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B. E. F. Fender, L. C. W. Hobbis and G. Manning

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The U.K. Spallation Neutron Source

By B. E. F. Fender†, L. C. W. Hobbis‡§ and G. Manning‡
† *Inorganic Chemistry Laboratory, South Parks Road, Oxford OX1 3QR, U.K.*
‡ *Science Research Council, Rutherford Laboratory, Chilton, Didcot, Oxon. OX11 0QX, U.K.*

Pulsed neutron sources offer an attractive route for the realization of effective fluxes greater than those currently available from high flux reactors. The spallation neutron source now under construction at the Rutherford Laboratory will produce intense bursts of fast neutrons through interactions of 800 MeV protons with a heavy metal target. The fast neutrons are slowed down in nearby hydrogenous moderators viewed by some 20 time-of-flight neutron scattering instruments. The spectrum of the moderated neutrons is strongly enhanced in the high velocity region compared with that from a reactor. The new source will be comparable with the best beam reactors for experiments with neutrons of mid-thermal energy, and will provide unrivalled potential for use of the epithermal neutrons. Areas of science that will benefit immediately are the study of liquids and amorphous materials, high energy excitations in crystalline materials, molecular spectroscopy, surface phenomena and kinetic processes, as well as a range of crystallographic applications.

1. Introduction

A high intensity pulsed neutron source is being built at the Rutherford Laboratory for use in condensed matter research. The main attraction is that by using a high intensity proton accelerator to produce intense bursts of neutrons from heavy metal targets, effective neutron fluxes can be generated that, for many neutron scattering experiments, will be significantly greater than those available from the best steady-state reactor sources that exist today or are likely to be built in the foreseeable future. This paper aims to explain how this comes about and outlines the Spallation Neutron Source (S.N.S.) project (Hobbis *et al.* 1977) which started in mid-1977.

So far, most condensed matter research with neutrons has been done with the use of steady-state reactors, but even the most powerful reactor beams are very weak in comparison with the photon intensity from a laboratory X-ray source and ever higher neutron intensities are therefore continually in demand. However, it is generally agreed that the steady-state reactor is already close to its technological and financial limits. The use of pulsed neutron beams provides a solution.

2. Pulsed sources

In a diffraction experiment at a reactor, a monochromating crystal is normally used to define a narrow wavelength band of neutrons incident on the sample, and the various Bragg reflexions must be sought at different scattering angles; most of the neutrons in the initial beam are discarded. In the corresponding pulsed source experiment, time-of-flight is used to

§ Present address: Science Research Council, Central Office, North Star Avenue, P.O. Box 18, Swindon SN2 1ET, U.K.

define the velocity (wavelength) of the diffracted neutrons and in principle none of the neutrons in the initial 'white' beam need be discarded; a fixed scattering angle can be used, although in practice several banks of counters are normally employed to improve counting rates. In the steady-state experiment a narrow wavelength band is used continuously; in the time-of-flight experiment a wide wavelength band is used for short periods.

For the ideal time-of-flight inelastic experiment, energy analysis by, for example, crystal reflexion measures final energy and is combined with overall time-of-flight data to define incident neutron energy in the so-called inverse geometry. Again a wide wavelength band pulsed incident beam is used. In contrast, in a steady-state triple-axis experiment a narrow wavelength band beam is incident on the sample. In inelastic experiments with choppers to define the incident energy, it is clearly the instantaneous pulsed source flux that has to be compared with the steady-state reactor flux.

TABLE 1. NEUTRON PRODUCTION PROCESSES AND SOURCES

			practical sources		
process	neutron yield per incident particle	target energy per neutron / MeV	source	fast neutron yield/10^{15} ns^{-1}	target power / MW
$(e\gamma)$, (γn) in heavy target	4×10^{-2}/60 MeV electron	1500	new Harwell linac	0.2	0.045
^{3}H (^{2}H n)α	*ca.* 10^{-4}/300 keV deuteron	*ca.* 10^4	intense neutron source project, Los Alamos	*ca.* 1	0.3
fission	(*ca.* 1/fission)	*ca.* 200	I.L.L., Grenoble	*ca.* 2000	57
proton spallation non-fissile target	*ca.* 14/800 MeV proton	*ca.* 30	S.N.S., Rutherford Laboratory	*ca.* 20	0.09
fissile target	*ca.* 30/800 MeV proton	*ca.* 55		*ca.* 40	0.35

The general reasoning above, supported by detailed examination of representative experiments, leads to the conclusion that a pulsed source may achieve the same effective flux as a steady-state source but with greatly reduced mean power. Practical pulsed sources can be either pulsed reactors or accelerator based systems in which the burst of fast (megaelectronvolt) neutrons is first moderated in a small hydrogeneous moderator whose surface(s) form the effective source for the experiments. Ideally the pulse lengths of the moderated neutrons should not exceed a few tens of microseconds so that the required energy resolution can be obtained with reasonably short flight paths (10–100 m). Relevant experience with pulsed reactors exists in the Soviet Union, where a small (30 kW) system has been working since 1969 and a much larger system (4 MW, 10^{16} neutrons cm^{-2} s^{-1} peak intensity) is now in the final stages of construction. Unfortunately, pulsed reactors produce an inherently long pulse (the neutron bursts from the 4 MW reactor will be 90 μs long before moderation) and it would require in any case a very substantial development programme before such a source could be built in the U.K.

On the other hand, particle accelerators are well suited to the production of intense neutron bursts of *ca.* 10 μs duration and at 10–20 ms intervals, which are convenient for time-of-flight experiments. The most competitive accelerator sources are based on the use of protons to produce neutrons by spallation reactions from heavy nuclei; the use of a fissile material target yields additional neutrons from high-energy fissions. The high yield of neutrons from these

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reactions, combined with the low energy dissipated in the target per neutron produced, enables a neutron spallation source to have a performance comparable with or better than a reactor but with a heat dissipation in the target some 100 times lower than that of the reactor core. These features are illustrated in table 1, which includes data for neutron production by electron accelerators.

The potential of proton-induced spallation as a neutron source has long been recognized (Bartholomew & Tunnicliffe 1966), but it is only in recent years that accelerator technology has advanced far enough to permit the realization of a practical alternative to the steady-state reactor. A pulsed source with a proton linac is now in the early stages of use at Los Alamos Scientific Laboratory (Russell *et al.* 1978) and sources of intensity comparable with that of the Harwell Linac (Windsor *et al.* 1978) are being prepared at Argonne National Laboratory (Carpenter *et al.* 1978) and in Japan (Ishikawa & Watanabe 1978). Steady-state spallation sources can also have attractions, although they need relatively high average proton currents to be viable.

On a pulsed source it is essential to exploit the time structure of the neutron flux; so much so that the moderator is designed to optimize $I/\Delta t^2$ rather than I, where I is the time-averaged neutron flux and Δt is some measure of the pulse width (e.g. full width half maximum or standard deviation). A thin moderator made of a material that gives a high mean energy loss per collision is required to minimize Δt in the thermal region. Such moderators, in practice hydrogenous, greatly undermoderate the spectrum resulting in a $1/E$ slowing down component which, unlike that of a reactor, is of comparable intensity to the Maxwellian component. A pulsed source designed to have the same instantaneous flux in the thermal region as a particular reactor will have a performance some 1000 times better at 1 eV. The pulse structure in the slowing down region is sharp (e.g. $\Delta t = 2$ μs at 1 eV with $\Delta t \propto E^{-\frac{1}{2}}$) giving an intrinsically good time resolution. In the Maxwellian region, the pulse shape deteriorates with an attendant degradation of intrinsic resolution. Moderators of sub-ambient temperatures are used to extend the slowing down region to lower energies or neutron absorbers are introduced to suppress thermalization. Target–moderator coupling can be improved and the leakage of partly moderated neutrons reduced by surrounding the assembly with a neutron-reflecting material (Be, D_2O). A decoupling layer is required to prevent contamination of the moderator pulse by neutrons returning at long times from the reflector. A pulsed source target assembly is illustrated schematically in figure 1 while figures 2 and 3 illustrate some moderator characteristics. Specific choices in the design of the S.N.S. target–moderator–reflector system are given in §3*e* below.

It is clear that the spectral characteristics of pulsed sources favour the use of epithermal neutrons although, if the source is sufficiently powerful, thermal neutron experiments will not be excluded.

3. Description of S.N.S. facility

The source will use an 800 MeV high intensity proton synchrotron accelerator to deliver individual 400 ns bursts of 2.5×10^{13} protons at 50 Hz onto a heavy metal target to produce a fast neutron yield of *ca.* 4×10^{16} neutrons s^{-1}. Four moderators close to the target and embedded in reflector will slow these neutrons down to epithermal and thermal velocities and yield pulse lengths in the range 1–100 μs. The moderated neutrons will pass through 18 channels in a massive shield to the individual neutron scattering instruments ranged at distances

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of 6–100 m from the moderators. Table 2 gives the main parameters of the facility. Figure 4 illustrates its layout.

The choice of the main parameters (energy, proton intensity, repetition rate) was made on the basis of neutron yield from the moderators, overall costs and the need to use as much as possible of the former Nimrod plant and buildings. Neutron yields increase linearly with proton energy above 100 MeV and increase with increasing target mass number. Fissile target materials give significantly higher yields than non-fissile. Proton energies greater than about 1 GeV are not advantageous because of their longer range in targets and consequent extended source distribution; 800 MeV was a suitable energy from yield considerations and allowed the synchrotron to be fitted into the Nimrod magnet hall. Repetition rates above 50 Hz were ruled out by the economics of the laminated magnets and the r.f. accelerating system. The synchrotron magnet aperture, and hence the proton burst intensity, has been set as high as costs permit.

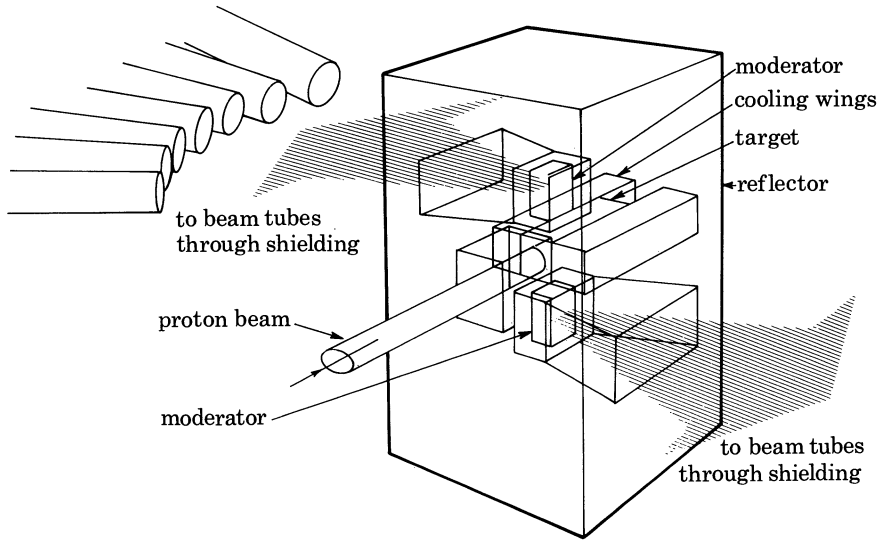

FIGURE 1. Schematic illustration of spallation target, moderator and reflector assembly, showing two moderators in wing geometry with single side viewing.

(*a*) *Synchrotron main ring*

The main synchrotron ring consists of a series of laminated bending and focusing magnets forming a ring of average radius 26 m. The proton beam circulates in a vacuum chamber maintained at no more than 5×10^{-7} Torr†. As the field in the bending and focusing magnets is increased, the beam is maintained centrally in the vacuum chamber by accelerating the protons with radio-frequency fields produced in r.f. cavities situated at six positions around the ring. The r.f. frequency, phase and amplitude are controlled to maintain the beam on a stable orbit as the field is increased from about 0.176 T at injection up to 0.7 T. This corresponds to the proton kinetic energy changing from 70 to 800 MeV as the circulation time changes from 1.49 to 0.65 μs. Bias windings on the ferrite in the r.f. cavities are used to sweep the accelerating frequency from 1.3 to 3.1 MHz. There are two equally spaced proton bunches circulating around the circumference of the accelerator ring.

† 1 Torr ≈ 133 Pa.

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Tight focusing of the beam is needed to keep it within the 25 cm × 12 cm vacuum vessel aperture. The necessary transverse forces are provided by the quadrupoles, which control the transverse or betatron oscillations, and in the azimuthal direction the synchrotron oscillations are controlled by the r.f. accelerating field. Tolerances of the magnet parameters (fields and physical locations) must be carefully controlled to avoid unacceptable disturbance of the beam, and the betatron oscillation frequencies must be chosen to avoid the excitation of resonances in the motion by the residual errors. Magnetic correction elements are provided in the accelerator ring to reduce the effect of magnetic field errors. (Resonance excitation due to space-charge

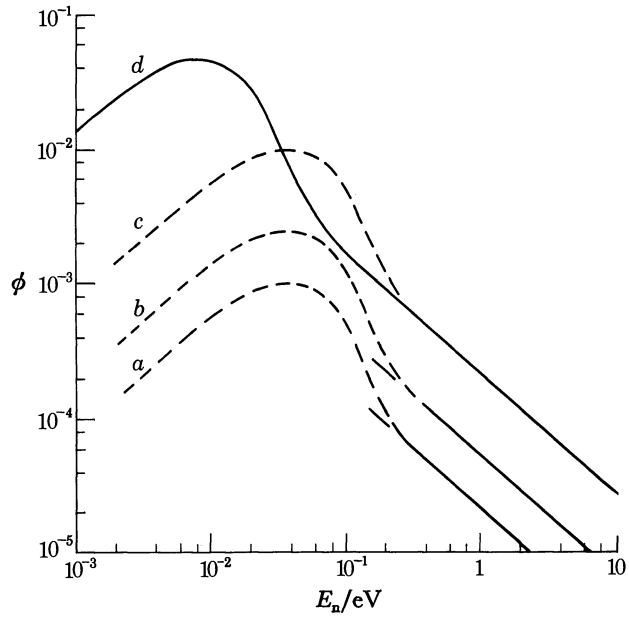

FIGURE 2. Computed neutron spectrum leaving moderators of 10 cm × 10 cm × 5 cm placed above a neutron source. The vertical scale is neutrons per steradian per electrovolt per fast neutron, and is for the total yield at 90° to the 10 cm × 10 cm face of the moderator. Curve (*a*) is for a bare water moderator at 300 K, 12 cm above a neutron source giving the spectrum expected from a small target (peak of the neutron spectrum at 1.4 MeV). Curve (*b*) is for the same moderator but with a neutron source characteristic of a large target (peak of the neutron spectrum at 0.14 MeV). Curve (*c*) is similar to (*b*) but with a reflector and decoupler. Curve (*d*) is similar to curve (*c*) but with a 10 cm × 10 cm × 5 cm moderator at 77 K. Experimentally measured spectra closely confirm the computations.

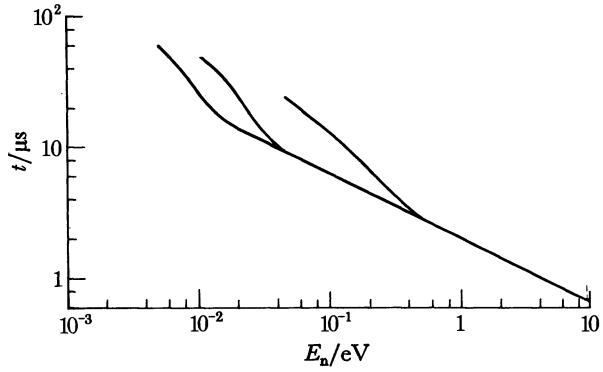

FIGURE 3. Full width at half height of the neutron time distribution leaving a 10 cm × 10 cm × 5 cm moderator as a function of neutron energy.

TABLE 2. S.N.S. MAIN PARAMETERS

injector

output energy	70.51 MeV
input energy	0.665 MeV
accelerated particle	H^-
pulse current	20 mA
pulse length	500 μs (max.)
r.f. frequency	202.5 MHz
injection method	foil stripper

main ring

number of superperiods	10
number of dipoles	10
number of doublet quadrupoles	20
number of trim quadrupoles	20
number of singlet quadrupoles	10
mean radius of synchrotron	26.0 m
repetition frequency	50 Hz
maximum proton energy	800 MeV
proton burst intensity	2.5×10^{13} per pulse

vacuum vessel

material	alumina ceramic
pressure	$< 5 \times 10^{-7}$ Torr

r.f. system

number of r.f. cavities	6
number of accelerating gaps/cavity	2
r.f. power (peak)	1.1 MW
r.f. frequency	1.34–3.09 MHz

extraction system

field in pulsed kickers (3)	0.040 T
kicker field rise time	0.225 μs
d.c. septum magnet field	1 T
proton burst length	0.4 μs

target station

target	Zircaloy-2 clad ^{238}U
target power	350 kW
fast neutron production rate (time average)	4×10^{13} s^{-1}
shield thickness nominal:	
forward direction	5 m
laterally	4 m
no. of beam channels	18

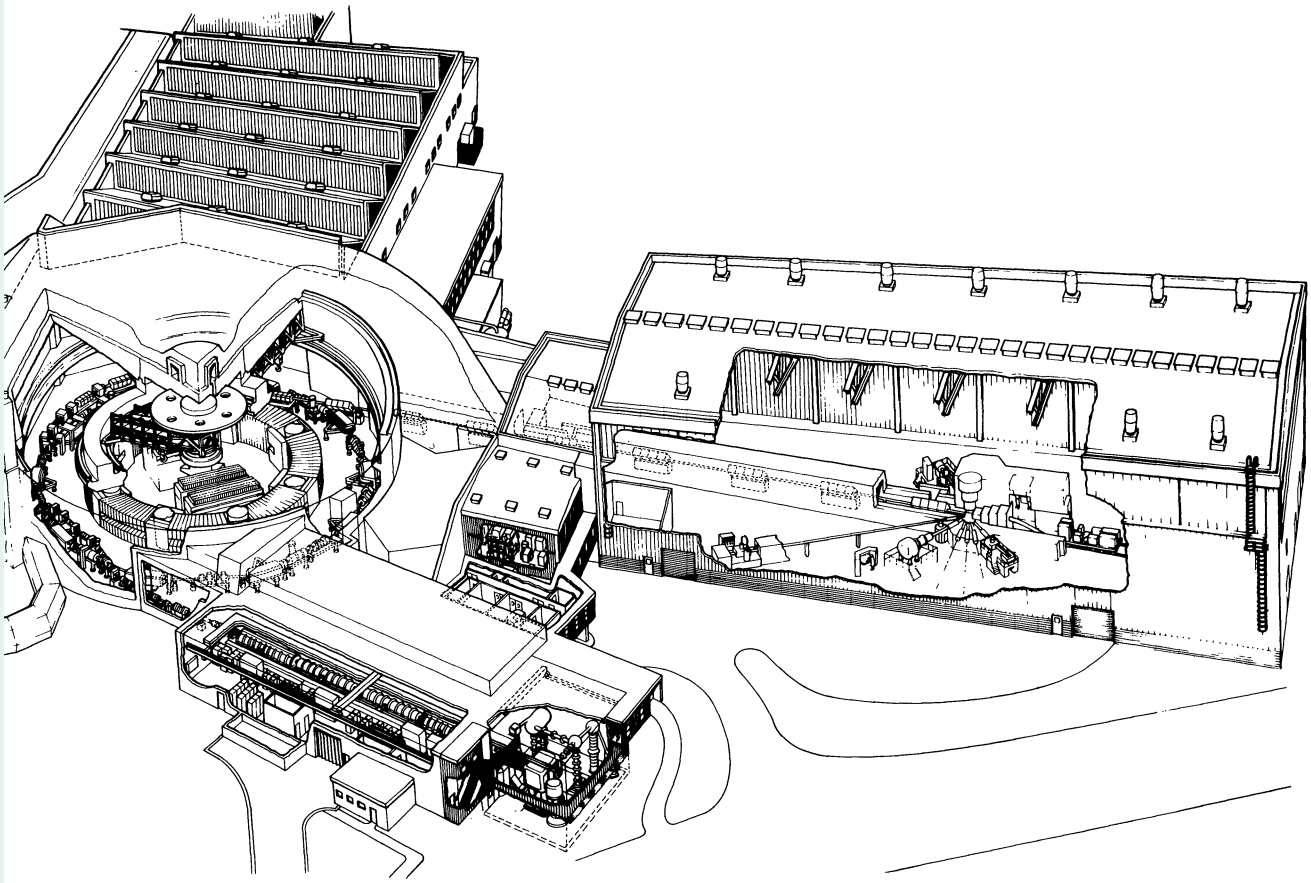

FIGURE 4. Illustration of the spallation neutron source that is being constructed at the Rutherford Laboratory. The linear accelerator used to inject the H^- beam is at the bottom of the diagram, the synchrotron ring is at the left and the spallation neutron target station at the right. Only a few of the neutron scattering instruments are indicated. The buildings were formerly used for the Nimrod 7 GeV proton synchrotron and particle physics experiments.

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effects cannot be so readily corrected.) The r.f. parameters must also be accurately controlled, with fast feedback loops playing an important part.

The magnets in the ring are tuned by a large capacitor bank and driven at approximately 50 Hz by a biased sinusoidal voltage. The d.c. component sets the minimum field corresponding to injection at 70 MeV. Circuit losses will be made up from a motor alternator set whose frequency must be carefully chosen to be compatible with the use of choppers in the neutron beams. A choice will be made between operation at mains frequency, at the natural resonant frequency of the magnet, or by locking onto a fixed frequency determined by a crystal oscillator, which also controls the choppers.

Inside the magnets, the vacuum vessels must be electrically insulating to avoid eddy current heating and will be made of high alumina ceramic chosen for its good vacuum properties and high thermal conductivity. Elsewhere, stainless steel chambers will be used. A pressure of less than 5×10^{-7} Torr is required to avoid beam/gas instabilities and will be realized with 30 triode ion pumps. An r.f. shield (Faraday cage) must also be provided inside the vessel to ensure that beam instabilities are not produced by electromagnetic coupling to its surroundings.

Non-destructive beam monitors are required to measure the beam intensity and position in space and time. They form an essential part of the beam control servo-circuits as well as giving diagnostic information needed during commissioning and fault finding.

(*b*) *Injection*

The former 70 MeV Nimrod injector (an Alvarez, axial field r.f. linac with drift tubes) will be used, uprated for 50 Hz operation, and will provide a pulse current of 20 mA (West 1979). Multi-turn injection (315 turns during 470 μs) is needed to achieve the required synchrotron intensity. To avoid a phase space limitation on the number of turns that can usefully be injected, negative hydrogen ions will be delivered by the linac and be stripped by a foil (thickness *ca.* 50 μg cm^{-2}) to form H^+ as they enter the ring. About 50 % of the beam will be trapped by the synchrotron r.f. system.

(*c*) *Extraction and beam transport*

The 800 MeV beam is extracted from the synchrotron by means of three full aperture ferrite kicker magnets with a rise time of *ca.* 200 ns followed by a d.c. septum magnet which together deflect the beam in the vertical plane into an external transport channel. The kicker field rises within the interbunch interval of *ca.* 250 ns, thus ensuring that the circulating beam is extracted within a single turn and a very short proton burst (*ca.* 450 ns) is delivered to the target. After extraction, the beam is transported by a channel containing 64 separate magnetic components over the distance of *ca.* 125 m to the target station. The extraction and transport system overall is achromatic and provides a 70 mm × 70 mm stable spot size at the target.

(*d*) *Intensity limitations*

In addition to any beam losses caused by failure to operate within the specified machine tolerances, there are many interactions that can cause the beam to become unstable as the beam current is increased (broadly speaking, space charge effects). The more important instabilities are:

(i) transverse incoherent space charge effects – a defocusing effect due to the mutual repulsion of protons within a bunch;

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(ii) transverse coherent effects – the beam produces an image current in nearby components and the whole bunch is excited into coherent motion by the antidamping effect of the fields between the image currents and the bunch;

(iii) longitudinal instabilities – these can arise when a bunch induces fields in nearby cavity-like objects, which then interact with the same or subsequent bunches.

In the S.N.S., the use of the vacuum vessel r.f. shield and care in component design will contain the effects of (ii) and (iii), leaving the space charge effect, (i), to determine the intrinsic intensity limit at a level calculated to be 2.5×10^{13} protons per pulse.

Some beam losses are inevitable during the processes of injection, r.f. trapping, acceleration and extraction, but they must be strictly limited because of the radioactivity and radiation damage induced in the machine and other nearby components. A special collector system is being designed to localize the low-energy losses, and, generally, a combination of component design, local shielding and special handling equipment is needed to ensure that an acceptable operating schedule can be maintained. Even with the advantage of a modern computer-based control system, commissioning up to routine operation at design level may take up to 2 years, about twice as long as for most accelerators. Neutron scattering experiments will, however, be possible throughout commissioning except for the very early stages.

(*e*) *Target station*

The fast neutron production target consists of *ca.* 30 plates of Zircaloy clad uranium-238 separated by cooling channels and forming an assembly 10 cm × 10 cm in cross section and 30 cm long with cooling manifolds on two sides. Neutron yields, energy deposition, residual activity and the nuclide inventory in a used target, have been computed by using codes developed from a well known Oak Ridge package, HETC (Chandler & Armstrong 1972). There is a significant contribution to the neutron production from high-energy fissions and from the target material outside the beam cross section. This target, dissipating 350 kW, will yield approximately 26 fast neutrons per incident proton, somewhat less than the frequently quoted 30 for solid uranium because of the diluting effects of the cooling channels and Zircaloy.

Of the fast neutrons, 0.6% have energies exceeding 100 MeV and are emitted within a 15° semiangle forward cone; the average energy of all neutrons is less than 1 MeV. These yield predictions are used as the design basis of the bulk shield, which must provide an attenuation of approximately 10^9. There will be 5.2 m of iron and concrete in the forward direction, 4.2 m radially and 3.9 m above the target. The shield will rest on a steel plinth 2 m deep, made from former Nimrod magnet sectors.

Radiation damage growth effects are expected to limit the useful lifetime of a uranium target to not less than 3 months. Induced activity after this time will be approximately 400 kCi, comparable with a DIDO type fuel element, so a remote handling cell is provided immediately downstream of the target station to replace the used targets. Alternative targets, e.g. of tantalum, will be available should they be required.

The moderator geometry adopted is a four-wing arrangement with two moderators above and two below a horizontal target. (Wing geometry is analogous to a tangential beam on a reactor.) The front moderators are in the region of highest neutron flux and each is viewed on both faces. The rear moderators are mounted parallel to the target and are viewed on only one face. By suitable angling of the front moderators to the axis of symmetry of the target, an 18 beam channel layout may be achieved. The radiation and background levels experienced

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will be lower than those from slab moderators (analogous to a radial beam on a reactor), where a direct view of the target through the moderator is possible. To meet the requirements of the proposed instruments, moderators with a wide spectral range are required. In the slowing down region, optimization requires the moderator to have a source area of *ca.* 100 cm^2 and a thickness of *ca.* 5 cm, and the moderator material to have as high a hydrogen density as possible. Radiation damage effects and the need to remove up to several hundred watts of induced heat limit the choice to H_2O, liquid H_2 and some metal hydrides. In the Maxwellian

TABLE 3. S.N.S. MODERATORS

moderator location		number of beam channels	material	$\phi(E)_{1\text{ eV}}$
upper front	A	6	ambient H_2O	2.2×10^{-4}
lower front	B	7	heterogeneously poisoned H_2O *or* cooled metal hydride	1.8×10^{-4}
upper rear	D	2	ambient H_2O *or* heterogeneously poisoned H_2O	1.3×10^{-4}
lower rear	C	3	liquid H_2	1.1×10^{-4}

$\phi(E)_{1\text{ eV}}$ is the yield of neutrons at 1 eV per electronvolt per steradian per source neutron for a 10 cm × 10 cm × 5 cm moderator with the hydrogen density of H_2O. For comparison, the S.N.S. single moderator reference design value for $\phi(E)_{1\text{ eV}}$ is 2.5×10^{-4}.

region, neutrons approach thermal equilibrium with the moderator material and a significant fraction of the pulse is contained in a long exponential tail. The resultant degradation of performance is avoided by lowering the physical temperature of the moderator or poisoning the moderator with a resonant absorber (Cd or Gd). A 20 K liquid hydrogen moderator of some 9 cm thickness is required specifically for the production of high intensities of long wavelength neutrons ($\lambda > 4$ Å†) for applications that do not demand the shortest possible pulse lengths.

The performance of the four-wing moderator system discussed above, as predicted by using programs based on the TIMOC Monte-Carlo code (Kschwendt & Rief 1970), is given in table 3. Calculations and measured results on benchmark systems (Boland *et al.* 1978) indicate an absolute accuracy of 20 % and relative accuracy of 5 %. The performances quoted are with a reflector of D_2O-cooled Be and decoupler energy 60 eV. (It is expected that the decoupler energy may be lowered somewhat, particularly for thermal instruments.) The flux of neutrons $n(E)$ having energies between E and $E+\Delta E$, on a sample at distance L is

$$n(E) = \phi(E)\,\Delta E n_f/L^2 \text{ neutrons cm}^{-2}\text{ s}^{-1},$$

where n_f is the fast neutron production rate in the target.

Comparison of the performance of pulsed and reactor sources is not straightforward. The direct comparison of the equivalent 4π flux emitted during the pulse and the steady 4π flux in the reactor shows that the intrinsic brightness of the S.N.S. is comparable with that of the Institut Laue–Langevin (I.L.L.) reactor in the thermal region, somewhat inferior in the low energy region served by the I.L.L. cold source, but is 10 times greater at 100 meV and 1000 times greater at 1 eV. Although intrinsic brightness is certainly not the sole factor in evaluating a source for a particular scientific experiment, it does in many cases provide a rough guide.

† 1 Å = 10^{-10} m = 10^{-1} nm.

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4. Instruments and techniques

(a) *Planned instruments*

It is expected that the S.N.S. target station will eventually be able to support 20–25 instruments on 18 beam channels. For initial operation, it is planned to install 10–12 instruments with an overlapping programme of further instruments to follow. Seven have already been chosen for construction to begin now. Brief descriptions are listed in table 4. Five of these initial instruments will exploit the special advantages of the S.N.S. in the epithermal part of the neutron spectrum. Two instruments, the low Q spectrometer and the high resolution quasi-elastic spectrometer, are biased towards the use of long wavelengths from a cold (20 K) moderator where the effective fluxes are not so high as those at I.L.L. Nevertheless, these two instruments incorporate design features to give performances comparable with the equivalent instruments at I.L.L. (the small angle scattering apparatus (D 11 and the inelastic spectrometer IN 10).

(b) *Envisaged instruments*

Instruments following those listed in table 4 will incorporate new developments, including experience from the Harwell Linac and the S.N.S. itself. Some beam channels will be retained for completely novel instruments when they emerge. Additional instruments already proposed include:

single crystal diffractometer;	constant Q spectrometer;
small-angle neutron diffractometer for liquids and amorphous materials;	high symmetry spectrometer;
	eV spectrometer;
medium energy inelastic spectrometer;	polarization spectrometer.

Of the additional instruments listed above, a second liquids and amorphous materials machine is at the planning stage; this will be a small-angle instrument for measurements in the low Q region ($Q \approx 0.5$ Å^{-1}). Four instruments await experience at the Harwell Linac before their detailed design can be finalized. Tests will be conducted on the Linac of a simple single crystal diffractometer, of elastic polarization analysis with the use of two samarium filters (Freeman & Williams 1978), and of the use of resonance detectors (Ta, U) for measuring very high energy (0.5–5 eV) transfers such as would occur in studies of high energy excitations in crystalline materials. A constant-Q spectrometer, a time-of-flight equivalent of the triple axis machine (Windsor *et al.* 1978), is being installed on the Linac for use in the U.K. research programme (figure 6); construction of the S.N.S. instrument will benefit directly from this experience.

(c) *Techniques*

A number of important developments are incorporated in the S.N.S. instrument designs, notably in the fields of computing, detectors and neutron choppers as outlined below. In addition, a wide range of sample environment equipment (cryostats, furnaces, magnets, pressure cells, etc.) will be provided, standardized as far as possible between instruments, with computer control of variable parameters available. The high data rates and the inherently pulsed nature of the S.N.S. will be especially suited to the use of pulsed, or time-varying, environment parameters.

The instruments will depend crucially on the use of computers to control experiments, to acquire and organize data, and to convert it into a state where users can analyse it. Many of

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Table 4. Initial batch of S.N.S. instruments

instrument	outline description
high intensity powder diffractometer	An instrument of 'conventional' design to measure powder diffraction profiles rapidly and with higher statistical accuracy than currently possible while retaining a reasonable resolution in the lattice parameter ($\Delta d/d \approx 6 \times 10^{-3}$). See figure 5.
high resolution powder diffractometer	To complement the high intensity diffractometer when high spatial resolution is needed. High resolutions ($\Delta d/d \approx 3 \times 10^{-4}$) are achieved by means of a 100 m long neutron guide.
liquids and amorphous materials diffractometer	An instrument of basically conventional design deriving from the series used successfully on the Harwell Linac. Q range 0.2–60 Å^{-1}.
low Q (small-angle scattering) spectrometer	A 'small angle scattering' instrument in demand for a wide range of science. Improvements will be realized on existing reactor instruments by means of a sophisticated detector system. Q range 0.0015–4 Å^{-1}, continuously accessible.
high resolution quasi-elastic spectrometer	An instrument exploiting the time-of-flight method to advantage while using back scattering from analyser crystals to give very high resolution: *ca.* 1 μeV within a 250 μeV window at final energy 2.07 meV (graphite analyser) or *ca.* 13 μeV within 960 μeV at 1.82 meV (silicon analyser).
high throughput inelastic spectrometer	The time-of-flight version of the well known beryllium filter machine used for medium to high energy transfer work (20–500 meV) when high energy resolution and Q definition are not needed, especially useful for chemical spectroscopy with high sample throughout.
high energy inelastic spectrometer	An instrument using the latest developments in chopper technology to achieve high resolution at high energy. For example with the 3° forward detectors and incident energy 1 eV, an energy resolution of *ca.* 4% is obtainable at final energy 0.4 eV and $Q \approx 5$ Å^{-1}.

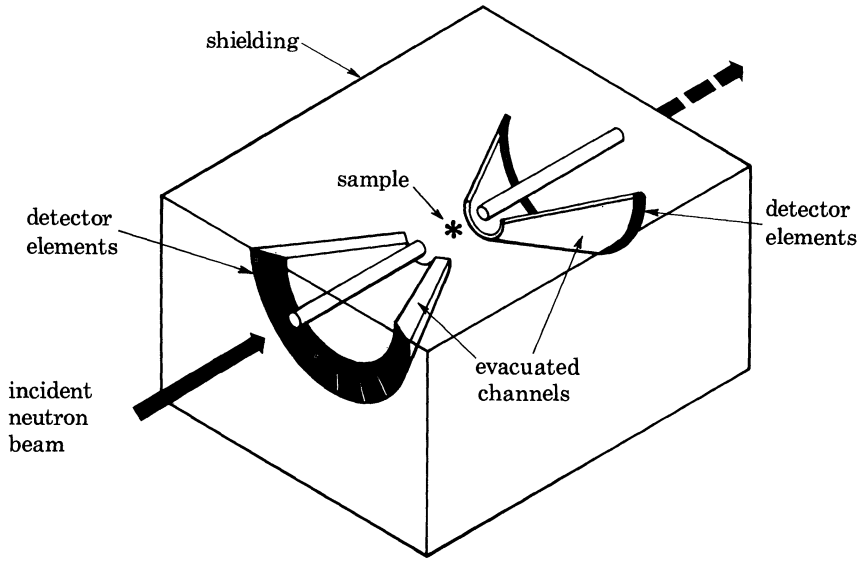

Figure 5. Sketch of the high-intensity powder diffractometer. The sample (indicated by the asterisk is viewed by two semicircular Li-glass scintillator detector banks situated at 30° and 150° to the incoming neutron beam and 1 m from the sample. The 150° detector is inclined in time-focusing geometry. The wavelengths of the diffracted neutrons are measured by time-of-flight. Resolution, $3 \times 10^{-3} < \Delta d/d < 10^{-2}$.

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the problems arising from the high data rates and the use of the time-of-flight mode could not be solved economically without the recent and continuing rapid developments in the computing field. Software development will also need to break much new ground for the treatment of time-of-flight data; work has begun on profile refinement of time-of-flight powder diffraction patterns.

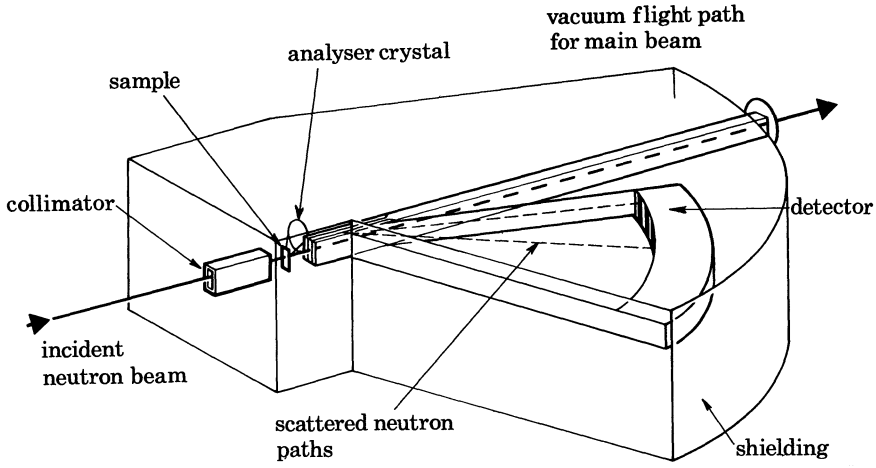

FIGURE 6. Sketch of the constant Q spectrometer planned for use on the S.N.S. in the field of lattice dynamics. The energies of inelastically scattered neutrons are measured by the analyser crystal and the detector array. The initial energies can then be calculated from the overall times of flight. The energy analyser is a large single crystal of germanium in transmission geometry and the detector bank uses 50 Li-glass scintillators, each 8 mm × 60 mm, mounted 1 m from the analyser.

Position sensitive detectors will be needed that are capable of detecting epithermal neutrons with good efficiency (up to 40 %), good gamma discrimination and short dead time (*ca.* 100 ns). Scintillation detector systems have been developed at the Rutherford Laboratory to meet these criteria. In a few cases, traditional gas counters will be used. The scintillator system modules have been tested in various experiments, including some at a pulsed spallation source, and will be incorporated for full-scale tests in some of the Linac instruments.

Several types of mechanical chopper are needed: a Fermi fast chopper with a burst time *ca.* 1 μs; fast neutron eliminators to reduce backgrounds; various disk choppers for selecting energy windows, time frames etc.; and mechanical velocity selectors for definining a variable wavelength window with resolution $\Delta\lambda/\lambda \approx 0.05$ to 0.5. The most demanding requirement is that of the Fermi fast chopper for the high energy inelastic spectrometer, where an energy resolution of the order of 1 % will be required at neutron energies up to 1 eV. A suitable slit package has been developed for this application by using aluminium–boron fibre composite in a rotor that can be driven by a standard Harwell spinning head (Jones *et al.* 1979).

5. SCIENTIFIC APPLICATIONS

(*a*) *Introduction*

The S.N.S. will have an impact scientifically, just because for many experiments the effective neutron flux is increased relative to the best reactor sources. However, the way that the extra intensity is utilized will vary greatly from experiment to experiment. In some cases the researcher will wish for an increased data collection rate not only simply to improve the statistics but also,

for example, to follow time-dependent phenomena; in other instances it will be the ability to measure weak scatterers that will be important. On several standard instruments such as the liquids and amorphous materials diffractometer, the choice of high count rates or the deployment of small or dilute samples remains open to the experimenter. In other instruments the availability of higher flux will be used to give improved resolution (e.g. in the high resolution powder diffractometer), or by using the epithermal bias of neutrons from a pulsed source, an extended range of energy or momentum transfers (e.g. in the high energy inelastic chopper spectrometer). Also quite apart from the emphasis on shorter wavelength neutrons, the use of a pulsed white beam is valuable for the simultaneous investigation of a wider range of energy and momentum transfer than can normally be obtained by using monochromated beams. Table 5 gives an indication of some of the areas of science that will benefit from these developments, which are further discussed below.

TABLE 5. THE IMPACT OF THE S.N.S. ON NEUTRON STUDIES

improvements envisaged	scientific areas affected
higher counting rates	(*a*) structure of fluids: more accurate partial radial distribution functions; the influence of temperature, pressure and concentration more easily studied; extension of isotopic substitution techniques (*b*) time-dependent structural changes readily followed (*c*) 'routine' molecular spectroscopy in the range 10–500 meV available
weak scatterers more accessible	(*a*) structural and dynamical studies of physisorbed or chemisorbed atoms and molecules (*b*) examination of dilute systems such as gases or matrix isolated molecules (*c*) general use of small samples where necessary, e.g. when rare isotopes are involved and amorphous thin films
better resolution in $Q, \hbar\omega$	(*a*) very high resolution powder diffraction, particle broadening effects (*b*) improved inelastic studies including separation of diffusional broadening and dispersion effects in the spectroscopy of molecular fluids and the minimization of multiphonon effects on solids (*c*) more powerful polarization analysis experiments for the separation of nuclear and magnetic scattering, coherent and incoherent scattering, magons and phonons; as well as the identification of magnetovibrational effects
more short λ neutrons; large $\hbar\omega$ (and/or Q)	(*a*) magnon studies up to 0.3 eV (*b*) improved chemical spectroscopy at high energies (*c*) spectroscopy in the electronvolt region (*d*) enhanced interatomic resolution in molecular fluids and amorphous solids (*e*) extended use of anomalous scattering techniques (*f*) studies possible on highly (neutron) absorbing materials
wide $Q/\hbar\omega$ window	(*a*) advantageous for certain studies of diffusion in molecular crystals and liquid crystals, polymers, intercalated compounds and biological membranes and for low-lying inelastic processes (*b*) more complete small-angle scattering data for studies in polymeric science, biology, metallurgy and the investigation of nucleation and growth processes

(*b*) *Liquids and amorphous solids*

In some simple systems, e.g. alkali halides, where the interactions can be described by pairwise potentials, the neutron results confirm the merits of the computer simulation studies. However, there is much to learn for most liquids, where chemical bonding is important. Similarly, Enderby's beautiful work on the structure of aqueous solutions is only a beginning

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(Enderby, this symposium). Subtle details of the structure, including the changes with concentration, pressure and temperature, can only be revealed by data of very high statistical accuracy; hence the need for high rates of data collection. Because of the limited fluxes, the systems studied so far involve elements with readily available isotopes that have relatively large differences in scattering lengths; higher fluxes will broaden the range of systems to include those with rarer isotopes and smaller scattering length differences.

An important consequence of the high epithermal flux from the S.N.S. is the opportunity that it provides to extend upwards the range of momentum transfer and so to enhance the resolution in real space. Again, there have been some excellent pioneering studies on molecular liquids principally by the group from the University of Kent (see, for example, Walford *et al.* 1978). Improved real space resolutions will also aid the determination of the structure of amorphous solids (which also benefit from the use of isotopic substitution techniques). Higher fluxes will open the way to the study of much smaller samples (e.g. thin films) and an investigation of the links between structure and preparative conditions as well as kinetic investigations of the structural rearrangements that occur before phase separation or crystallization.

There will also be increased interest in the dynamics of fluids, whether it be in the study of diffusion processes, with the use of the high-resolution quasi-elastic spectrometer, or in the examination of vibrational modes, with the use of the high-energy inelastic spectrometer (at low Q). The latter instrument will also be suitable (at very high Q) for experiments on quantum liquids, where measurements of the proportion of ^{4}He atoms in liquid ^{4}He with the zero momentum state can be envisaged.

(*c*) *Crystallography*

The new source will provide outstanding facilities for neutron powder diffraction. On the high intensity instrument it would be possible to collect a complete set of good quality data in a moderately complicated structure (e.g. Al_2O_3) in about 30 s. As a result, a major use of the instrument is likely to be the use of variations in ambient conditions, e.g. electrical field and mechanical stress, to follow relaxation effects structurally. The high intensity available will also greatly improve the prospects for accurately detecting very weak features arising, for example, from atoms or molecules adsorbed on a surface, so that it is possible to envisage present studies (Bomchil *et al.*, this symposium) being extended to the investigation of the build-up of chemisorbed layers on relatively low surface area metals.

The high resolution powder diffractometer is designed to extend to the full the power of profile analysis methods, which have proved so successful in recent years (Cheetham & Taylor 1977) and which are now available for time-of-flight instruments (R. B. Von Dreele, personal communication, 1979). An improvement in resolution up to $\Delta d/d$ of 3×10^{-4} will both make it much easier to determine unknown structures and increase the number of independent structural parameters that can be refined to perhaps as high as 200. This instrument and the high-intensity diffractometer will be equipped with ring detectors, which can detect anisotropy in the radial scattering, thus providing excellent opportunities for textural studies of which the recent stress effects in bone provide a very good example (Bacon *et al.* 1979).

The success of time-of-flight single-crystal diffraction will depend on the development of area detectors and on solving the problems of data collection. However, given that wavelength-dependent structure factors would be routinely available for extinction corrections, very accurate measurements are in principle possible. In these circumstances a single crystal

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diffractometer on the S.N.S. would be particularly powerful for structure determination involving unit cells up to 20 Å and for the determination of very high resolution data.

(*d*) *Molecular spectroscopy*

The ubiquity of hydrogen and its large incoherent cross section for neutrons means that there is potentially a heavy demand for neutron (proton) spectroscopy. Bands that are weak or forbidden (for symmetry reasons) in the infrared or Raman regions may be seen by neutrons, and optically opaque materials such as metals are often transparent to neutrons.

At present, neutron spectroscopy is curtailed by a limited energy range, relatively low count rates and poor resolution. The S.N.S. high throughput inelastic spectrometer will enable normal spectroscopic measurements in the energy range $10\,\text{meV} < \hbar\omega < 500\,\text{meV}$ to be made in minutes rather than hours, although still with modest resolution. It is therefore possible to envisage experiments involving a series of samples that parallel those employing standard laboratory infrared instruments. The possibility for improving resolution at the expense of counting times will exist and, of course, the high intensity will be particularly valuable in the examination of hydrogenous molecules (or atoms) in dilute solution or as an absorbed species.

(*e*) *Polymer science and biology*

One of the recent successes of neutron scattering has been the very rapid growth in experiments on polymers and biological materials. This has been associated to a large extent with instruments at the I.L.L. that make use of long wavelength neutrons. Although the flux of cold neutrons is more modest from the S.N.S. it is nevertheless clear that a powerful low Q instrument can be built that is capable of sustaining programmes similar to those described by Jacrot (this symposium). Because the S.N.S. instrument employs a wide band of wavelengths, it will cover, in one experiment, a much larger Q range than D 11 at the I.L.L. This is important when the dimensions of the scattering particles are deduced from an analysis based on both Guinier and Porod data together with the evaluation of an integrated intensity. For quasi-elastic and low-energy inelastic measurements the high resolution quasi-elastic scattering spectrometer will also, because of its versatility, prove to be competitive with I.L.L. instruments.

(*f*) *Solid state physics*

Many of the neutron experiments currently carried out involve magnon and phonon studies on triple-axis spectrometers. In §4 the equivalent time-of-flight spectrometers are mentioned; these instruments, which will allow larger energy transfers to be studied, will have many applications. One of the most exciting features of the S.N.S. however, is the prospect that the effective fluxes will be high enough to carry out useful polarization analysis experiments. In magnetic inelastic scattering the following areas of interest can readily be identified in (i) the separation of coherent magnetic excitations from other scattering (for example, in cases where the magnon energies overlap considerably with high energy optic phonon branches), (ii) the measurement of single particle excitations in ordered magnets (of considerable significance to the theory of magnetism in transition metals) and (iii) the measurement of inelastic paramagnetic scattering in both ordered magnets above the transition temperature and in dilute alloys. Again, the results of such experiments are likely to challenge directly our theoretical understanding of magnetism at the atomic level. Polarization analysis also allows the separation of spin incoherent scattering from coherent scattering so that for some elements, especially

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hydrogen, nuclear inelastic scattering gives information about the self and pair dynamic correlations. The inelastic polarization analysis experiments, in terms of instrument design, will be among the most demanding on the S.N.S.

Somewhat less demanding, but still important, are total scattering polarization analysis measurements, which allow an identification of the elastic magnetic scattering. For paramagnets and spin glasses and for amorphous ferromagnets with large magnetic anisotropy, it is very difficult to separate the elastic magnetic component of the scattering without polarization analysis.

Spectroscopy in the electronvolt region is a unique possibility where very high energy transfers (0.5–5 eV) are needed for investigating high-energy excitations in crystalline materials, including interband transitions in semiconductors, and may also be useful for the study of single particle distribution functions, e.g. in liquid helium.

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