Acta Cryst. (1983). A**39**, 89–90

On the Coupling Between Multiple Scattering and Absorption

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(*Received* 29 *March* 1982; *accepted* 27 *July* 1982)

Abstract

In a recent paper [*Acta Cryst.* (1982), A**38**, 248–252], Borie discusses extinction in absorbing materials. He argues that the problem has been improperly analysed by Becker & Coppens. It is shown here that Borie's argument is wrong: Becker & Coppens solution is correct as far as absorption–extinction coupling is concerned, for crystals of general shape.

If x and y are the coordinates along the incident and diffracted directions, the propagation equations (in the case of intensity coupling) are:

$$\frac{\partial I_0}{\partial x} = -(\sigma + \mu) I_0 + \sigma I$$
$$\frac{\partial I}{\partial y} = -(\sigma + \mu) I + \sigma I_0. \quad (1)$$

Borie (1982) considers the case of a crystal whose edges are parallel to the incident and diffracted directions, and looks for a detailed solution of (1). Such a case is of course purely abstract and is of no practical interest. Moreover, we are not interested in $I(x,y)$ at any point at the surface of the crystal. The recorded intensity is the flux of the outgoing beam across the exit surface. Balibar (1968) and later Becker (1977) have shown that one can eliminate the boundary conditions by decomposing the beam into a superposition of point sources. Under the assumption that entrance and exit surfaces do not overlap significantly (small Bragg angle) we can write (Fig. 1)

$$P = \int_v I(S \to M)\, \mathrm{d}v_m, \quad (2)$$

where $I(S \to M)$ is the intensity at M originating from the point source S. m is defined uniquely. The boundary condition for I_0 is

$$I_0 = \delta(y). \quad (3)$$

In the kinematic limit, only one scattering occurs at m, leading to

$$\begin{cases} I_{0k}(x,0) = \exp(-\mu x) \\ I_k(x,0) = \sigma \exp[-(\sigma + \mu)x]. \end{cases} \quad (4)$$

I have shown (Becker, 1977) that the solution for $I(S \to M)$ is

$$I(S \to M) = \sigma \exp[-(\sigma + \mu)(x + y)] J_0(2\sigma\sqrt{xy}), \quad (5)$$

where J_0 is a modified zero-order Bessel function. We get generally

$$P = \sigma \int \mathrm{d}v \exp[-(\sigma + \mu)(t_1 + t_2')] J_0(2\sigma\sqrt{t_1 t_2'}), \quad (6)$$

where t_1 and t_2' are the path lengths along the incident and diffracted directions. The result (6) is very general and contains no approximation. It is identical to the result of Becker & Coppens (1974).

Borie's argument is that (5) and (6) are incorrect. In the case of the geometry he studies, he gets a very complicated function [his equation (8)]:

$$I(x,y) = \exp[-(\sigma + \mu)(x + y)] \times \sum_{p=1}^{\infty} \left(\frac{\sigma + \mu}{\sigma}\right)^{p-1} \left(\frac{y}{x}\right)^{p/2} J_p(2\sigma\sqrt{xy}). \quad (B8)$$

My argument is that

$$I(x,y) = \sigma \int_0^y \exp[-(\sigma + \mu)(x + v)] J_0(2\sigma\sqrt{xv})\, \mathrm{d}v \quad (7)$$

since we have to take all points S that contribute to the outgoing beam at M.

From the well-known expression

$$J_p(z) = J_{p-1}(z) - \frac{p}{z} J_p(z), \quad (8)$$

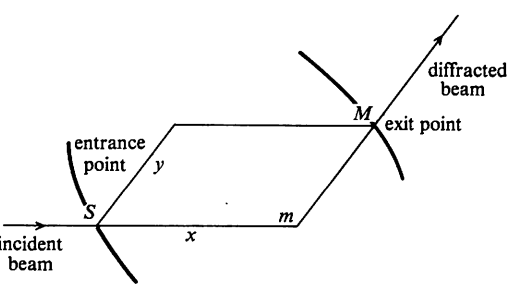

Fig. 1. Laue geometry for a point source.

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0567-7394/83/010089-02$01.50

the partial derivative of ($B8$) with respect to y is equal to (5). Therefore, we have two proofs that Borie is wrong in his argument.

It may be quite difficult to obtain any analytical expression for $I(x,y)$. But remember that we are only interested in the integral (6) often with an extra integration over the divergence angle ε. Therefore the correct procedure is to look for numerical approximations to the integral (6). In the case of strong absorption, we have shown (Becker & Coppens, 1974) that no general solution can be found. However, when $\mu\bar{T}$ is not too large, we have shown that most of the coupling between absorption and multiple scattering can be dealt with by using the general extinction expressions and just replacing the mean path length $\bar{T} = t_1 + t_2'$ by its absorption-weighted value

$$\bar{T}_\mu = \frac{1}{A_v} \int \mathrm{d}v\, T \exp(-\mu T)\, \mathrm{d}v, \qquad (9)$$

where A is the absorption factor. When dealing with accurate structure-factor determination, such conditions are generally fulfilled.

In conclusion, very complicated expressions such as those derived by Borie, using Werner's method, are believed to be of little practical use. In contrast, I want to repeat that the method of point sources, which eliminates boundary conditions, is certainly of strong potential usefulness (Becker & Dunstetter, 1982).

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Acta Cryst. (1983). A**39**, 90–94

Improved Corrections for Thermal Diffuse Scattering

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(*Received* 9 *March* 1982; *accepted* 28 *July* 1982)

Abstract

Programs have been written to calculate TDS corrections from Long Wave eigenvectors and modelled frequency Dispersion of the acoustic branches (LWD approximation). Calculations on naphthalene crystals with neutral and with charged atoms were carried out to check the convergence of the lattice dynamical calculations and of the numerical integration procedures used in the programs.

1. Introduction

It has been shown by Kroon & Vos (1979; referred to as KV) that corrections of X-ray diffraction intensities for thermal diffuse scattering (TDS) can be calculated in very good approximation by the LWD method. This method has in common with the long-wave (LW) method that only acoustic branches are taken into account and that eigenvectors for $g = g(\text{small})$ are used for all values of the wave vector $\mathbf{g}$. In contradistinction to the LW method, the LWD method accounts for the real frequency dispersion $v_j(\mathbf{g})$ instead of taking the linear relation

$$v_j(\mathbf{g}) = v_j(\hat{\mathbf{e}})\, g \qquad (1)$$

where $\hat{\mathbf{e}}$ is a unit vector along $\mathbf{g}$ and $v_j(\hat{\mathbf{e}})$ is the acoustic velocity along $\hat{\mathbf{e}}$ for branch j ($j = 1$–3).

Frequency dispersion curves and eigenvectors can, in principle, be obtained by inelastic neutron scattering. Long-wave eigenvectors can also be deduced from the elastic constants of the crystal considered (Wooster, 1962; Born & Huang, 1968). In favourable cases both quantities can be obtained by lattice dynamical calculations. Such calculations can, for instance, be made for crystals consisting of rigid-body molecules with uncharged atoms with the program *LATDYN* written by Kroon (1977).

The LWD method can easily be incorporated in programs which compute TDS corrections according

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0567-7394/83/010090-05$01.50