spherical wave theory (*e.g.* Kato, 1964), the relation (7) is particularly useful to know the intensity distribution of traverse topographs.

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*Acta Cryst.* (1968). A**24**, 160

# Specimen Motion Effects in Neutron Diffraction*

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(*Received* 16 *June* 1967)

Observations are reported on two effects of specimen motion upon neutron diffraction processes. These include the necessary realignment of a single crystal in maintaining Bragg reflection conditions and the shift in the long wavelength cut-off characteristic of the transmission through a polycrystalline sample. The observations are compared with those to be expected from an analysis of Doppler and velocity compounding effects.

## Introduction

Among the three forms of radiation commonly used in crystal diffraction research, namely X-rays, electrons and neutrons, the characteristics of the latter are convenient in demonstrating the dynamical effects of specimen motion on the diffraction process. This arises because the transport velocity of slow neutron radiation is of the same order of magnitude as the laboratory speeds to which crystal specimens can be accelerated. Thus Doppler effects and velocity compounding or aberration effects can be expected to be sizable. A previous study (Shull & Gingrich, 1964) has demonstrated measurable changes in the polycrystalline diffraction pattern with specimen motion and the measured shifts in the position of the Debye–Scherrer reflections were shown to agree with those expected from analysis of the reciprocal lattice construction.

Additional observations on specimen motion effects are supplied in the present report. The present experimental investigations are of two forms, (1) demonstration of the realignment of a single crystal necessitated in maintaining Bragg reflection with crystal motion and (2) illustration of the shift in the long wavelength cut-off edge of the transmission cross section of a polycrystalline specimen. The reported effects are of practical usefulness in neutron technology as will be discussed.

* This research was supported by the National Science Foundation and forms the basis for undergraduate theses submitted by two of us (KRM and JGR) to M.I.T. May 1965.

## Single-crystal realignment in Bragg reflection

If a single crystal is set in motion, then it is to be expected that the crystal must be realigned to maintain Bragg reflection of an incident monochromatic neutron beam. This is most conveniently analyzed from the reciprocal lattice construction diagramed in Fig. 1. In this Figure **v** represents the incident neutron velocity, **V** the crystal velocity, and **τ** the reciprocal lattice vector of the diffracting planes. The diagram illustrates the case where **V** and **τ** are collinear, implying that the crystal velocity is perpendicular to the Bragg reflecting planes. In the crystal frame of reference, the neutron

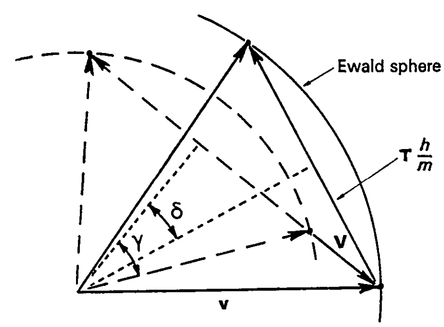


Fig. 1. Reciprocal lattice construction illustrating the reorientation necessary in maintaining Bragg reflection from a moving crystal. The incident neutron velocity is **v**, the crystal velocity is **V** and the reciprocal lattice vector is **τ**. The dashed line construction corresponds to the moving crystal case with a tilt angle $\delta$ of **τ** to keep the reciprocal lattice point on the Ewald sphere.

velocity becomes **u** by velocity compounding and the crystal orientation must be changed by an angle $\delta$ from the stationary crystal case in maintaining the reciprocal lattice point on the Ewald sphere of reflection.

For the present experimental case of $V$ being small compared with $v$ it can be shown to good approximation that

$$\delta = \frac{V}{v} \cdot \frac{1}{\cos \gamma}, \tag{1}$$

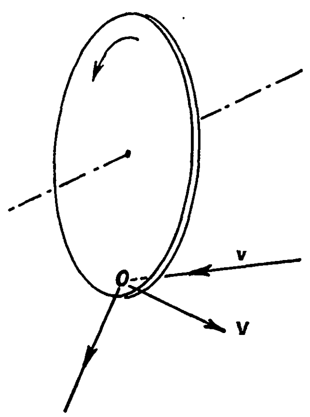


Fig. 2. Diagram of rotating crystal disc assembly for obtaining motion collinear with the reciprocal lattice vector. The disc is a sodium chloride crystal rotating around a [100] axis with (220) diffraction from the fourfold internal planes.

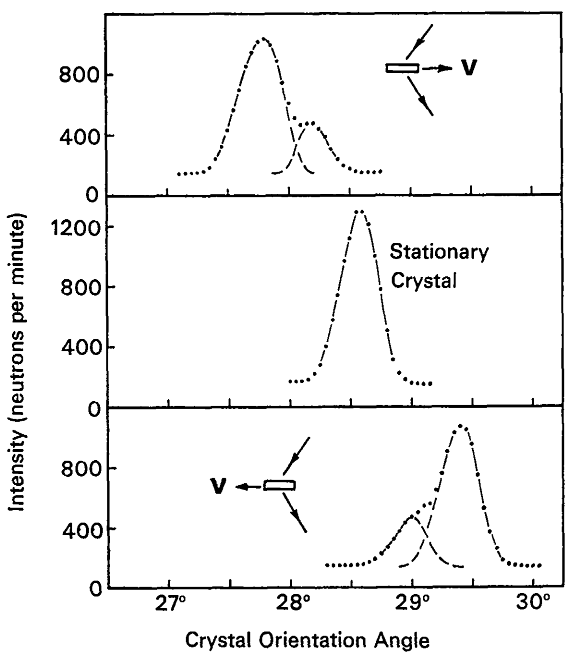


Fig. 3. Rocking curves for the (220) NaCl reflection for stationary (see text) crystal and for crystal moving parallel and anti-parallel to reciprocal lattice vector. The secondary peaks in the shifted patterns arise from the $\lambda/2$ component in the incident beam. The crystal velocity was 24·5 m.sec$^{-1}$ compared with the neutron velocity of 1978 m.sec$^{-1}$ for the primary wavelength of 2·00 Å.

$\gamma$ being the Bragg angle. A reversal of the direction of **V** changes the sign of $\delta$ without changing its magnitude in first approximation.

This crystal orientation shift has been studied experimentally with a sodium chloride crystal set in motion. For this purpose a crystal disc of diameter 7·60 cm was rotated about its cylindrical axis while diffracting in transmission a neutron beam striking it near its periphery, as shown in Fig. 2. The circular face of the crystal disc contained (100) planes and diffraction was studied with internal (220) planes. Upon rotation of the disc, the fourfold (220) planes come into consecutive Bragg reflection and the diffracted beam was of pulsed nature with four pulses per revolution of the crystal.

Rotational speeds up to 7500 revolutions per minute were utilized and with the mean radial position of 3·12 cm for the illuminated crystal area (circular of diameter 0·63 cm), this provides a translational velocity of 24·5 m.sec$^{-1}$ perpendicular to the (220) planes. Neutrons of wavelength 2·00 Å, from a monochromating crystal of germanium set in (220) reflection were used so that $v$ was of magnitude 1978 m.sec$^{-1}$.

Fig. 3 shows rocking curves of the crystal for the two directions of motion along with that of a slowly moving crystal illustrating the necessary realignment. The latter was accomplished by maintaining a slow rotation of the crystal disc so that the intensity was again being delivered to the detector in burst fashion. This slow rotation of the crystal produced a crystal velocity of 0·10 m.sec$^{-1}$, which was negligibly smaller than the specimen speed of 24·5 m.sec$^{-1}$; the latter is characterized by the shifts illustrated in the Figure. The secondary peaks in the shifted, rocking curve patterns are caused by the $\lambda/2$ or 1·00 Å component in the neutron beam from the monochromating germanium crystal and this component is shifted only half as much as the primary $\lambda$ component. In essence this demonstrates that the motional pattern is displaying the spectrum of the incident radiation. For the crystal speed of 24·5 m.sec$^{-1}$, the calculated values for the shift are 49·1 and 49·5 minutes of arc, to be compared with measured shifts of 47·7 and 49·2 minutes of arc respectively for the two directions of crystal motion given in the Figure.

A study of the shift as a function of the crystal speed has been performed and Fig. 4 summarizes the comparison between experimental values and those to be expected. The agreement is satisfactory within the precision of the measurement. It may be mentioned that along with the orientation shifts which are seen there are integrated intensity and peak width modifications just as had been observed in the polycrystalline sample study (Shull & Gingrich, 1964).

Further experiments were carried out with the rotating disc crystal when it was reoriented to permit crystal motion perpendicular to the scattering vector or within the Bragg reflecting planes. An analysis of the reciprocal lattice vector diagram for this case shows that no orientation shift is to be expected in spite of the fact that Doppler and aberration angle effects are still in play, the two effects cancelling each other. The rocking curves of Fig. 5 illustrate the absence of a shift for a crystal velocity of 16·2 m.sec$^{-1}$ compared with that for a slowly moving crystal.

### Long wavelength cut-off shift with specimen motion

When the transmission cross section of polycrystalline material is examined with long wavelength neutrons, pronounced discontinuities are to be expected when the wavelength corresponds to back reflection from the innermost Bragg reflections. These effects are most pronounced for specimens whose transmission is dominated by coherent scattering as in the case of beryllium, first demonstrated by Fermi, Sturm & Sachs (1947). For wavelengths beyond $\lambda_c = 2d_{\max}$ corresponding to back reflection from planes of maximum interplanar spacing, no coherent scattering is possible and the transmission cross section drops abruptly to a level dictated by the absorption, incoherent and inelastic scattering, and physical inhomogeneities. The presence of this cut-off edge is frequently exploited in neutron technology as a means of producing a long wavelength neutron filter.

It is to be expected that the wavelength associated with the cut-off will be shifted if the specimen is in motion relative to the beam. Again this can be analyzed with reciprocal lattice construction and the most interesting case corresponds to that where the specimen motion is collinear with the incident neutron velocity. Oppositely directed shifts are to be expected with a reversal of the relative direction of motion.

This has been studied experimentally by imparting specimen motion to a sample of polycrystalline iron for which the cut-off wavelength is normally located at 4·046 Å corresponding to back reflection from the (110) planes. A 12 inch diameter disc was placed in rotation and the transmission cross section was measured as a function of incident neutron wavelength for a peripheral region of the moving disc. An average

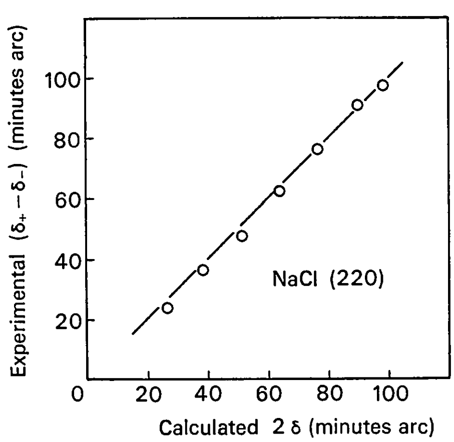


Fig. 4. Comparison between the observed total shift in crystal orientation upon reversal of motion direction and that calculated for different crystal velocities to a maximum value of 24·5 m.sec$^{-1}$.

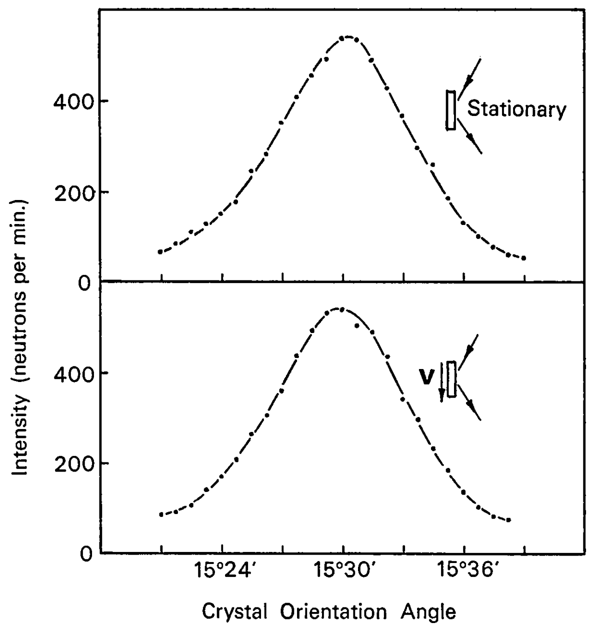


Fig. 5. Rocking curves for the (200) NaCl reflection for stationary crystal and for crystal moving parallel to Bragg reflecting planes. No shift is expected because the Doppler and velocity-compounding effects counteract each other. A neutron wavelength of 1·51 Å was used and the crystal velocity was 16·2 m.sec$^{-1}$.

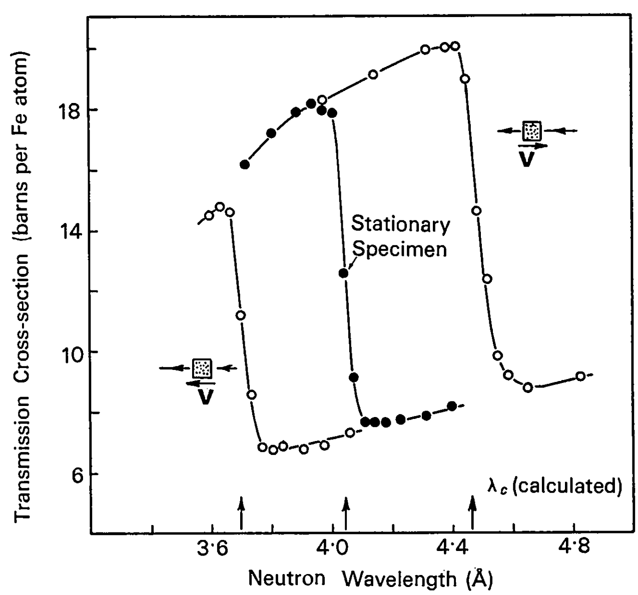


Fig. 6. Transmission cross section of a polycrystalline iron sample with and without sample motion parallel and antiparallel to the neutron velocity. The discontinuity in the cross section corresponds to back reflection by the (110) planes and this is shifted along the neutron wavelength scale with specimen motion. The expected positions of the cross section edge are shown by the vertical arrows.

speed of 91·8 m.sec$^{-1}$ (component along the neutron direction) at the examined region was used, and the transmission cross section was studied for the two cases where the specimen motion was parallel and anti-parallel to the neutron velocity. Monochromatic neutrons in this wavelength region were obtained by Bragg reflection from a mica crystal, polycrystalline beryllium being used to filter out the higher order reflected neutrons.

Fig. 6 shows the measured transmission cross sections for the stationary and moving specimen cases along with the wavelength positions where the cut-off is to be expected. Agreement between experiment and calculation is again evident. It is significant that the magnitude of the cross section discontinuity is changed in the expected manner with specimen motion. Thus it is demonstrated that the cut-off wavelength can be easily shifted by suitable specimen motion and this can be exploited in producing window filters of adjustable width. This has been suggested independently by Iyengar (1964). In considering the case of polycrystalline specimen motion perpendicular to the incident neutron velocity, no shift in the cut-off edge is to be expected in first approximation. It is interesting that this case changes the back-reflected Debye–Scherrer circular rings into elliptical rings.

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*Acta Cryst.* (1967). A**24**, 163

# The Role of Lattice Vibrations in Dynamical Theory of X-rays

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(*Received* 18 *July* 1967)

A consistent dynamical theory of X-rays is developed which takes into account in explicit form the processes of Thomson scattering, photoelectric absorption, and Compton scattering as well as inelastic scattering of X-rays by phonons. Special attention is paid to analysis of the role played by lattice vibrations and by temperature. Owing to inelastic scattering by phonons, the temperature dependence of the coefficients of dynamical equations is not determined by Debye–Waller factors but has a more complicated behaviour. A detailed analysis is given of the influence of lattice vibrations on the effect of anomalous transmission.

## 1. Introduction

In recent papers by the present authors (Afanas'ev & Kagan, 1965; Kagan & Afanas'ev, 1965, 1966) a dynamical theory has been developed which describes the motion of $\gamma$-quanta and neutrons in a regular crystal when the interaction of the particles with individual nuclei has primarily resonance character. In those papers it turned out to be possible consistently to include the vibrations of nuclei in the dynamical theory. In this aspect a considerable simplification of the problem had been achieved under an assumption that the inelastic part of the scattering cross-section by an individual nucleus was large as compared with the elastic one – as is the case in most of the situations. A complete solution of the dynamical problem in a vibrating crystal, free from this assumption, has been given in a more recent paper (Afanas'ev & Kagan, 1967).

As has been noted in the papers quoted, all the aspects of the dynamical theory of X-rays, connected with vibrations of the atoms, are identical with those of the resonance problem if the width of the resonance level is large compared with the characteristic energy of the phonons. This circumstance made it possible to give, in the last paper (Afanas'ev & Kagan, 1967), final results for the coefficients of the dynamical theory of X-rays.

Keeping in mind the great interest attached to this problem in the physics of X-rays, we give in the present paper a detailed analysis of the influence of lattice vibrations, and thus of temperature, on the dynamical theory of X-rays and particularly on the effect of anomalous transmission (Borrmann, 1941, 1950).

## 2. Derivation of general equations

To describe the electromagnetic field inside the crystal we use the usual set of Maxwell equations, as in the first paper mentioned (Afanas'ev & Kagan, 1965). Converting to space and time Fourier components, we get:

$$(k^2-\omega^2/c^2)\mathbf{E}(\mathbf{k},\omega)-\mathbf{k}[\mathbf{k}\mathbf{E}(\mathbf{k},\omega)]=i\,\frac{4\pi\omega}{c^2}\,\mathbf{j}(\mathbf{k},\omega)\,. \quad (2.1)$$