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by

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A SET OF THERMAL NEUTRON-SCATTERING EXPERIMENTS FOR THE WEAPONS NEUTRON RESEARCH FACILITY

by

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ABSTRACT

Six classes of experiments form the base of a program of thermal neutron scattering at the Weapons Neutron Research (WNR) Facility. Three classes are to determine the average microscopic positions of atoms in materials and three are to determine the microscopic vibrations of these atoms. The first three classes concern (a) powder sample neutron diffraction, (b) small angle scattering, and (c) single crystal Laue diffraction. The second three concern (d) small κ inelastic scattering, (e) scattering surface phonon measurements, and (f) line widths. An instrument to couple with the WNR pulsed source is briefly outlined for each experiment.

1. INTRODUCTION

It is now accepted that thermal neutrons are a unique form of radiation that must be made available to materials scientists if they are to have a complete set of diagnostic tools. Thermal neutron scattering complements infrared, microwaves, low energy electron diffraction (LEED), Raman scattering, x-ray diffraction, and other physical measurement techniques. Thermal neutrons are used to detect microstructure (crystal structure, magnetic ordering, liquid short-range order) as well as microdynamics (dispersion relations, frequency distributions, diffusion, molecular levels). Many examples¹ now exist of the power and effectiveness of thermal neutrons. For example, Guinier² outlined how neutrons complement x rays for diffraction; a recent Brookhaven National Laboratory (BNL) conference³ emphasized neutron scattering in the biological sciences; Shirane⁴ demonstrated how neutron scattering has elucidated the mechanisms of phase changes; and a recent meeting⁵ of the National Science Foundation (NSF) at the Massachusetts Institute of Technology (MIT) showed the additions that neutrons have made in molecular spectroscopy.

As with x-ray diffraction and Raman scattering, the capability of thermal neutron scattering depends on the magnitude of the flux or current of radiation available. Neutron diffraction was introduced three decades after x-ray diffraction started, hence the available flux of thermal neutrons lags behind that of x rays. The flux of neutrons on target runs about three orders of magnitude below x rays, and this gap is widening with the step up of x-ray intensities by application of synchrotron radiation. Even though neutron scattering suffers from lack of flux, it is still needed because of its unique capabilities.

Figure 1 shows the increase in flux from thermal neutron sources over the years. Note that effective beam source flux of steady state fission reactors rose rapidly in the 1940s and early 1950s, but now has reached a plateau at about 10^{15} n/cm² s. Steady state sources are not expected to rise above this plateau in the foreseeable future. Note from Fig. 1 that charged particle reactions were the earliest sources of thermal neutrons. These reactions, when incorporating the flux magnifications of time-of-flight (TOF) techniques, have progressed steadily over the years. Because of their advantages, more intense pulsed sources are being proposed and built.

Fig. 1.

Progress of the effective thermal neutron flux at the source of beam tubes that can be used for thermal neutron scattering. For steady state sources this is the average flux and for pulsed sources it is the peak flux

The WNR is one of the pulsed sources currently being built.

Table I lists some of the pulsed neutron sources that have been used for thermal neutron experiments and new sources that are proposed or under construction. Figure 2 shows the increase in flux that these pulsed sources have attained over the years. Until the newest sources under construction are in operation, the effective flux of thermal neutrons from pulsed sources will lag well behind steady state fission reactors. This lag in flux is probably why there has been only a limited amount of definitive scientific data forthcoming from pulsed sources. Figures 1 and 2 demonstrate that pulsed sources promise to reach higher effective flux levels. These gains in flux of pulsed sources and the promise of fluxes above the steady state sources, explain the renewed interest^{6,7} in pulsed sources.

Figure 3 shows the relative epithermal flux produced by several fission reactors and pulsed neutron sources. Fission reactors have not been very effective in conducting experiments with epithermal neutrons. However, hot sources at steady state reactors, particularly at the Institut Laue-Langevin (ILL), have increased flux to a level where experiments are now feasible using epithermal neutrons. Pulsed fission reactors have been omitted from Fig. 3 because their long pulses render them ineffective at epithermal energies. For steady state reactors, epithermal flux is low compared to thermal flux, whereas for pulsed neutron sources, epithermal flux is relatively high compared to thermal flux. Thus, pulsed sources have much greater potential at

epithermal energies than do steady state fission reactors. Figure 3 suggests that very high epithermal flux from pulsed sources may open unexplored regions for investigation. Pulsed sources, like the WNR, have certain advantages compared to steady state reactors; they produce higher fluxes of epithermal neutrons, achieve good resolution more easily at these epithermal energies, cause fewer stringent safety and licensing conditions, and have lower capital and operating costs for comparable effectiveness.

The WNR realizes these advantages and fits into the chronological progression of pulsed sources (shown in Table I and Figs. 1 and 2), beginning operation in 1976. Its effectiveness will closely equal the best steady state reactors at thermal energies and it will be up a factor of 5 from previous operating pulsed neutron sources used for thermal neutron scattering. The WNR will be the first fully operational source of the new class of very high energy, high current, proton-induced neutron sources. It can provide experience in shielding design, beam tube layout, source handling, moderator and cold moderator development, and TOF experimental development. The WNR can carry forward a most effective program of thermal neutron scattering provided the right experiments and instrument design are initiated.

The following sections propose six classes of experiments and experimental equipment that the author deems most effective and feasible. Excluded is the type of experiment where one can see a predicted effect with neutrons, but in which the data never becomes a real test of theoretical predictions. Also excluded are outstanding basic science experiments which, although they demonstrate a unique property of matter, do not lead to a set of diagnoses or applications. Classes of experiments have been selected which are judged to be, or become, sets of definitive measurements challenging theorists to improve their calculational methods and potentials (or force fields) or they have been selected to lead to applied instruments and methods.

In the following sections, instruments for each class of experiments are outlined; time constraints prevent elaboration in this report. For the instruments, TOF methods and components have been employed wherever possible. TOF methods limit orders and spurious scattering, and are effective for multidetector, low angular resolution experiments and for absolute intensity measurements. As the WNR is a pulsed system, its experimental strength depends on efficient use of TOF methods.

Of the six classes of experiments, three are static or structure determinations and three are dynamic or inelastic scattering experiments (see Table II).

TABLE I

SOME PULSED NEUTRON SOURCES USED FOR THERMAL NEUTRON-SCATTERING EXPERIMENTS

Source	Years of Operation	Type	Power on Target	Effective Thermal Neutron Beam Tube Flux	Remarks
GGA	1955 - 1965	Electron linac	5 kW	5×10^{12}	Inelastic scattering measurements with phased chopper
IBR-5	1960 - 1965	Pulsed reactor	5 kW	1.6×10^{13}	Many and varied experiments
RPI	1963 - 1968	Electron linac	15 kW	1.5×10^{13}	Scattering law measurements with phased chopper
Old Harwell Linac	1967 -	Electron linac	5 kW	5×10^{12}	Diffraction measurements
IBR-30	1969 - 1972	Pulsed reactor and accelerator	10 kW	1×10^{14}	Many and varied experiments
Tohoku	1971 -	Electron linac	10 kW	1×10^{13}	Diffraction
Toronto	1971 -	Electron linac	10 kW	1×10^{13}	Rotating crystal spectrometer
India-30	1972 -	Pulsed reactor	10 kW	1×10^{14}	
ISIS-I	1972 - 1975	500 MeV proton cyclotron	- - -	1×10^{12}	Demonstrations of capabilities
→ VNH	1976 -	500 MeV proton linac	- - -	5×10^{14}	Nearing completion
IBR-II	1976 -	Pulsed reactor and accelerator	4000 kW	1.3×10^{16}	Nearing completion
ISIS-II	1976 - 1980	500 MeV proton accelerator	- - -	5×10^{14}	Lab supported
New Harwell Linac	1978 -	Electron linac	40-70 kW	5×10^{13}	Funded
Harwell Linac and Booster	1980 -	Add booster to New Harwell linac	- - -	1.5×10^{15}	- - -
ORNL	1978 -	Electron linac	40 kW	5×10^{13}	Linac operational, now proposed for thermal neutron scattering
ORNL and Booster	1980 -	Add booster to ORNL	- - -	1.5×10^{15}	Proposed
IPNS	1980 -	500 MeV proton accelerator	- - -	2×10^{16}	Proposed
LIFE	1990 -	Laser imploded fusion reactor	- - -	1×10^{18}	Feasible if laser fusion succeeds
Fission	1990 -	Laser imploding fission reactors	- - -	1×10^{18}	No serious development evident in unclassified literature

Each class is described, an experimental layout proposed, special features outlined, experimental progress mentioned, and subsets of experiments described.

II. NEUTRON DIFFRACTION

Neutron diffraction is the determination of the periodic atomic character of a material by measuring the preferential elastic scattering of neutrons from this periodic character. This scattering obeys the Bragg relation

$$\lambda = 2d_{hkl} \sin \theta \quad (1)$$

where λ is the wavelength of the neutrons, d_{hkl} is the distance between planes indexed hkl , and θ is one-half the scattering angle. From this, one can determine the lattice of crystals or short-range order of liquids.

Intensity of the Bragg scattering peaks is

$$I_{hkl} \propto e^{-2W} \left| \sum_{\rho} b_{\rho} \exp[2\pi i(hx/a_0 + ky/b_0 + lz/c_0)] \right|^2 \quad (2)$$

where I_{hkl} is the intensity of scattering for the Bragg peak with hkl as its index, b_{ρ} is the scattering length of the ρ 'th atom in the unit cell, and e^{-2W} is the Debye-Waller factor. By measuring the intensities,

Progress of effective thermal neutron flux at the source of beam tubes that can be used for thermal neutron scattering from pulsed neutron sources.

one can locate the atoms in the unit cell. One can also determine the Debye-Waller factor and thus the average oscillation of the atoms about their central location. To know the lattice, space group, and Debye-Waller factor, is to know all about the average positions of the atoms in a crystal. Knowledge of crystal structure is basic to our understanding of crystalline materials. Thus, measuring this property is related to materials studies. X-ray and neutron diffraction have had great success in identifying crystal structures, both for single crystal

Fig. 3.
Progress of effective epithermal neutron flux at the source of beam tubes from several neutron sources.

TABLE II
PROPOSED CLASSES OF THERMAL
NEUTRON-SCATTERING EXPERIMENTS
FOR WNR

Neutron Diffraction

Powder samples
Small angle scattering
Single crystal Laue

Inelastic Scattering

Small λ scattering
Phonon measurement of scattering surface
Line widths

samples and for powders. There seems to be no limit to the use of x-ray and neutron diffraction, hence three different classes of experiments for WNR are proposed to measure the structure of materials by neutron diffraction.

III. NEUTRON DIFFRACTION: POWDERED SAMPLES

A. Description

In a neutron diffraction experiment, if the sample is a powder rather than a single crystal, information about the distance between the planes is measured; however, the angle between planes is not directly measured in the experiment. Quite often astute guessing can overcome this lack of knowledge of the angle. In other experiments, the lattice has already been measured; now the object is to determine the space group from the intensities of the Bragg peaks. Powder diffraction is a powerful tool for simple crystal structures, for observing the change in peak intensities as a function of a physical parameter, or for when single crystals cannot be obtained.

In conventional diffraction, λ is fixed and θ is varied to determine the d's of the Bragg equation. But when pulsed neutrons are available, θ can be held fixed and the λ 's of those neutrons which are preferentially scattered from a white spectra can be used to determine the d's and intensities.

B. Experimental Equipment

Figure 4 shows a hypothetical diagram of the TOF powder diffraction instrument. Neutrons are produced in the source and moderated by the

Fig. 4.
TOF powder sample, neutron diffraction instrument for WNR.

moderator. Some of the neutrons from the moderator pass down the flight path, scatter from the sample, and are detected by the counters. The source and moderator are arranged so that the sample does not see the source with its γ flash but does see the flux of neutrons from the moderator. For the flight path, the angle of divergence is small enough and the length long enough to obtain high resolution, $\Delta d/d$. One large area detector receives neutrons scattered at different angles; the detector is positioned so that the neutrons scattered from one set of crystalline planes all arrive at the same time. The detector can also cover a large part of the Debye-Scherrer cone in the ϕ angle. This large-area, clam-shell detector greatly increases the counting rate. A monitor is placed behind the sample to measure incident flux distribution. The flight path in front of the sample should be evacuated.

C. Special Features

To achieve very good d resolution⁸ and intensity statistics, efficient detection will be needed. This is provided by large area detectors which can be multiwire proportional counters with ^3He gas in a common envelope. Besides covering a large part of angle θ , they should cover as much of angle ϕ as is practical. Because burst width is proportional to TOF, good time resolution—and thus d resolution—are achieved at small as well as large d 's. This characteristic of the pulsed source should be made use of to measure Bragg peaks with indexes as large as possible. Data in the unresolved region should also be preserved because newly developed computerized fitting methods⁹ of the resolved and unresolved regions can provide a powerful means for obtaining precise space groups. Measuring the scattered and unscattered flux simultaneously

provides more precision because both observe identical volumes of the sample.

D. Previous Experience

The TOF method of powder neutron diffraction has been shown to be very effective. However, the full potential of powder neutron diffraction has not been fully appreciated or realized to date, perhaps because many experimenters use conventional variable θ spectrometers that do not easily go to small d 's or achieve high resolution. Moreover, many experimenters are familiar with x-ray diffraction in which the electronic structure f^2 rapidly suppresses the higher-order peaks. They have yet to reorient their thinking to make use of the good resolution and large scattering vector κ available to neutron diffraction using pulsed source TOF.

E. Subsets of Powder Diffraction Experiments

1. **Physical Properties of Ordinary Crystals.** In many experiments the investigator follows the physical phenomena of interest by tracking crystal structure changes. The TOF diffraction instrument shown in Fig. 4 will allow rapid tracking of these properties on relatively simple samples (<25 atoms per unit cell). A complete and accurate pattern might be obtained in 1 to 30 min. At this speed many parameter steps or sample changes will be possible.

2. **Samples Under High Pressures.** TOF diffraction is well adapted to studying samples under high pressure.¹⁰ For these sample cells, the neutron is a more penetrating probe than x rays. In addition, for TOF diffraction, entrance and exit ports need be cut at only a few angles. These ports do not compromise the strength of the binding rings as much as when a band has to be cut to allow θ scans. Al_2O_3 has excellent high pressure qualities for cells and anvils while having low neutron attenuation. At the Materials Testing Reactor (MTR) in Idaho it was shown that the straight piston system could go to 40 kbar and a Bridgman anvil to 85 kbar, still allowing good diffraction patterns to be obtained. Detectors with an area less than that indicated in Fig. 4 will be used; nevertheless, poorer resolution can be tolerated.

3. **Samples at High Temperature.** Roullet¹¹ has demonstrated that TOF powder neutron diffraction had advantages for studying samples at high temperature.¹² Because the samples are at extreme

conditions, and may change or drift during measurement, data from diffraction scans of the angle will vary as the detector scans from a peak at one angle to the next. This makes interpretation difficult. However TOF observes all peaks simultaneously, obtaining an averaged pattern which can be more easily interpreted. With the high counting rates expected, data can be obtained in a shorter time, thus limiting variations.

4. Complicated Structures. The structure of samples having thousands of atoms per unit cell is presently determined by x-ray diffraction from single crystals. This requires measurement of tens of thousands of reflections. To take advantage of the space selection, single crystals are used to separate peaks that may be closely spaced in plane spacing distance. For x rays, the peaks must be observed at smaller d 's before Ω^2 reduces the intensity beyond the point of detection.

With the new capabilities introduced by pulsed neutron sources, it should be possible to push the complexity of powdered samples studied to many more atoms per unit cell than has been achieved by neutrons in the past.^{13,14} With increased epithermal flux, high plane spacing resolution will allow observation of many more reflections at larger indexes. Information can be extracted from the unresolved region by the raw data fitting methods presently used. Because neutron diffraction does not attenuate by the electronic structure factor f^2 , Bragg peaks at large d 's will still be observable.

Figure 5 is an example of recent measurements of Pr_2O_3 made by Yarnell¹⁵ using a good resolution, variable-angle spectrometer at the Los Alamos

Fig. 5.

A powder sample diffraction pattern of Pr_2O_3 taken with a good resolution conventional neutron diffraction instrument at the steady state Omega West reactor. The ladder of hash marks indicates positions of expected peaks.

Scientific Laboratory (LASL) Omega West Reactor. Both the powder pattern and the ladder of expected peaks are shown. Even though the diffraction pattern does not resolve all the peaks, the pattern is interpreted by the data fitting method. With a TOF spectrometer of higher resolution, the pattern in this region can be resolved and an additional area of unresolved peaks containing information will be available.

5. Diffraction with Polarized Beams. The ability to distinguish polarization of scattered neutrons would add a powerful diagnostic and filtering capability.¹⁶ With an effective polarizer (such as $\text{MgLaNO}_3 \cdot (\text{H}_2\text{O})_x$ crystals) the TOF diffractometer can adapt well to such modifications. A polarizer placed in the flight path of the incident beam defines the polarization of the incident neutrons and a polarizer placed in the flight path behind the sample analyzes the polarization of the neutrons after scattering.

Neutrons scattered coherently from hydrogen atoms preserve their spin orientation, whereas neutrons scattered incoherently from hydrogen atoms flip their spin. Coherent scattering by hydrogen atoms is a very small percentage of incoherent scattering. It is the ability of neutrons to locate hydrogens, even though the coherent scattering is small, that is one of the unique capabilities of neutron diffraction. The coherent signal as compared to the incoherent background of scattering from hydrogen would be greatly enhanced by using polarized beams and analysis to observe only the scattering that occurs with no change of polarization.

6. Electron Density Maps. Neutron diffraction locates the positions of the nuclei of atoms in crystals whereas x-ray diffraction maps the distribution of the electron density. Careful measurements of both followed by subtraction of nuclear from electron density leaves a map of the nonnuclear centered distribution of the electron distribution. These maps are important for showing the distribution of the valence electrons.

7. Conclusion

The TOF neutron diffraction experiment, using powder samples, provides access to a whole set of experiments that will produce definitive data. It takes advantage of the strong capabilities of pulsed sources, such as the use of epithermal neutrons, the use of large area detectors—to obtain high counting rates, and the adaptability to special sample cells.

IV. NEUTRON DIFFRACTION: SMALL ANGLE SCATTERING

A. Description

Some of the periodic characteristics of materials have repeat distances that are very large. This is particularly significant for biological materials, polymers, and radiation damage centers.¹⁷⁻²⁶ To reach these large d 's (10-1000 Å), the Bragg relation $\lambda = 2d \sin \theta$ shows that large λ 's ($\sim 5-10$ Å) and very small θ 's ($< 10^\circ$) are required. To reach these conditions requires special experimental instruments.

B. Experimental Equipment

Figure 6 shows a hypothetical diagram of a small angle scattering instrument for WNR. Neutrons are produced by the source and moderated in the moderator. Some fly down the flight path, scatter from the sample, and are caught by the detector. It is assumed that all scattering is elastic; inelastic scattering is small enough to be ignored. At small angles, the concept of putting the detectors on the surface of constant TOF for each d cannot be used because that surface is now at glancing angle. A detector sensitive to both space and time (hereafter called an S-T detector) is employed. Part of the S-T detector is a computer which identifies the location and time of each captured neutron and converts this S-T information into d by the Bragg relation. Then the number of captures or events per d is stored in the computer.

This system integrates the events corresponding to equal d spacings that had larger λ and θ with those for smaller λ and θ . The flux decreases as λ increases, although the scattering decreases as θ increases, therefore this integration will tend to equalize the number of events over the range of d 's and improve the statistical accuracy.

Fig. 6.

A small angle diffraction instrument for WNR.

C. Special Features

Integration of data taken at different λ 's and θ 's but for the same d 's is one feature of the small angle spectrometer. Integration significantly increases the counting rate of the experiment. The flight paths will be evacuated to limit air scattering. It is important to develop and use an S-T detector so that data from many scattering angles and for many incident wavelengths can be obtained simultaneously.

D. Previous Experience

Small angle scattering with neutrons has been long in coming; however, much physical data is now being obtained since its initiation at Jülich and perfection at Grenoble. Flux requirements are modest enough, however, to permit good performance in intermediate flux reactors. Small angle scattering has not been tried by true TOF; velocity selectors have only been used to select one incident wave length. The experiment proposed here is a true TOF experiment.

E. Subsets of Experiments

1. **Samples in Special Environments.** The proposed instrument, in addition to measuring the long range order of biological samples and polymers, can measure small angle scattering from samples under extreme conditions. These latter samples can either be under high pressure or at high temperature.

2. **Radiation Damage.** Small angle scattering can detect the size and shape of damage centers. If the sample is oriented (a single crystal), the damage centers may be oriented and the diffraction will define their size and shape. It should be possible to construct shielded casks with small entrance and exit ports so that scattering can be seen from extremely radioactive samples.

3. **Magnetic Scattering.** With a polarizer in front of the sample and a polarized sample, specific long range magnetic properties might be observed.

F. Specific Instrument

Figure 7 shows a small angle scattering instrument which is used to evaluate magnitudes of the components to be built. A guide tube or collimator of a cross sectional area 0.5 cm by 0.5 cm and 10-m long

Fig. 7.
Small angle diffraction instrument.

defines the beam from the moderator to the sample. The divergence of this tube is $\Omega = 0.5/1000 = 5 \times 10^{-4}$. Neutrons interact with the sample and some are scattered through small angles X/R .

An S-T detector is placed at distance $R = 10$ m. Counts from the detector are sorted into bins of constant d . Thus more of the total spectra is used, since counts from large angles and large λ are added to those of small angle and small λ . The computer program should accept only a band of λ to limit the spread in resolution (see Fig. 8). Thus the computer acts like a band pass filter.

It is desirable to achieve constant plane spacing resolution

$$\frac{\Delta d}{d} = \text{constant} = \left[\left(\frac{\Delta X}{R} \right)^2 + \left(\frac{\Delta S}{L} \right)^2 + \left(\frac{\Delta \text{TOF}}{\text{TOF}} \right)^2 \right]^{1/2} \quad (3)$$

with each term contributing about the same magnitude. Resolution from the burst spread

Fig. 8.
Expected resolution from the diffractometer
shown in Fig. 7.

$\Delta \text{TOF}/\text{TOF}$ will be nearly constant because for long times-of-flight

$$\Delta \text{TOF} = \text{constant TOF}^Y \quad (4)$$

where Y is 1.0 for thin moderators increasing to 1.6 for thick moderators.

Detector width resolution $\Delta X/R$ can be made constant by computer sorting in X bins when the width of each bin X is proportional to ΔX .

$$\Delta X = \text{const} \cdot X \quad (5)$$

It is not evident that the resolution associated with incident beam divergence $\Delta S/L$ can be made constant and that this will broaden the resolution at large d . Figure 8 plots estimates of $\Delta d/d$ for the layout shown in Fig. 7 assuming $\Delta \text{TOF} = (1/50) \text{ TOF}$. This gives a $300 \mu\text{s}$ burst at $\lambda = 3 \text{ \AA}$. The S-T detector is ~ 1 m edge to edge, which seems reasonable. Its minimum resolution ΔX_{min} might be 2 mm.

G. Conclusion

A small angle scattering instrument at WNR can open up a whole class of significant experiments on the material properties of biological molecules, polymers, and radiation damage. TCF methods adapt well to these measurements.

V. NEUTRON DIFFRACTION: SINGLE CRYSTAL LAUE

A. Description

In the Laue method of diffraction, a white beam of radiation strikes a single crystal; the radiation that is Bragg scattered by many planes is observed as spots on a space-sensitive detector. The strength of this method is the direct measurement of the angle between planes, which is a great help in determining the lattice. Its weakness is that the intensity of each spot contains several orders of scattering; thus the intensities of each d_{hkl} are not reliably determined. Moreover, for x rays, the flux distribution of the white beam of x rays is not well known. TOF Laue neutron diffraction can overcome these weaknesses. In place of the space-defining detector, an S-T sensitive detector will be used. TOF will sort the orders in each spot, while a beam monitor precisely measures the flux spectra of the white beam of neutrons.

B. Experimental Equipment

Figure 9 shows a hypothetical diagram of a TOF Laué diffractometer for WNR. Neutrons made in the source and moderated by the moderator fly down the flight path, scatter from the single crystal sample, and are detected by the S-T detector. The instrument need not have extremely good space or time resolution but should have high counting rates to obtain good intensity statistical resolution.

C. Special Features

TOF modification of the Laué method can sort the multiple orders in each peak which make it a complete and very powerful diffraction instrument. Its high counting rates allow use of small samples which in turn reduce self absorption. Its use of all neutrons and favorable thermal neutron-to-gamma ratio reduces exposure time, thereby reducing radiation deterioration of the sample.

D. Previous Experiences

In x-ray Laué diffraction, no space detector is presently available that can also distinguish x-ray energies. Thus, order separation in the x-ray measurements is not possible. For neutrons, the TOF Laué method has been shown to work but it has not been adapted for extensive use because no S-T detector has been available. Nunes²⁷ tried using a correlation chopper to distinguish order with limited success. Building an S-T detector for neutron diffraction appears within the state of the art.

Fig. 9.

A TOF Laué diffraction instrument for use on WNR.

E. Subsets of Experiments

1. Ordinary and Complex Samples. With the single crystal Laué instrument, ordinary crystals can be run quickly and with complete data. The instrument has the rate capability to tackle the most complex samples.

2. Polarized Scattering. By adding polarized filters to the Laué spectrometer, one can select coherent scattering and filter out incoherent scattering by the preservation-of-polarization principle. This may allow detection of very weak peaks which arise from hydrogen scattering from a much greater incoherent background.

3. Phase Determinations. X-ray and neutron diffraction measurements of Bragg peaks give the square of the scattering effect. The phase relation, which is needed for a unique determination of the atomic positions within the unit cell,²⁸ is lost by measuring the square. In the past, astute guessing has been used, but as the crystals become more complex direct methods are needed.

Neutron scattering from a few isotopes is accompanied by large absorption. This absorption adds an imaginary part to the scattering length and produces anomalous scattering which contains information about the phase. By measuring the scattering above and below the resonance, scattering length and additional phase information can be obtained.

In addition to anomalous scattering, there is also Schwinger scattering²⁹ (interference between nuclear and electronic potential) which produces a right- and left-handedness to some scattering. This also may be used to determine phase. With the TOF Laué method, it should be possible to take advantage of anomalous and Schwinger scattering. The TOF method will measure at different λ 's, some above the resonance energy and some below. This may provide the means for extracting the phase.

4. Samples Under High Pressure. It should be possible to use the Laué diffractometer to observe the crystal structure of samples under very high pressure. Figure 10 shows a sample cell which should be able to hold a sample at 100 kbar. A similar pressure system was built and tested at MTR. The figure shows a Bridgman anvil design with Al_2O_3 anvils in which the incident beam and scattered beams enter and leave along the anvil axis.

Fig. 10.

High pressure region of a Bridgman anvil press that could be used for TOF Laue patterns.

E. Conclusion

The TOF Laue method appears particularly well suited to measure neutron diffraction patterns from single crystals with a pulsed neutron source. This will compete favorably with the full circle method of steady state reactors.

VI. INELASTIC SCATTERING

Turn now from microstructure measurements to microdynamic measurements. Inelastic neutron scattering is the excitation or deexcitation of molecular quantum states in a material when a neutron scatters from the material. In these cases, the neutron loses or gains energy upon scattering; measurement of this loss or gain detects the quantum states of the material. If the scattering is coherent as well as inelastic, measurements record information about direction of the wave or location of the vibration in microscopic zones of the material. When the number of vibrations is recorded, a function related to the frequency distribution—the frequency spectra—is also recorded.

One of the unique powers of neutron inelastic scattering is that the neutron has the proper range of relations between its energy and momentum to detect the coupled relation between the energy and momentum of waves in the material. Electromagnetic radiation does not have this match and has been unable to do this so far.

Inelastic scattering measures the microdynamics of a material. Data obtained from inelastic scattering places stringent requirements on the force models and potential functions used to describe the material. Three sets of inelastic scattering experiments are proposed for WNR.

VII. INELASTIC SCATTERING: SMALL κ METHOD

A. Description

For inelastic scattering, one wants to measure as accurately as possible the excitation of a discrete energy state of a molecule. The resolution with which the scattered neutrons can be defined is a function of the resolution of the spectrometer as well as a "recoil resolution" characteristic of the sample and interaction parameters. The recoil resolution is appreciable for samples that show diffusion, such as molecular gases or liquids.

Recoil resolution is

$$\Delta E_{\text{recoil}} \propto \left(\frac{\kappa^2 T}{M_{\text{eff}}} \right)^{1/2} \quad (6)$$

where ΔE_{recoil} is the recoil resolution, κ is the wave vector of scattering, T is the temperature of the sample, and M_{eff} is an effective mass of the sample molecules. To improve recoil resolution one reduces the temperature and κ or increases effective mass. However, lowering temperature or increasing effective mass usually takes the sample to a new phase, thus changing the experiment. To reduce κ for any given energy exchange value, one must go to smaller scattering angles and higher incident energies. Higher incident energies are in the region where a pulsed source like WNR should excel. For solids where recoil resolution should be zero, small κ measurements of molecular spectra still have an advantage; multiphonon scattering backgrounds are reduced relative to the single scattering events.

B. Experimental Equipment

Figure 11 shows a hypothetical diagram of a proposed small κ instrument. Neutrons from the source are moderated by the moderator and fly toward the sample. These are interrupted by a chopper phased to the source. The phase lag of the chopper is set so that only a burst of monoenergetic neutrons is passed. This burst scatters from the sample, some neutrons exchange energy, and this energy change is measured by time of flight to the counter.

Fig. 11.

A small κ inelastic scattering instrument for WNR.

C. Special Features

The small κ method is designed to measure interpretable molecular spectra data. Evacuated flight paths eliminate air scattering. Use can be made of a tall sample container and a detector which is only sensitive to time whose area can be large because good space resolution is not important. A chopper needs to be developed to give good timing in the 0.05-0.5 eV range. Programs have been written to fit the data; they can be used for precise definition of energies and intensities.

D. Experience

The small κ method of molecular spectroscopy, which improves resolution by taking data at small κ 's, was successfully conducted at the MTR. At a recent NSF meeting⁵ Dr. Bruce Hudson stated that the MTR small κ data is the only molecular spectroscopy data so far produced by neutrons that can be interpreted both for energy exchange and intensity. The MTR measurements were on a thermal reactor, hence the upper limit of usable flux was about 0.1 eV. WNR will have high performance above 0.1 eV where recoil resolution can be further improved.

E. Subgroups of Experiments

1. Molecular Gases. The small κ method can produce definitive molecular spectroscopy data for molecules in the gas phase.³⁰ Modes of greatest interest are the optically forbidden rotational and vibrational modes that are inaccessible to infrared and Raman. The modes will be measured for dilute gases where intermolecular effects are negligible.

2. Molecular Liquids and Dense Gases. Similar molecular states will be measured as in the preceding paragraph. In addition, a determination will be made of the intermolecular effects which

were introduced by the molecules being in dense gases or liquids. In solids that still have a diffusive mode (for example, NH_3 molecules that can still rotate or librate), these transitions will be resolved.

3. Solids. The small κ method may be advantageous for measuring the frequency spectra of solids. Small κ measurements suppress multiphonon scattering relative to single phonon spectra thus making the latter more distinguishable. They are the only way to measure $\chi(\vec{q}, \omega)$ for magnetic metals where the limit is always $Q \lesssim 4 \text{ \AA}$, perhaps $Q \lesssim 2 \text{ \AA}$, and it is desirable to have $\hbar\omega \gtrsim 500 \text{ meV}$.

F. Conclusion

The power of the small κ method has been demonstrated. When using instruments of high resolution, its application promises to produce excellent molecular spectroscopy data.

VIII. INELASTIC SCATTERING: SCATTERING SURFACE METHOD

A. Description

The "constant Q " method of measuring dispersion relations for single crystals has become very popular and has many advocates. (Q and κ are the same.) Steady state reactors with three-axis spectrometers use this method whereby three of the four parameters of the spectrometer are adjusted so that each data point of the sample is taken at the same position in reciprocal space while the energy change is stepped through a set of energies.

A similar approach, but not quite as well aimed, can be conducted with TOF at a pulsed neutron source. Schmunk and Brugger³¹ at MTR showed how the scattering surface method could be used to obtain data in the desired $\vec{Q}$ direction which is near but not exactly at the desired $\vec{Q}$ magnitude.

B. Experimental Equipment

Figure 12 shows a hypothetical TOF scattering surface instrument. Neutrons from the source are moderated and fly toward the sample. A chopper, phased with the source, passes bursts of monochromatic neutrons which are scattered by the single crystal sample. Some of these neutrons that scatter coherently and inelastically are detected by the sets of counters. These counters are set to detect inelastic scattering surfaces that cross a given $\vec{Q}$

Fig. 12.

A TOF scattering surface instrument for measuring phonons in fixed directions of reciprocal space.

direction of the reciprocal lattice near the desired magnitude of $|\vec{Q}|$. If dispersion relation curves are to be traced out, the slight miss in the magnitude of $\vec{Q}$ (and thus $\vec{q}$) will make little difference in the instrument's ability to trace the full curve. However, if the experiment calls for phonon energy at an exact $\vec{Q}$ (both direction and magnitude), 3 to 12 different runs for a set of E_0 or crystal orientations will be needed to obtain data for extrapolation to the exact $\vec{Q}$.

C. Special Features

Angular resolution needs to be good in the scattering plane but relaxed above and below it, hence sets of tubular counters can be used. Banks of counters at a number of angles can run simultaneously. The central position of each bank of counters must be adjustable and programmable in the Q plane. The sample will be mounted on a programable axis that moves when the arm to the counter banks moves.

D. Past Experience

To date, the success of the "constant Q " method which uses three-axis spectrometers with steady state reactors and the limited intensity of pulsed sources, has discouraged application of the scattering surface method.

E. Subsets of Experiments

Subsets of experiments are numerous. The scattering surface method used with pulsed sources should open up all the possibilities of inelastic

neutron scattering for which the constant Q method, using three-axis spectrometers with a steady state reactor, is being used.

F. Conclusions

The scattering surface method enables a TOF system to approach a three-axis spectrometer in measuring the energy of phonons at a prescribed $\vec{q}$.

IX. INELASTIC SCATTERING: LINE WIDTHS

A. Description

Whenever motion of atoms in a material experience anharmonic forces (barrier penetration, diffusion, translations), the anharmonicity will cause discrete elastic and inelastic scattering to exhibit a broadening.³²⁻³⁶ For translational motions, such as atoms in a gas, the broadening is very large, dominating the scattering, and producing tens of meV of broadening. (It is to limit this translational broadening of the molecular vibrations of molecules in gases that the small κ method outlined in Sec. VII was developed.) For diffusion, as in a liquid, the elastic and inelastic peaks associated with molecular vibrations are broadened by units of meV (the elastic peak in this case is called quasielastic). For barrier penetration (such as methyl librations in solid neopentane) the rotational levels are broadened by units of meV. For dispersion relations, inelastic scattering peaks which arise from excitation of a lattice wave may be broadened by μeV ³⁷ because of phase transformations or other anharmonic effects. Measurement of these broadenings may provide valuable information about the anharmonicity of the forces.

B. Instruments

1. TOF Instrument. Instruments to measure tens of MeV are not needed since translational motion is well understood; additional measurements are of limited interest. Instruments to measure units of MeV are described in Secs. VII and VIII which will suffice to measure broadening caused by diffusive motions, librations, and very anharmonic phonons. However, to reach μeV broadening, special instruments are needed.

One such special instrument is proposed in Fig. 13. Neutrons from the source are moderated to cold neutrons by the cold moderator. Bursts from WNR

Fig. 13.

TOF instrument for line width measurements of high resolution.

will not be short enough to give the required high resolution, therefore two choppers are used as a velocity selector, one inside the target shielding and one in front of the sample. A burst of cold neutrons travels down the guide tube. The second chopper passes only those of one velocity which scatter from the sample; the gain or loss of energy is determined by measuring the TOF to the detector. Tall guide tubes are needed to accept all of the neutrons from the highest intensity part of the moderator.

For liquids or powders, one guide tube behind the sample is adequate. To measure line widths of low level phonons it would be advantageous to have a number of guide tubes and detectors for application of the scattering surface method.

2. TOF Instrument Resolution. If the choppers have burst times of $10 \mu\text{s}$ each, guide tube lengths of 10 m each, and E_0 and E_f are 0.005 eV (1000 $\mu\text{s}/\text{m}$), the resolution of E_0 is

$$\Delta T_0 = \left[\left(\frac{10}{10^4} \right)^2 + \left(\frac{10}{10^4} \right)^2 \right]^{1/2} = 1.4 \times 10^{-3} \quad (7)$$

$$\Delta E_0 = 2.8 \times 10^{-3} E_0 = 14 \mu\text{eV} \quad (8)$$

ΔE_f includes the $14 \mu\text{eV}$ of ΔE_0 , as well as flight path uncertainties, channel widths, etc. It might be reasonable to predict a resolution of $2 \times 14 \mu\text{eV}$ or $\sim 30 \mu\text{eV}$ for the total instrument.

3. Diffraction Instrument. Figure 14 shows a hypothetical diagram of a line width spectrometer for very high energy resolution measurements. Neutrons from the source are moderated by the moderator and fly toward the sample. The moderator rotates as fast as possible, say with an edge speed near 500 m/s. A 5-cm-wide moderator would exit from the beam in 100 ms, thereby cutting off the tail of cold neutrons for burst times $> 100 \mu\text{s}$.

The instrument operates as follows. Moderated neutrons fly down a 100-m-long flight path formed by a neutron guide and strike the sample from which neutrons are quasi-elastically scattered. The energy of the scattered neutrons is analyzed by a large area curved silicon crystal analyzer,³⁸ which makes use of the high resolution of the back-scattering analyzer. The crystal focuses on a counter just beyond the sample. A filter removes orders and faster neutrons.

C. Subsets of Experiments

1. Diffusion in Liquids. An understanding is needed of the different types of motion which contribute to quasi-elastic scattering. Data for a number of ranges of κ provide this understanding and can yield definitive information about the mechanism of diffusive motions in liquids.

2. Molecular Librations in Liquids and Solids. The effects of liquid-like behavior are determined by measuring the width of the quasi-elastic peak at very small κ . Then the broadening of the inelastic peaks, which is corrected for liquid-like behavior, would reveal the diffusive motion of molecular reordering and molecular librations. This motion should give some information of the anharmonicity of molecular

Fig. 14.

Diffraction analyzer for line width measurements of high resolution.

libration potential. The same processes will hold true for the solid but without the effect of liquid diffusion.

3. Phonon Widths. In solids, near or at phase changes, the phonon peaks should show a broadening which indicates an increased tendency of the atoms to move from their crystal sites. These broadenings are in μeV ; their measurement should provide valuable information about the potential shapes near these phase changes.

D. Conclusion

The WNR could make an effective study of anharmonic potentials by measuring widths of quasi-elastic and phonon peaks.

X. MODULAR SYSTEM

Methods outlined in Secs. III-IX maximize the use of TOF methods while minimizing the use of diffraction components (crystal monochromators and analyzers). Many of the experiments have common components; thus interchange of modules is possible and, indeed, beneficial. Two lengths-of-flight paths will accommodate most instruments: long paths for high resolution and short for low resolution, high count rate experiments. The choppers can be modules added at the end of these flight paths, most of which will benefit from being evacuated.

A. S-T Detectors

To adopt the modular approach requires special attention to development of several modules. S-T sensitive detectors are needed to capture the full power of pulsed sources.³⁹ BNL and ILJ. have developed delay wire or crossed wire detectors that are space sensitive; it may be possible to make them fast enough to be time sensitive as well. A search should be made in the areas of high energy physics, nuclear medicine, and aerospace development for systems that can be modified to form a large S-T detector.

B. Choppers

The second module to develop is a chopper with timing resolution to 0.5 eV. Noncadmium materials

must chop the thermal and epithermal neutrons. Choppers need not be as heavy as those at steady state reactors because the average fast flux which comes down the beam tube is much lower. Design of such choppers does not seem prohibitive. Ways must also be developed of phasing these choppers to bursts from the accelerator, a trivial matter for linacs triggered by the chopper, but a questionable undertaking for the configuration at the Los Alamos Meson Physics Facility (LAMPF).

XI. INITIAL IMPLEMENTATION

Physics Group P-11 at LASL has acquired surplus TOF equipment from MTR. The group plans to use the equipment to initiate, test, and develop the classes of experiments outlined in Secs. III-IX. Acquired were (a) an evacuated flight path, (b) ~ 12 each 25-cm-long and 10-cm-long ^3He counters, (c) several Fermi choppers, and (d) shielding for the choppers. The evacuated flight path has the following parameters: sample-to-detector distance of 2 m, a sample shield, holders for 25-cm-long and 10-cm-long ^3He counters, and a $\Delta\theta$ of $\sim 25^\circ$. Figure 15 shows equipment arrangements for the three classes of neutron diffraction experiments.

Fig. 15.

MTR equipment arranged for neutron diffraction measurements. Dimensions refer to the length of detectors to be used.

A. Powdered Samples

A longer flight tube is fitted with collimators behind the moderator and in front of the sample. The MTR evacuated flight path is fixed to rotate about the sample position; it is rotated to a scattering angle of 90° where the vertical counters better match the Debye-Scherrer cones. The flight tube is modified so that the counters fall on the surface of the same TOF for each d . The 25-cm counters are used because ϕ position is not critical. A monitor is placed in the incident beam 2 m behind the sample.

The counters are hooked to a common preamplifier and TOF data is recorded. This provides a powder sample diffraction instrument that could prove to be a quality research and analytical diffractometer.

B. Small Angle Scattering

Next, the small angle flight path is rotated to zero degrees. Slits at the moderator and sample are narrowed and the 25-cm counters are replaced with 10-cm detectors, each connected to a separate timing channel. This allows observation of larger plane spacings ($d < 200 \text{ \AA}$). This could be a useful analytical instrument.

C. Single Crystal Laue

To demonstrate the TOF Laue method, the small angle flight path is rotated back to some finite angle θ and a single crystal sample is placed at the sample position. One or more detectors observe Bragg peaks and sort the orders. Without a better detector to cover more space while still being time sensitive, this arrangement can only be a demonstration.

D. Small κ

Turning now to inelastic scattering, Fig. 16 shows an arrangement of the MTR equipment. For a small κ measurement, with the longer flight path, rotate the small angle flight path to 0° . Insert the 25-cm detectors and connect them in common to a time channel. Insert a Fermi chopper in front of the sample and phase it with LAMPF. The equipment is ready for molecular spectra measurements. A long flight path is needed to compensate for the large burst at the moderator.

Fig. 16.

MTR equipment arranged for neutron inelastic scattering measurements.

E. Scattering Surface

To demonstrate the scattering surface method, insert the 10-cm detectors in the small angle flight path and connect each to a time channel. Place a single crystal sample at the sample position. To straddle a $\vec{q}$ direction, orient the sample, rotate the flight path, and set E_0 by adjusting the phase of the Fermi chopper. Phonons across the desired $\vec{q}$ can then be measured. This may well constitute an analytical instrument without further modification.

F. Line Widths

To measure quasi-elastic line widths or line widths of phonons, replace the 10-cm counters in the arrangement of the preceding paragraph with 25-cm detectors. The sample to be measured is placed at the sample position and the chopper phase set to deliver the desired E_0 . This equipment can only observe meV of width and not μeV .

XII. CONCLUSIONS

Six promising classes of experiments in slow neutron scattering have been presented for WNR

research. Lattice and space groups of crystalline samples can be determined by a high resolution, powder diffraction instrument. Large distance ordering in polymers, biological samples, and radiation-damaged samples can be measured with the small angle scattering instrument. The x-ray Laue method can be improved by the single crystal neutron TOF Laue method.

Molecular spectra will be measured for highly symmetric molecules by the small κ method. The constant Q method that has proven so powerful on steady state reactors will be supplemented in the WNR by the scattering surface method. Diffusive and anharmonic motions in materials will be observed in line-width measurements.

The experimental instruments should be built as modules to allow interchange of components. Special effort must go into development of choppers and S-T sensitive detectors. Each proposed experiment can be initiated with the MTR instruments procured by WNR.

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