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Numerical simulation study of the performance of a small neutron three axis spectrometer

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ABSTRACT

This article describes Monte Carlo computer simulations comparing the performances of a conventional neutron three axis spectrometer (TAS) and a micro-TAS, a μTAS, designed to be as compact as seems practical. The simulations show that the μTAS delivers performance (intensity at equal resolution) equivalent to that of a normal TAS. The μTAS should be very cheap to build and a "farm" of several such small machines at a single conventional instrument position should greatly increase the TAS beam time available from a given source. A μTAS can deliver significantly larger beam angular divergence at the sample and detector, thus extending the accessible resolution-intensity range, whether using flat or curved monochromating crystals.

1. Introduction

Neutron scattering is a powerful tool in scientific studies of condensed matter because the neutron is a penetrating probe, scatters from both atomic nuclei and magnetic moments and has energy and momentum similar to those of excitations in solids. Neutron scattering remains something of a technique of "last resort" because neutron sources are both very expensive and very feeble and neutron transport from the source to instrument detectors is extremely inefficient. Thus, performance improvements for neutron scattering instruments are highly desirable.

Neutron three axis spectrometers (TAS) [1], consist of a source, crystal monochromator, sample and analyser and a detector. Beam restrictions (slits or Soller collimators) are often placed in the four instrument arms to control the allowed beam divergence. In the early years of neutron scattering, TAS were often used as workhorses because they can measure any accessible combination of sample energy and wave-vector transfer and they have great flexibility in intensity-resolution trade-off. However, conventional TAS measure only one point at a time and neutron inelastic scattering cross-sections are extremely small so counting is usually very slow indeed even by the standards of a field used to slow data acquisition. The need for often difficult to obtain large single crystal samples to overcome these inherently low count rates further restricts TAS usefulness. Most neutron scattering research is now done using more specialised and less versatile but much faster machines. TAS remain useful because of their unique ability to closely examine scattering with a particular wave-vector and energy transfer and thus definitively answer specific questions.

TAS are usually very large, heavy instruments of order 5 m long weighing 10's of tonnes. This large size was originally dictated by the need for heavy monochromator shielding against fast neutrons and gamma rays at reactor sources (typically 1 m thick) and by the large beam areas needed to illuminate big samples. Space must be allowed for beam elements such as collimators and monitors and for sample environment on the instruments. In practice, it is quite difficult to reduce monochromator-sample distances to less than 2.5 m. Building such large specialised machines, which need great positioning accuracy, needs expensive custom made parts. Using a guide tube source reduces the monochromator shielding needs and monochromator-sample distances of about 1.75 m are achievable but other dimensions are normally unchanged. Such large distances limit the beam angular divergence and thus the beam intensities possible.

On an optimised spectrometer, to increase count rates one must increase source intensity, reduce transmission losses to the detector or reduce resolution (increase angular or wavelength spread). TAS now often accept poor resolution to increase counting speed and even larger angular divergence and lower in-plane

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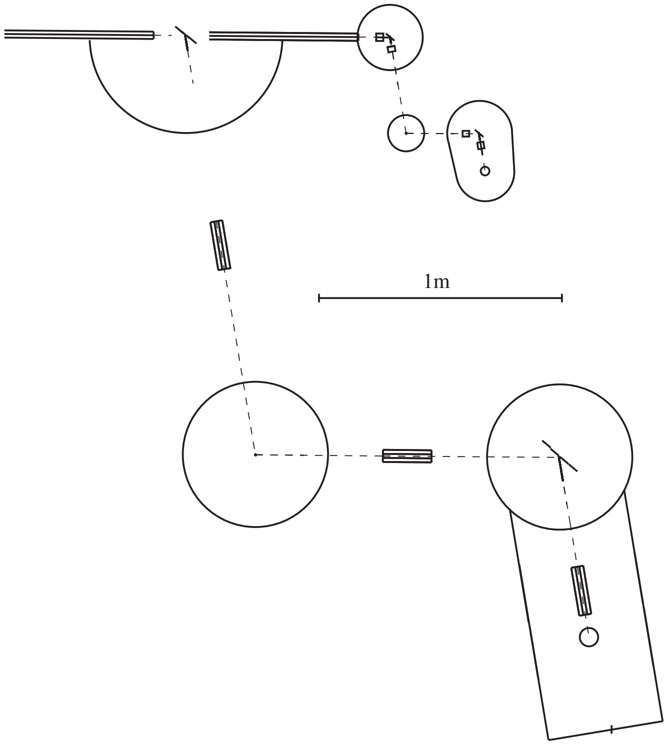

Fig. 1. Schematic diagram showing the standard TAS and μTAS on a guide drawn to the same scale.

resolution than is currently possible would sometimes be useful. TAS count rates have been greatly improved, most recently by work concentrating on using large double curved monochromators and analysers [2], developing effective multi-detector arrangements [3–7] and using Monte Carlo computer simulations to seek better instrument set-ups [8–11]. These intensity gains have made it possible to use smaller samples (now typically $5\times 10\,\mathrm{mm}^2$ – wide × high), which is important because interesting new materials are often only available as small crystals. Several as yet incomplete development avenues for TAS are the perfection of focussing monochromators and analysers, finding optimum instrument configurations and reducing instrument length to increase the range of angular divergence accessible. This article explores the effect of reducing TAS size to the current practical limit.

Fig. 1 illustrates the μTAS ("micro-TAS") instrument proposed here compared in plan view to a conventional size TAS. A μTAS should benefit from reduced construction cost, larger natural beam divergences, increased monochromator focussing gains and possibly reduced noise. A μTAS needs only a small beam area so efficiency in using the available neutrons may be increased by siting several such independently functioning μTAS at a single normal beam position, thus creating a "TAS farm" as shown schematically in Fig. 2.

2. Design considerations for a μTAS

This section discusses the feasibility of building a μTAS designed for samples with a maximum size of $5\times 10\,\mathrm{mm}^2$ ($W\times H$). Shielding thickness and sample environment size are the main restrictions to reducing TAS size. The shielding must be thick enough to keep the instrument background low. Radiation shielding on neutron scattering instruments must attenuate gamma rays, fast neutrons and slow neutrons. Because radiation shields are usually quite large, the cost of materials is an important consideration. Efficient compact shields for low energy γ-rays simply need a high density but high energy γ-ray shields work better if they include heavy nuclei so lead is a good choice fulfilling both these needs. γ-rays of about 2 MeV require the thickest shields. Slow neutrons can be effectively shielded by thin layers of strongly absorbing materials like Gd, Cd, B or Li but neutron capture almost always produces secondary γ-rays, which must then be shielded. While Li emits no γ-rays it has a relatively small neutron absorption cross-section. B emits only low energy γ-rays and is usually the slow neutron shielding material of choice. Shielding fast neutrons with energy below 1 MeV is best done using hydrogenous material like paraffin wax or polyethylene (PE) to slow the neutrons. Boron is often included to capture the slowed neutrons without the emission of energetic gamma rays. Neutrons of energy above 1 MeV are most practically shielded by a large thickness of iron or an even larger thickness of hydrogenous material. A reactor face shield must control intense fast neutron and γ-ray fluxes and is usually made from thick heavy concrete or borated paraffin with iron included. A reactor face position is not likely to be practical for a μTAS.

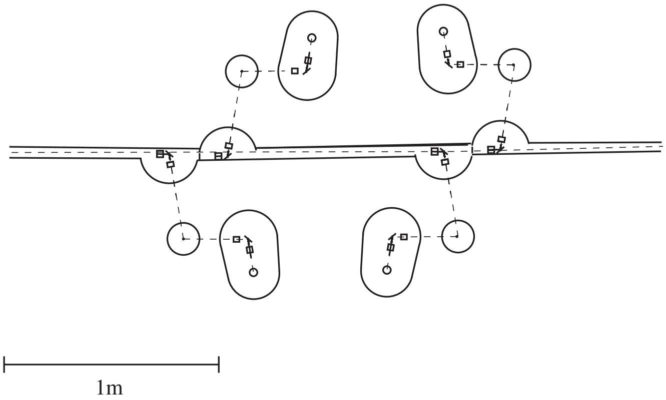

Fig. 2. Schematic diagram of a μTAS "farm". Each machine would use a separate small section of the total guide beam and operate independently.

Guide tube beams are designed to have no direct line of sight to the reactor so fast neutrons are few and careful shielding of the guide tube itself should mean that fast neutrons and primary gamma rays are of little concern for an instrument in a guide hall. Monochromator shielding on a guide tube need only manage scattered thermal neutrons and any secondary γ-rays produced. The best practical thermal neutron shield (such as a beam stop) is a sheet of boron backed by a lead block. Both calculation and experience show that a 5 or 10 mm thick layer of boron containing plastic is sufficient to effectively shield the full beam from a normal neutron guide (of order $10^{10}\,\mathrm{n\,cm^{-2}\,s^{-1}}$) and 10 cm of lead is enough to shield the secondary gamma rays produced. Instrument monochromators produce secondary γ-rays, which must be shielded but if the monochromator material choice is restricted to graphite, silicon or even germanium this problem is not too severe. Copper monochromators require substantial shielding and probably need to be avoided for the μTAS.

Experience shows that TAS in guide halls can have background of 1 count per minute or less, except when the detector shield itself moves into the main instrument beam. This background comes mainly from detector electronic noise, air scattering from the main beam, scattering from the sample environment and scattering from instrument components such as beam elements and the shielding itself. Background from the sample itself cannot be avoided. TAS analysers and detectors usually use borated polyethylene (B-PE) shields between 10 and 20 cm thick although B-PE is a fast neutron shield so its use is probably based on