Acta Cryst. (1975). A**31**, 523

Anomalous reflexion in a neutron triple-axis crystal spectrometer. By E. Maliszewski, J. Sosnowski and S. Bednarski, *Institute of Nuclear Research, Świerk, Poland*

(*Received* 28 *July* 1972; *accepted* 21 *February* 1975)

The origin of the anomalous peaks occuring in a neutron crystal spectrometer is explained by the use of reciprocal-space geometry. The anomalous peaks are due to Bragg reflexion in the sample of the incident neutrons with wavelengths different from the central value of the nominally monochromatic beam.

Introduction

In phonon dispersion relation investigations by means of one-phonon coherent inelastic scattering of neutrons two fundamental conservation laws are used: the energy conservation law

$$\frac{\hbar^2}{2m}(k^2-k_0^2)=\hbar\omega \qquad (1)$$

and the momentum conservation law

$$\mathbf{k}-\mathbf{k}_0=\boldsymbol{\tau}+\mathbf{q}\,, \qquad (2)$$

where $\mathbf{k}_0$ and $\mathbf{k}$ are the wave vectors of the incident and scattered neutrons respectively, ω and $\mathbf{q}$ are the frequency and wave vector of the phonon, $\boldsymbol{\tau}$ is the reciprocal-lattice vector and m is the neutron mass. When equations (1) and (2) are satisfied a maximum in the differential cross section for inelastically scattered neutrons is observed. A neutron triple-axis crystal spectrometer is widely used to determine the dispersion relations of phonons. However, there are several ways known (Cowley, 1969) in which peaks can arise from the contributions other than a purely one-phonon process, and one further way in which anomalous peaks may arise is analysed in this note.

The energies and wave vectors of the incident and scattered neutrons are determined with an accuracy depending on the resolution of the spectrometer. This resolution, as has been shown in many papers (see *e.g.* Cooper & Nathans, 1967; Bjerrum-Møller & Nielsen, 1970) is determined by the geometry of the experiment: the mosaic spread of crystals and divergences of collimators. Monochromators and analysers used in neutron triple-axis spectrometers should have high reflectivity and a suitable mosaic spread. They are specially prepared and even distorted for this purpose. The finite resolution of the spectrometer causes each neutron peak to contain contributions from a range of wavelengths around the central value.

Experiment and results

It may happen in the course of measurements of inelastically scattered neutrons that some lattice plane of the crystal satisfies the Bragg reflexion condition for neutrons of the wavelength scattered by the analyser, and that this wavelength falls within the range of values contained in the incident beam. This plane of the sample will analyse the incident neutrons and, if at the same time the scattering angle is suitable (double or approximately double the incident angle) so that the neutrons Bragg-reflected in the sample fall on the analyser, an anomalous neutron group will be observed. Such a situation has occured in our spectrometer.

The Bragg condition may be satisfied for wavelengths from the 'tails' of the distribution of incident wavelengths. These wavelengths may differ considerably from the nominal incident wavelength even as a result of the generally Gaussian-like shape of the mosaic distribution of single crystals. It is known (Riste & Otnes, 1969; Dorner, 1971) that monochromators made of metallic single crystals (Zn, Pb, Cu) grown by the Bridgman method have such a real mosaic distribution which produces more extended 'tails' of the Bragg peaks than the crystal monochromators prepared from other materials (pyrolytic graphite, Ge, Be). However, the contribution of these neutrons to the scattering processes in comparison with the neutrons of wavelength of the central value is usually not observable except when they take part in the coherent elastic process accompanied by the inelastic one. Then, the inconspicuous intensity of these neutrons in the distribution of incident, nominally monochromatic, neutrons is compensated by the difference between the two scattering cross sections. Thus, the counting rate for these two processes can be comparable.

The anomalous neutron groups were first observed in inelastic neutron scattering experiments for bismuth (Sosnowski, Bednarski & Czachor, 1968). In connexion with detailed investigation of phonon dispersion relations in Pd–1 % Fe (Maliszewski, Sosnowski & Czachor, 1971) the origin of the anomalous peaks was investigated. They were also observed in Pd and Al single crystals when one-phonon coherent scattering in the (1$\bar{1}$0) scattering plane was measured along the transverse acoustical branch in the [111] direction.

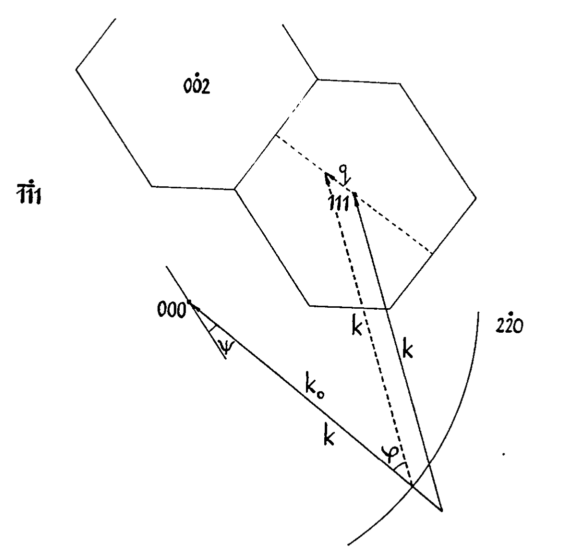

Fig. 1. Reciprocal-lattice diagram for the (1$\bar{1}$0) plane of Pd. Dashed lines show the 'simulated' wave vectors in the one-phonon process. Bold lines are for the real Bragg scattering from the (111) plane.

The divergences of the four collimators were from 30′ to 40′ and the mosaic spreads of the crystals between 10′–20′, as mostly used in neutron spectrometry. Monochromatic neutrons of the wavelength 1·52 Å were obtained from a (0002) plane of the zinc single crystal which gives a regular shape for the rocking curve. For the analyser, zinc and copper single crystals were used.

In the (1$\bar{1}$0) reciprocal planes of Pd (a=3·89 Å) and Al (a=4·05 Å) the geometries of the anomalous peaks arising are shown in Figs. 1 and 2 respectively. Incident and scattered neutrons are described by their wave vectors ($k_0=1/\lambda_0$). The triple-axis crystal spectrometer was 'constant-Q' operated in the mode in which the momentum transfer is held fixed and incident angle ψ, scattered angle φ and wave vector **k** are changed simultaneously. The diagrams show, in the reciprocal-space geometry, the momentum conservation law for two typical 'simulated' coherent inelastic scatterings with the energy gain and loss by neutrons (dashed lines) and for the actual Bragg scattering from the (111) planes of Pd and Al (bold lines). The 'simulated' and real scattered wave vectors **k** are parallel and equal. They were measured during the scanning of the one-phonon scattering for q=0·09 Å^{-1} in Pd (energy gain) and for q=0·05 Å^{-1} in Al (energy loss). The incident angles [on plane (111)] and one half of the scattering angles are in this case ψ=17°30′; 20°37′ and $\varphi/2$=17°27′; 20°38′ for Pd and Al respectively, which correspond to observed neutron scattered wavelengths 1·35 and 1·65 Å.

In Fig. 3 one-phonon and anomalous neutron groups are shown for Pd (q=0·08 Å^{-1}, ψ=22°52′) and Al (q=0·05 Å^{-1}, ψ=20°37′, case illustrated in Fig. 2). As can be seen, the intensity of the elastic and one-phonon peaks may be comparable; this also refers to the half width of a well focused phonon group but generally anomalous peaks are sharper in the Q-constant scanning method.

From these 'simulated' inelastic processes the dispersion curve may be derived which for Pd is a straight line with a slope higher than that of the phonon transverse acoustic branch in the [111] direction. The observed anomalous peaks were tested for another well-known process: the Bragg reflexion of incident neutrons in the monochromator and in the specimen followed by diffuse scattering in the analyser. For this purpose the zinc crystal analyser was exchanged for a copper single crystal (002 plane), and then for a polycrystal zinc plate of the same shape as the zinc analyser. In the case of the copper analyser, the anomalous peaks were observed at the expected Bragg angles for its reflexion plane; however, they disappeared with the polycrystal zinc plate. Therefore the neutron wavelengths given by the zinc analyser are real. The intensity curve of the anomalous peaks drawn against Bragg angle 2θ for the zinc analyser resembles the part of the curve obtained from incoherent scattering of monochromatic neutrons by vanadium. The latter test additionally confirms the explanation of the anomalous peaks illustrated in Figs. 1, 2 and distinguishes this case from an inelastic process which may occur in the monochromator. However, the inelastic process in the monochromator generally gives no regular dispersion curve, but rather single points.

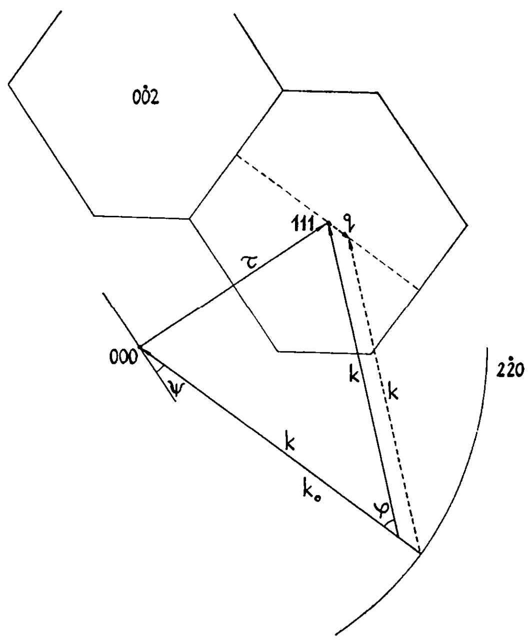

Fig. 2. Same plot as Fig. 1, for the reflexion in Al.

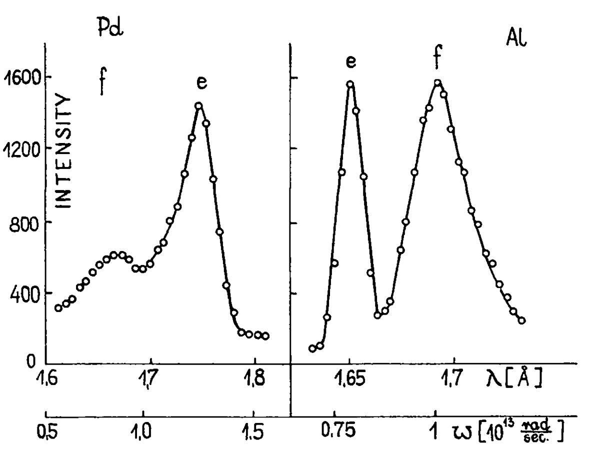

Fig. 3. The anomalous elastic peaks (e) and one-phonon groups (f) for Pd and Al.

Conclusions

Such anomalous peaks can simulate a regular dispersion curve for some elementary excitations or a slitting of the phonon branch which in this direction can also arise in another way (Cowley & Pant, 1970). The anomalous peaks may also produce misleading results when they contribute to the neutron groups obtained on a crystal double-axis spectrometer during measurements of magnon dispersion relations by the diffraction method. Thus it seems worth while to point out the origin of the anomalous peaks; they can easily be analysed and avoided if one is aware of them. They may be avoided by making the measurement at other pertinent points in reciprocal space or by changing the incident wavelength. Besides, it seems that the arrangement of the spectrometer in which anomalous peaks occur may be useful for the study of the real mosaic distribution in single crystals.

We are indebted to Dr J. Leciejewicz for his kind interest in this work.

References

BJERRUM MØLLER, H. & NIELSEN, M. (1970). *Instrumentation for Neutron Inelastic Scattering Research*, p. 49. Vienna: IAEA.

COOPER, M. J. & NATHANS, R. (1967). *Acta Cryst.* **23**, 357–367.

COWLEY, E. R. & PANT, A. K. (1970). *Acta Cryst.* A**26**, 439–442.

COWLEY, R. A. (1969). *Modern Solid State Physics*, Vol. 2, Edited by R. H. ENNS, and R. R. HAERING, p. 43. New York: Gordon and Breach.

DORNER, B. (1971). *J. Appl. Cryst.* **4**, 185–190.

MALISZEWSKI, E. F., SOSNOWSKI, J. & CZACHOR, A. (1971). *J. Phys. F. Metal Phys.* **1**, 339–344.

RISTE, T. & OTNES, K. (1969). *Nucl. Instrum. Meth.* **75**, 197–202.

SOSNOWSKI, J., BEDNARSKI, S. & CZACHOR, A. (1968). *Neutron Inelastic Scattering*, Vol. 1, p. 157. Vienna: IAEA.

International Union of Crystallography

Acta Crystallographica
Journal of Applied Crystallography

Prices of back numbers

The special sale of Volumes 1–23 (1948–1967) of *Acta Crystallographica* has ended. However, these volumes are still available at a price of Danish Kroner 240 per volume, and a reduced price of Danish Kroner 120 per volume for personal subscribers. Single parts of these volumes are not available. The prices of later volumes of *Acta Crystallographica* and of the *Journal of Applied Crystallography* will remain unchanged, at least until the end of 1975. Prices of all back numbers are given below. The prices are fixed in Danish Kroner and the U.S. dollar equivalents given below are subject to exchange-rate fluctuations.

Acta Crystallographica

Complete volumes, regular price per volume

Vols. 1–23	D.Kr. 240	($ 46.00)
Vols. A24–A25	D.Kr. 200	($ 37.00)
Vols. B24–B25	D.Kr. 500	($ 94.00)
Combined Vols. 24–25	D.Kr. 600	($113.00)
Vols. A26–A28	D.Kr. 250	($ 47.00)
Vols. B26–B26	D.Kr. 850	($160.00)
Combined Vols. 26–28	D.Kr. 1000	($188.00)
Vol. A29	D.Kr. 250	($ 47.00)
Vol. B29	D.Kr. 950	($178.00)
Combined Vol. 29	D.Kr. 1100	($207.00)
Vol. A30	D.Kr. 265	($ 50.00)
Vol. B30	D.Kr. 1000	($188.00)
Combined Vol. 30	D.Kr. 1160	($218.00)

Complete volumes, reduced prices for individuals

Vols. 1–23	D.Kr. 120	($23.00)
Vols. A24–A25	D.Kr. 100	($19.00)
Vols. B24–B25	D.Kr. 250	($47.00)
Combined Vols. 24–25	D.Kr. 300	($56.00)
Vols. A26–A28	D.Kr. 100	($19.00)
Vols. B26–B28	D.Kr. 340	($64.00)
Combined Vols. 26–28	D.Kr. 400	($75.00)
Vol. A29	D.Kr. 100	($19.00)
Vol. B29	D.Kr. 380	($72.00)
Combined Vol. 29	D.Kr. 440	($83.00)
Vol. A30	D.Kr. 110	($21.00)
Vol. B30	D.Kr. 420	($79.00)
Combined Vol. 30	D.Kr. 480	($90.00)

Ten-year index Vols. 11–23 (1958–1967)

Regular price	D.Kr. 120	($20.00)
Reduced price for individuals	D.Kr. 60	($10.00)

The reduced-rate subscriptions are ordinarily only available to members of recognized scientific societies, who must give a written undertaking accompanying their subscription application that the journal is for their personal use and will not be made available to libraries, institutions, *etc.* Orders should be addressed to Munksgaard International Publishers Ltd., 35 Nørre Søgade, DK-1370 Copenhagen K, Denmark or any bookseller. Orders for complete volumes from subscribers in North America may alternatively be placed through Polycrystal Book Service, P.O. Box 11567, Pittsburgh, Pa. 15238, U.S.A.

Single parts

The price of single parts are as follows:

Vols. A24–A31	D.Kr. 79	($15.00)
Vols. B24–B31	D.Kr. 150	($28.00)

Journal of Applied Crystallography

Complete volumes, regular price per volume

Vols. 1–4	D.Kr. 240	($46.00)
Vols. 5–7	D.Kr. 300	($56.00)

Complete volumes, reduced prices for individuals

Vols. 1–4	D.Kr. 120	($23.00)
Vols. 5–7	D.Kr. 150	($28.00)

Single parts

The price of single parts is as follows:

Vols. 1–8	D.Kr. 90	($17.00)