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RECENT PROGRESS ON eVS

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ABSTRACT
The development of eVS at ISIS is reviewed.

I. INTRODUCTION

The electron volt spectrometer (eVS) is dedicated to measuring atomic momentum distributions in condensed matter. At sufficiently high energy and momentum transfers the impulse approximation is valid and the scattering is identical to that which would be obtained from a free gas of atoms, with a momentum distribution identical to that of atoms in the target system. The neutron scattering cross-section is then related in a simple way to the atomic momentum distribution function by conservation of energy and momentum, as in 'billiard ball' collisions. These 'Deep Inelastic Neutron Scattering' measurements are possible only on pulsed neutron sources such as ISIS, which have sufficient intensities at the neutron energies required for the impulse approximation to be valid. eVS is an inverse geometry spectrometer, where the filter difference technique is used to analyse the energy of scattered neutrons at energies greater than 4 eV. This enables energy transfers between 10 and 30 eV and momentum transfers greater than 100 $Å^{-1}$ to be obtained.

The technique is particularly valuable for the investigation of hydrogen potentials in, for example, hydrogen bonds or metal hydrides. It gives direct information on the hydrogen wavefunction, which is complementary to the information on energy eigenfunctions obtained by conventional neutron spectroscopic techniques. A preliminary measurement on the anisotropy of the proton momentum distribution in a single crystal of $KHCO_3$, has given very promising results, despite the non-ideal instrument geometry [1]. The rms momentum components parallel and perpendicular to the hydrogen bond were found to be significantly different and were in excellent agreement with calculations using a potential derived from previous neutron spectroscopic measurements.

The time-of-flight scans for the measurements on $KHCO_3$ are shown in Figure 1. In the impulse approximation the neutron scattering function $S(Q,\epsilon)$ is peaked along the 'recoil line', $\epsilon = Q^2/(2M)$ where M is the atomic mass. This corresponds to scattering from a stationary atom with conservation of energy and momentum. The atomic motion Doppler broadens $S(Q,\epsilon)$ into a function of width $\simeq pQ/M$, at constant Q, where p is the rms atomic momentum. The recoil line and the measured FWHM of $S(Q,\epsilon)$ are also shown in Figure 1. The position at which the scans cross the recoil line determine the energy and momentum transfers at the peak position. It can be seen from this that an energy transfer of $\simeq$ 20 eV and momentum transfer of 50 $Å^{-1}$ were obtained at the highest scattering angle. These values are respectively 100 and 10 times greater than those obtainable on reactor sources and should ensure that the impulse approximation can be used with confidence.

Typical time-of-flight scans are illustrated in Figure 2 It can be seen that the hydrogen peak (the left hand peak) is well separated from the peak obtained from K, C, O and Al atoms in the sample and sample holder. This easy separation of the hydrogen scattering is one of the advantages of the technique. As the scattering angle increases, the hydrogen peak moves to higher energy transfers (and hence shorter times since eVS is an inverse geometry instrument).

It is anticipated that many of the experiments during the next year will measure the anisotropy of the proton momentum distribution in single crystals. eVS has been redesigned for such measurements. Two banks of detectors at ±45° allow for the simultaneous measurement of the distribution of momentum components along directions separated by 90°, with good resolution. More sophisticated data analysis should facilitate the measurement of the shape of the atomic momentum distribution, rather than simply mean momentum components.

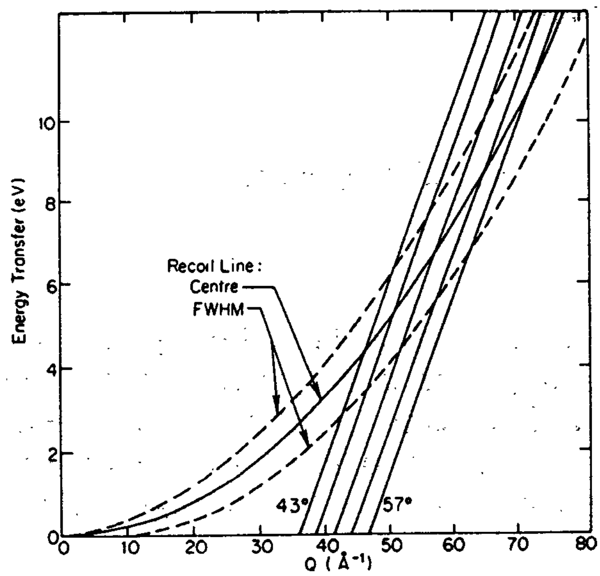

Figure 1. Time-of-flight loci from the 4.906 eV Au resonance analyser used in the momentum distribution measurements on a single crystal of $KHCO_3$.

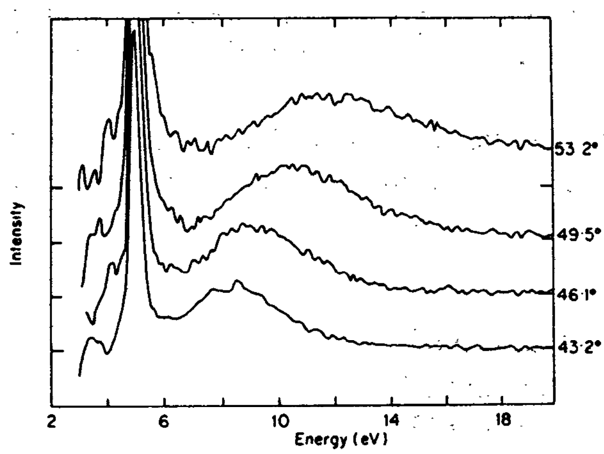

Figure 2. Recoil scattering from $KHCO_3$ with momentum transfer along the hydrogen bond. Scattering from hydrogen occurs at high energies/short times and is well separated from that due to heavier atoms.

References

[1] P Postorino, F Fillaux, J Mayers, J Tomkinson and R S Holt
Anisotropy of the Proton Momentum Distribution in Single Crystal $KHCO_3$
J Chem Phys 1990 (in press)