On the Inelastic Scattering of Neutrons by Crystal Lattices

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Previous theoretical results on the inelastic scattering of neutrons in ideal crystals are reviewed. Restrictive conditions imposed by crystal interference on inelastic scattering are discussed. It is found that if the velocity of the incident neutrons is smaller than the sound velocity in the crystal, neutrons from a monochromatic, well-defined beam are scattered by inelastic processes into sharply limited areas. On the other hand, inelastic scattering of faster neutrons should give rise to diffuse spots similar to those observed in inelastic scattering of x-rays.

OWING to the comparatively great mass of neutrons the theory of inelastic scattering of neutrons by crystal lattices differs from the corresponding theories for electrons and for x-rays. Theoretical treatment[1] of the scattering of neutrons in crystals has led to two simple results. First, elastic collisions are predominant if the neutron energy is less than ME_0^2/E_v (M = mass number of an appropriate atom in the crystal, $E_v \equiv$ vibrational energy of such an atom in the crystal; the latter quantity becomes equal to kT at high temperatures and to the zero-point energy E_0 at low temperatures). Second, the total scattering probability of neutrons having sufficiently low energies becomes zero if the temperature of the crystal is equal to 0°K. While the absence of elastic scattering processes at sufficiently low neutron energies follows from the impossibility of fulfillment of the Bragg interference conditions, the disappearance of the inelastic scattering processes is owing to the relatively great value of the mass of the neutron.

The purpose of the present note is a discussion of the restrictions on inelastic scattering processes imposed by the crystal interference conditions. We shall see that these restrictions not only lead at low neutron energies to the disappearance of the scattering probabilities, but continue to operate at somewhat higher neutron energies. Actually they influence the inelastic scattering processes whenever the velocity of the neutron is not great as compared to the sound velocity in the crystal.

The following considerations will be restricted to crystals in which the neutrons are scattered in the same way by each lattice cell. This condition is fulfilled if no atomic species occurring in the crystal is a mixture of isotopes and if all nuclear spins are equal to zero.

We shall consider only such inelastic processes in which one quantum of a lattice vibration is emitted or absorbed. These processes are more probable than processes involving emission or absorption of several quanta if $a_m|\Delta k|$ is small compared to one.[2] Here a is the mean vibrational amplitude of an atom in the crystal. Different atomic species possess different a values and a_m is the greatest of these values. The quantity $|\Delta k|$ is the amount by which the neutron's wave number k has changed during the collision. The inequality $a_m|\Delta k| \ll 1$ is the general condition for processes involving a greater number of vibrational quanta to be progressively less probable. The condition is the same for neutrons, electrons, and x-rays. If one considers scattering through all possible angles the average value of $|\Delta k|$ will be equal to the initial wave number k. The above condition may then be replaced by $a_m k \ll 1$. If one now averages over the orientations of the crystal one may compare the average number of elastic collisions, which occur with high probability in the neighborhood of certain orientations, with the number of inelastic collisions, which occur with small probability, but in many cases for all orientations. It is then found that the average number of elastic collisions is great compared to the average number of inelastic collisions if $a_m k \ll 1$. This condition is valid as long as the crystals are small enough so that the dynamical

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[1] G. C. Wick, Physik. Zeits. **38**, 403 (1937); I. Pomerantschuk, Physik. Zeits. d. Sowjetunion **13**, 65 (1938).

[2] See Pomerantschuk, reference 1.

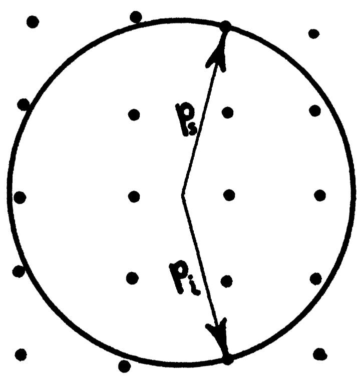

FIG. 1. Momentum of incident and scattered quantum.

theory of crystal interference need not be applied. For neutrons the condition $a_m k \ll 1$ may be transformed into $E_n E_v \ll M E_0^2$, where E_n is the energy of the incident neutron and M is the mass number of that atomic species which vibrates with the greatest amplitude. Thus we see that in the energy region where processes involving one lattice quantum are more probable than processes involving several quanta the elastic processes are, in turn, even more probable than the one-quantum processes.

We shall now review the theory of inelastic scattering processes involving one quantum of a lattice vibration for electrons and for x-rays. This theory is in its essential parts similar to the theory of neutron-scattering, but the relatively small velocity of the neutrons makes the latter theory somewhat more complicated. The influence of lattice vibrations on x-ray scattering has been discussed recently by Zachariasen[3] whose treatment we shall summarize below.

The Bragg interference conditions for an elastic scattering process can be stated simply with the help of the reciprocal lattice. This is a lattice in momentum space; the vectors connecting any two of its points are the momentum changes which an incident particle (photon, electron, or neutron) can suffer during an elastic scattering process. The vector p_i in Fig. 1 shows the momentum of an incident x-ray quantum. We construct the reciprocal lattice in such a way that one lattice point coincides with the end point of the vector p_i. Those lattice points which lie in the plane of the drawing are shown in Fig. 1. After an elastic scattering the momentum of the scattered photon may be represented by a vector which connects the origin of p_i with a point on the surface of the sphere of radius $|p_i|$ drawn around the origin of p_i as center. The circle in Fig. 1 shows the intersection of this sphere with the plane of the drawing. If this sphere passes through a lattice point of the reciprocal lattice which is different from the end point of p_i, then the interference conditions are fulfilled and elastic scattering takes place. In Fig. 1 the vector p_s shows the momentum of a scattered x-ray quantum.

If the sphere mentioned above does not pass through any lattice point different from the end point of p_i, no elastic scattering occurs. Inelastic scattering, however, is still possible. In this case the interference conditions require that the momentum represented by the vector p_L in Fig. 2 shall be given to a lattice vibration. This may happen either by the emission of a vibrational quantum carrying the momentum p_L or by the absorption of a quantum with momentum $-p_L$. The vector p_L is constructed by connecting the end point of p_s with the closest point of the reciprocal lattice. (The momentum of a lattice vibration is defined as its wave number vector k_L multiplied by Planck's constant h.)

The intensity of the inelastic scattering[3] is proportional to the square of the amplitude of

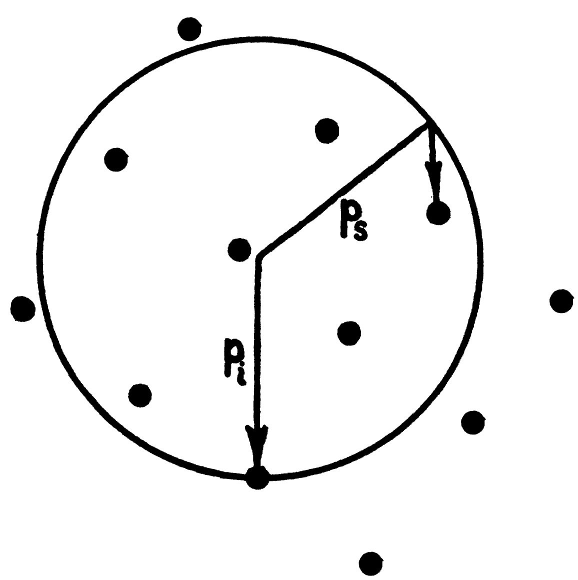

FIG. 2. Inelastic scattering.

[3] W. H. Zachariasen, Phys. Rev. 57, 597 (1940).

the lattice vibration which has been emitted or absorbed during the process. In thermal equilibrium the amplitude of the vibrations increases with decreasing frequency. Thus the most probable inelastic scattering processes will be those in which a vibration of small frequency, and therefore of small wave number, participates.[4] Returning to the notation of Fig. 2 one may say that the intensity of inelastic scattering is greatest if p_L is as small as possible, or in other words if the Bragg condition is as nearly fulfilled as possible. This explains[3] the diffuse spots observed by Preston[5] around Laue spots and also in other positions in which the Bragg conditions are nearly fulfilled.

In using Fig. 2 it was tacitly assumed that the magnitudes of the momenta $|p_i|$ and $|p_s|$ are equal; or in other words the energy change of the x-ray during the inelastic scattering process has been neglected. This is permissible for x-ray quanta and also for electrons because in all cases of practical interest the energy of these particles is great compared to any vibrational quantum of the lattice. For neutrons, however, the change in energy must be taken into account.

We shall restrict this discussion to the inelastic processes of highest intensity, i.e., to those processes in which vibrations of small frequency participate. Then the change in the neutron energy ΔE_n remains relatively small and is given by

$$\Delta E_n = v_n \Delta p_s,$$

where v_n is the velocity of the incident neutron and Δp_s, defined by the relation $|p_s| \pm \Delta p_s = |p_i|$, is the distance between the end point of p_s and the sphere of radius $|p_i|$ around the origin of p_i. On the other hand ΔE_n must be equal to the quantum of lattice vibration

$$\Delta E_n = h\nu = hk_L v_L = p_L v_L,$$

where v_L is the sound velocity in the lattice. Since we consider vibrations of small frequencies and long wave-lengths sound dispersion need not be taken into account. But even so v_L will depend on the state of polarization of the lattice vibration and also on the orientation of the vector p_L.

[4] We consider only the acoustical branch.

[5] G. D. Preston, Proc. Roy. Soc. **A172**, 116 (1939).

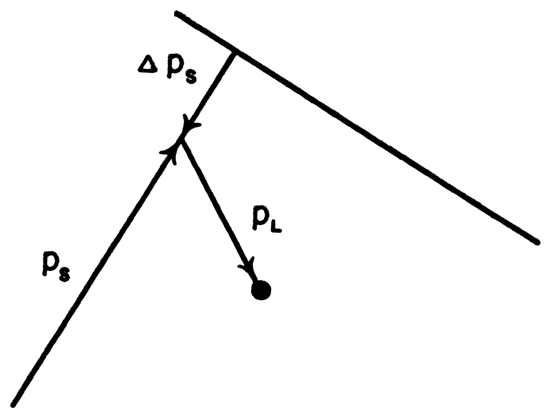

FIG. 3. Inelastic scattering, enlarged scale.

From the two above equations we find

$$\Delta p_s / p_L = v_L / v_n. \tag{A}$$

To represent the relevant momentum vectors for inelastic neutron-scattering we show in Fig. 3 the region around the end point of p_s on an enlarged scale. Because of the change in scale the circle appearing in Fig. 1 and Fig. 2 may now be replaced by a straight line. Only one point of the reciprocal lattice is shown in Fig. 3. This point is supposed to be very close to the circle which appears in the figure as a straight line. The vector p_s coincides in direction with one of the radii of the "circle" and is, therefore, drawn at right angles to the straight line. In the particular case shown in Fig. 3, p_s ends inside the circle. Thus $|p_s| < |p_i|$ which means that E_n is diminished and emission of a sound wave has taken place. Processes in which a vibrational quantum is absorbed are represented by vector diagrams in which the end point of p_s lies outside the circle.

In order to obtain a crude picture of the possible inelastic processes we shall assume the sound velocity v_L to be a constant. Then for a definite velocity v_n of the incident neutrons the lengths of the vectors Δp_s and p_L have, according to (A), a constant ratio. Approximating the sphere around the origin at p_i by a plane, one finds that the end points of the vector p_s lie on a surface of the second order. If $|\Delta p_s|/p_L = v_L/v_n < 1$ this surface is a rotational hyperboloid. Its two sheets lie on opposite sides of the plane which we have substituted for the sphere, and the two sheets correspond to processes involving absorption and emission of vibrational quanta. (See

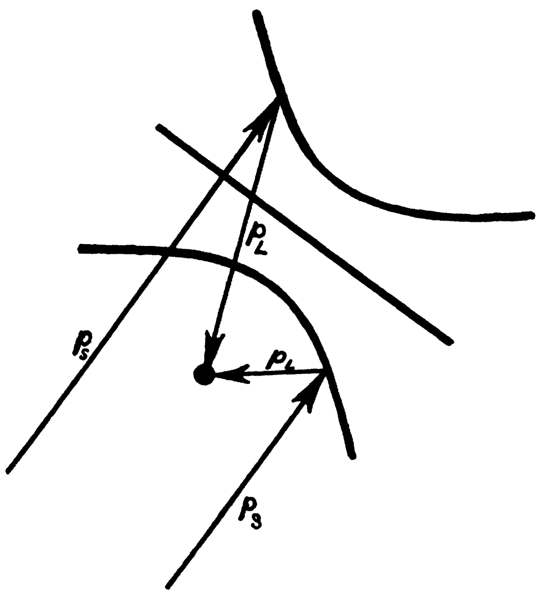

FIG. 4. Absorption and emission of vibrational quanta.

Fig. 4.) For similar reasons as mentioned above in connection with x-ray scattering those processes will be most probable in which the Bragg conditions for elastic scattering are most nearly satisfied. Thus we shall expect greatest intensity for inelastic scattering processes in the neighborhood of the sharp maxima corresponding to elastic scattering. With increasing v_n values the two sheets of the hyperbola mentioned above approach the plane (or sphere) defined by the relation $|p_s| = |p_i|$. In this limiting case the theory of inelastic neutron scattering becomes identical with the corresponding theory for x-rays or electrons. If, on the other hand, $\Delta p_s/p_L = v_L/v_n > 1$ the end points of the possible p_s vectors lie on a rotational ellipsoid surrounding the point of the reciprocal lattice. This whole surface will lie on one side of the sphere around the origin of p_i. The ellipsoid will lie completely inside the sphere if the same is true of the reciprocal lattice point, and completely outside the sphere if the reciprocal lattice point lies outside. In the former case only such inelastic processes occur in which a quantum is emitted, in the latter case only absorption is to be expected. In addition the finite extension of the ellipsoid limits the possible angular deviations of the inelastically scattered neutrons from the directions in which elastic scattering may occur. If, therefore, the incident momentum p_i is given, the inelastically scattered neutrons will be scattered into sharply delimited areas. The intensity per unit solid angle will actually become infinite at the rim of these areas. This is owing to the fact that near the rim an extended part of the surface of the ellipsoid corresponds to p_s vectors whose direction varies but very little. The integrated intensity over the whole spot remains, of course, finite. Figure 5 shows the end points of possible p_s vectors for the case $(v_L/v_n) > 1$.

If $v_L/v_n > 1$ and if at the same time p_i is small enough, it may happen that no points of the reciprocal lattice lie inside the sphere of radius $|p_i|$. Then according to our above argument only such inelastic processes are permitted in which a vibrational quantum is absorbed. If in

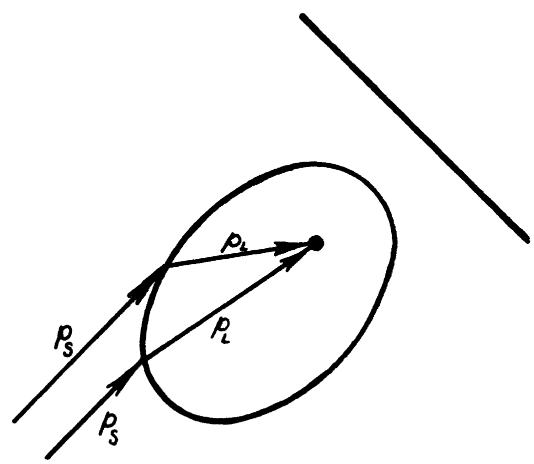

FIG. 5. End points of possible p_s vectors for $(v_L/v_n) > 1$.

addition the temperature of the lattice is very low so that no lattice vibrations are available, no inelastic scattering processes may occur. For sufficiently small p_i values the Bragg interference conditions cannot be satisfied so that elastic scattering cannot occur either. One may, therefore, expect that under these conditions neutrons will not be scattered at all. This particular result is essentially the same as that which has been obtained by Wick.[1]