TWO METHODS FOR MAKING ACCURATE MEASUREMENTS OF INELASTIC SCATTERING

H. Maier-Leibnitz

Two methods for making accurate measurements of inelastic neutron scattering are proposed. The first method leads to an increase in resolution by improving the triple-axis spectrometer. The second method employs backscattering from a vibrating crystal. Parameters are presented for appropriate apparatus.

INTRODUCTION

Some, but by no means all, experiments require extremely accurate measurements. Examples are: a) quasielastic scattering with small energy transfer to study hindered rotations and slow motions in liquid crystals or in organic matter; b) anharmonic effects: width and shape of phonon lines; c) molecular spectroscopy. The main difficulty arises from insufficient intensity.

The resolution is determined by the following factors:

Target area	2 Measurements 1 important
Solid angles	4 Measurements 2 important
Δk	2 Measurements 2 important
In time-of-flight experiments: time of flight instead of Δk	2 Measurements 2 important

In a poorly arranged experiment the intensity must increase as ε^{-5}, where ε is the resolution. Consequently it is necessary to try to produce focusing, that is, to decrease the number of variables affecting the resolution. Such a decrease is always possible if anything is known about the scattering law $S(k, \omega)$, e.g., that at some point in k space grad $\omega(k) = 0$ along the direction of propagation of the phonon. One method of increasing the intensity is focusing with a triple-axis spectrometer. This is a well-known procedure, but we hope to make it more widely applicable. Here the number of important variables is reduced to two. A second method uses backscattering from a vibrating crystal. In this case only one variable is important, namely the time of arrival at the detector.

1. GENERALIZED FOCUSING BY A TRIPLE-AXIS SPECTROMETER [1]

We consider three improvements of a triple-axis spectrometer: the monochromator and analyzer crystals are bent, the distances between the crystals and the target are variable, and the Soller collimator slits are eliminated. The crystals can be bent to a radius of about 3 m as is frequently done in x-ray or γ-ray spectroscopy, or with a temperature gradient [2]. In the latter case the thickness of the crystal is not an obstacle as it is in mechanical bending. Bent crystals have two advantages: 1) nearly perfect crys-

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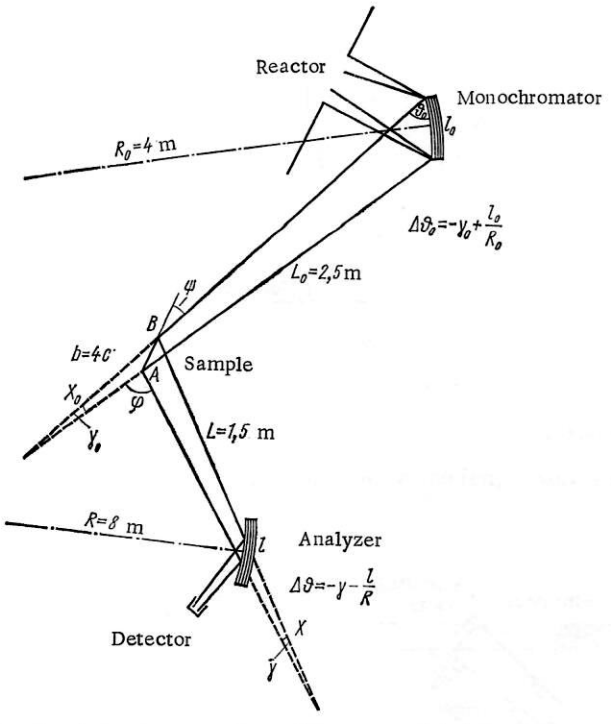

Fig. 1. Actual geometry of improved triple-axis spectrometer experiment.

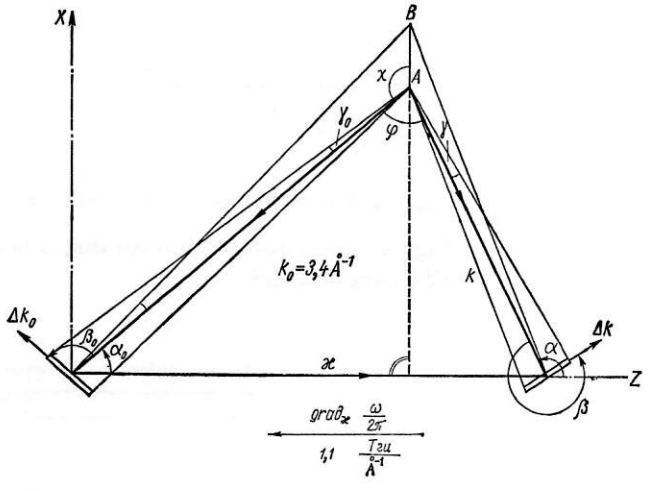

Fig. 2. Momentum diagram corresponding to the geometry of Fig. 1.

tals can be used instead of mosaics, since bending replaces the mosaic spread which is frequently required to obtain good integral reflection; 2) the magnitude and direction of the radius of curvature are convenient variables for making the triple-axis spectrometer more flexible.

A schematic diagram of the spectrometer is shown in Fig. 1. Figure 2 is a diagram in momentum space for two points on the target and for incident and reflected neutrons. It is assumed that the spread of wave vectors Δk_0 and Δk along the direction of neutron propagation is small (10^{-3}). The ends of the wave vectors range over a thin disk rather than an ellipsoid as is generally assumed.

Among the wave vectors of neutrons incident on and reflected from the second point of the target are some which are related to one another by energy and momentum transfer in the same way as the average $\mathbf{k}_0$ and $\mathbf{k}$ vectors of neutrons incident on and reflected from the first point.

Because of a certain angular spread of the primary and scattered beams the vector $\boldsymbol{\varkappa}$ is also spread about its average value $\boldsymbol{\varkappa}_0$, but within the limits of this spread there is a well-defined relation between ω and $\boldsymbol{\varkappa}$

$$\omega = \omega(\boldsymbol{\varkappa}), \tag{1}$$

which in first approximation can be written

$$\omega = \omega(\boldsymbol{\varkappa}_0) + \Delta\boldsymbol{\varkappa}\,\mathrm{grad}\,\omega. \tag{2}$$

Equation (1) is the same for $\boldsymbol{\varkappa}$ vectors which refer to the first and second points of the target, but the average $\boldsymbol{\varkappa}$ will be somewhat different in the two cases. The focusing principle [3-5] consists in bringing agreement at a given point $\boldsymbol{\varkappa} = \boldsymbol{\tau} + \mathbf{q}$, where $\boldsymbol{\tau}$ is the reciprocal lattice vector and $\mathbf{q}$ is the wave vector of the phonon, between grad ω from Eq. (2) and the value of the gradient which is already known approximately from preliminary data on the dispersion function. To do this, it is necessary to select most of the parameters shown in Fig. 2, except for one quantity, for example k_0. Then this scheme must be translated into the language corresponding to the experimental configuration of Fig. 1. The general formulas for this translation were derived by Marx [1]. It turns out that this is possible even without using all the parameters. For example it is not necessary to change the plane of the section of the sample if it is required to

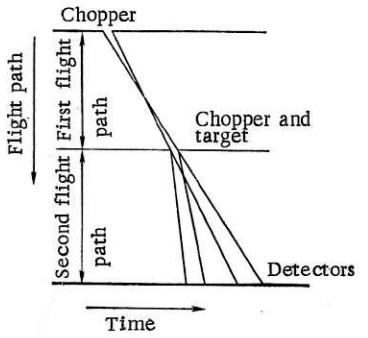

Fig. 3

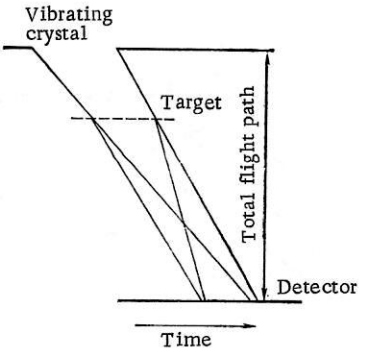

Fig. 4

Fig. 3. Conventional time-of-flight method.

Fig. 4. Principle of compacting a beam into bunches by means of a vibrating crystal.

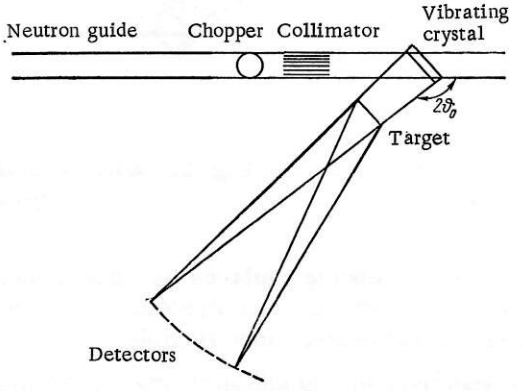

Fig. 5. Possible geometry of an experiment with a vibrating monochromator crystal.

change $\varkappa$ and ω. It is also possible to satisfy the condition grad $\omega = 0$. This condition can be satisfied with flat crystals only if the monochromator and analyzer are so placed that the scattering from each is at exactly 180°.

Numerical values are indicated for all possible parameters in the special case shown in Fig. 2, which corresponds to the actual configuration shown in Fig. 1. It is clear that the dimensions of the apparatus must be large because of the large radii of curvature of the crystals. The mechanical parts are arranged in the following way: the spectrometer consists of stands for the crystals, sample, and detector. The stands rest on a rather flat floor and are connected by light-weight arms of variable lengths. The positions of the arms and the values of the angles are checked optically. The stands are shifted after they are raised slightly on air bearings. Clearly this "dancing spectrometer" is no more expensive than an ordinary triple-axis spectrometer. The same setup can also be used in the conventional manner with flat crystals and moderate resolution; instead of focusing it is also possible to use multiple detector systems where one or more analyzing crystals serves each of several detectors.

BACKSCATTERING FROM A VIBRATING CRYSTAL [6]

The highest resolution achieved so far was obtained with a triple-axis spectrometer [7] in which the scattering from the monochromator and analyzer was at 180°.

This corresponds to the condition grad $\omega = 0$ mentioned above. In this case neither the dimensions of the target nor the size of the crystal worsen the resolution, which amounts to $5 \cdot 10^{-7}$ eV for 2 MeV neutrons. The energy is varied by moving one of the crystals.

Peterlin [6] studied the possibility of applying the time-of-flight method from the point of view of flexibility and gain in intensity. It is well known that for the same resolution in $\varkappa$ and ω the intensity is the same for both triple-axis and conventional time-of-flight spectrometers (Fig. 3), except that in the latter case there is a further attenuation by a factor $T_m f$, where T_m is the time interval after a pulse during which the detector receives useful information and $1/f$ is the time interval between pulses of primary neutrons. Peterlin observed, and we do not know whether this was shown earlier, that the intensity in time-of-flight experiments can be significantly increased if the neutron beam is transmitted in bunches to the detector rather than to the target (Fig. 4). The beam can be compacted into bunches by vibrating the monochromator crystal with the acceleration [8]

$$\frac{dv}{dt} = \frac{v^2}{L}, \tag{3}$$

where v is the neutron velocity and L is the distance from the monochromator to the target and to the detector. The configuration is shown approximately in Fig. 5. For small scattering angles the time of arrival at the detector after elastic scattering is the same as for the direct path, and the scattering angle, and therefore $\varkappa$, is the same for all points of the target. The time of arrival of neutrons whose energy has been shifted by a small amount $\hbar\omega$ is changed by the same amount for all points of the target and for all scattering angles, and is approximately the same for neutrons of all velocities present in the incident beam. The resolution in $\varkappa$ is determined by the angular spread of the primary beam and the radius and length of the neutron guide; the dimensions of the detector must correspond to this resolution.

In practice a gypsum crystal was used as a monochromator. Its [020] plane gives sufficiently intense reflection and the lattice constant is large so that backscattering occurs for $\lambda = 15.2$ Å, v = 261 m/sec, E = 0.568 MeV. The use of slow neutrons permits a short flight path L without significantly increasing the acceleration described by Eq. (3). Gypsum obviously forms rather good crystals. The mosaic width measured with gamma rays [9] is 10" so that for scattering at 180° the relative line width $\Delta\lambda/\lambda$ should be approximately the same ($\sim 10^{-4}$) as the theoretical width for an ideal crystal.

We list the basic data for the proposed design.

Gypsum crystal [020]	d = 7.59 Å
Neutron velocity for backscattering	261 m/sec
	E = 0.578 MeV
Dimensions	3 × 8 × 0.3 cm
Bragg angle	$\theta = 88°$
Frequency of vibrations	f = 131 Hz
Amplitude	2 cm
	V_{max} = 16.5 m/sec
	$(dv/dt)_{max}$ = 13600 m/sec^2
Time of irradiation of crystal	690 μsec
Length of flight path (for an angular resolution of 10^{-2} rad; $\Delta k = 0.4 \cdot 10^{-2}$ Å^{-1}):	
total	5.0 m
between sample and detector	3.8 m
Target area	3 × 6 cm
Time of flight	19.2 μsec
Radius of curvature of crystal	R = 10 m
Increase in pulse length because of crystal thickness	9.8 μsec
Total length of pulse	12.2 μsec
Time resolution $\Delta t/t$	$6.4 \cdot 10^{-4}$
Intensity at target	$>10^4$/sec

The large value of the Bragg angle ($\theta = 88°$) is very important for good compacting of the reflected beam into bunches. The pulse length is determined mainly by the thickness of the crystal, on which the intensity depends linearly. For neutrons emerging from the crystal at the same instant the accelerated crystal is

similar to a crystal whose lattice constant has a nonzero gradient. Neutrons are reflected from the crystal for 690 μsec so that the gain from bunching is approximately 690/12.2 = 56. The relative spread of velocities in the primary beam is $3.6 \cdot 10^{-2}$. Small refinements can be introduced. For example the crystal can be cut at an angle α with the reflecting planes in order to compensate the defect that $\theta \neq 90°$; θ_0 can be changed to adjust the bunching to the final scattering angles; the frequency of vibrations of the crystal can be changed to compensate the error which arises when ω is sizable, etc.

In quasielastic scattering the range of ω which can be studied is usually small and the loss factor $T_m f$ mentioned earlier becomes important. It can offset the whole gain from bunching. Therefore from the point of view of intensity the method discussed is equivalent to that of Alefeld, Bir, and Heidemann.

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