For example if we wished to study the quasi-elastic peak for a polymer and its width was 1μeV, should we go to the ILL or to ISIS? Some data on counting rates, energy ranges and experimental times would be useful.

A(U.Steigenberger): For Mica 002 the energy transfer range is 90 meV, which is an order of magnitude larger than that of IN10, the lutedine data were taken in 12 hours. Of course the flux at $\lambda = 20$Å is much bigger at ILL, in particular because the ISIS moderator was not designed to provide neutrons at this wave length.