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Constant intensity curves in critical scattering and von Laue diagrams. By JERZY KOCIŃSKI, *Institute of Physics, Warsaw Technical University,* 00-662 *Warszawa, Koszykowa* 75, *Poland*

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Abstract

Neumann's principle is applied for drawing an analogy between the constant intensity curves of critical scattering and the von Laue diagrams of X-ray scattering in single crystals.

In previous years, critical scattering of X-rays and neutrons in single crystals of various substances has been investigated (Yamada, Shirane & Linz, 1969; Pura & Przedmojski, 1973, 1975*a*, 1975*b*; Przedmojski & Pura, 1974, 1975; Fuji & Yamada, 1971; Jablonka, Ciszewski, Sikorska & Sobaszek, 1977). The curves of constant intensity of critical scattering, drawn in the reciprocal-lattice space, exhibit a symmetry which can be connected with the point-group symmetry of a crystal class.

A possible connection between the characteristics of critical scattering in single crystals and crystal symmetry was earlier suggested (Wojtczak & Kociński, 1970, 1971; Kociński & Wojtczak, 1973), and a group-theoretical approach to this subject has been recently formulated (Kociński & Marzec, 1977). It is here aimed to look at the problem of symmetry of the constant intensity curves from the point of view of Neumann's principle (Birss, 1966).

The customary application of this principle is limited to establishing relations among the components of a property tensor. It seems, however, that this principle can be extended so that it covers the symmetry properties of single components of a property tensor. An example in favour of such a suggestion is furnished by the cross-section formula for the Bragg scattering:

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}=\frac{(2\pi)^3}{V}\sum_{\mathbf{K}}|F(\boldsymbol{\kappa})|^2\,\delta(\boldsymbol{\kappa}-\mathbf{K}), \qquad (1)$$

$$\boldsymbol{\kappa}=\mathbf{k}_0-\mathbf{k},$$

where $\mathbf{K}$ denotes a reciprocal-lattice vector, and where the remaining symbols have their usual meaning. This cross-section formula is invariant with respect to the symmetry operations of a crystal class, and the corresponding symmetry is exhibited by the von Laue diagram. The dots in such a diagram correspond to the discontinuous change of the scattering vector from one value of the reciprocal-lattice vector to another.

In order to indicate the analogy with critical scattering, one can compare formula (1) with the critical scattering cross section, written in the elastic approximation, for a simple cubic Bravais lattice (Wojtczak & Kociński, 1970):

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\sim\frac{A\kappa_1^3}{[\frac{1}{3}\kappa_1^2+q_x^2][\frac{1}{3}\kappa_1^2+q_y^2][\frac{1}{3}\kappa_1^2+q_z^2]},\quad T>T_c, \qquad (2)$$

where κ_1 denotes the Ornstein–Zernike parameter. This cross section served for interpreting experimental data (Pura & Przedmojski, 1973, 1975*a*, 1975*b*; Przedmojski & Pura, 1974, 1975). On the basis of (2) from the condition

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}=f(\mathbf{q})=\text{constant}, \qquad (3)$$

$$\mathbf{q}=\mathbf{k}_0-\mathbf{k}-\mathbf{K},$$

one can determine the constant intensity curves in the reciprocal-lattice space, which are connected with the continuous change of the scattering vector around a reciprocal-lattice point. These curves exhibit the point-group symmetries of the cubic system. The pattern of dots in the von Laue diagram can now be compared with such a constant intensity curve or a set of them.

It seems that the point-group symmetry of the constant intensity curves represents a general characteristic of critical scattering in any crystal.

We note that the data (Yamada, Shirane & Linz, 1969) were also interpreted in terms of a dynamical model (Hüller, 1969) which supplements the phenomenological group-theoretical approach (Kociński & Marzec, 1977).

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