For instance, we note that, for $n=6$, the coefficient of D_0, which gives the number of the sixth order elastic coefficients of an isotropic solid (R_{∞}^{i}) in the reduced form of the representation $[[V^2]^6]$, is 7, but not 6.

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On Zachariasen's 1967 paper on the general theory of X-ray diffraction in crystals.

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It is believed that there is an error in the paper by W.H.Zachariasen [*Acta Cryst.* (1967) **23**, 558] and attention is drawn to relevant work published elsewhere.

The paper entitled *A General Theory of X-ray Diffraction in Crystals* by W. H. Zachariasen has recently been called to my attention. The purpose of this communication is twofold:

(1) To point out what I believe to be an error in his paper concerning the physics of diffraction in perfect crystals, and
(2) to call to the attention of X-ray crystallographers certain aspects of two papers (Werner & Arrott, 1965; Werner, Arrott, King & Kendrick, 1966) a thesis (Werner, 1965) and a laboratory report (Werner & Arrott, 1964) on neutron diffraction which have a direct bearing on the extinction problem.

The pair of coupled differential equations [equations (4*a*) and (4*b*) of Zachariasen] describing the flow of energy (X-ray photons, electrons, neutrons) in a crystal are a generalization (Hamilton, 1957) of the equations written first by Darwin (1922) to describe secondary extinction in extended flat plates.

These transport equations are rigorous as long as the energy flows along the two directions $\mathbf{t}_1$ and $\mathbf{t}_2$; that is, along the incident beam direction and along the direction of the emerging diffracted beam. In a perfect crystal region this is *not* the case. The energy flows in a direction normal to the tie point which is excited. In a general case where the incident beam is divergent, and the crystal is of finite size, numerous points on the dispersion surface are excited and the coherent wave field inside the crystal will depend in a detailed manner on the geometry of the crystal. This problem has been treated extensively by Kato (1952, 1960) in a series of papers on both electron and X-ray diffraction. Consequently, if one wants to deal with the flow of energy in a perfect crystal using a transport equation, this equation must take into account the coherent nature of the wave field and the manifold of directions in which the radiation is flowing.

The pair of coupled differential equations mentioned above describe the secondary extinction (or multiple scattering) problem in mosaic crystals fairly rigorously. The power series solution given in Zachariasen's equations (14*a*) and (14*b*) was written down and expressed in terms of modified Bessel functions in the references given in (2) above. The secondary extinction coefficient was calculated for crystals of various shapes (Werner, 1965, chapter 6) as examples of the general applicability of the theory. The exact solution for the parallelogram-shaped crystal shown in Zachariasen's Fig. 2 was given.

Certain mathematical subtleties of this multiple reflection problem in crystals of finite size are important. Although the power series expansion (modified Bessel functions) is a general solution of the differential equations, there exist certain lines in the crystal region where there are discontinuities in the derivatives of the current densities. Consequently, an analytical solution which applies everywhere in the crystal cannot be written, and the solution can only be continued from region to region in a piecewise sense.

It should also be pointed out that in these earlier papers the differential equations were put in integral form. A series solution of these integral equations was given which is a simple and direct prescription for calculating the current densities (and subsequently the extinction coefficients) in terms of once, three-times, ... $(2n+1)$-times reflected neutrons (X-ray photons, electrons). Consequently, an internal check on the accuracy of the successive approximations is contained in the calculation.

It is my opinion that these calculations are potentially useful to crystallographers, and will readily conform to specialized applications and extensions.

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