

blue incomplete extinction when the crystal plates are examined on the polarizing microscope in white light.

Conclusions

Optical activity has been observed for the first time in a crystal of class $\bar{4}$ and the effect has the correct directional properties for this symmetry. Optical activity has now been demonstrated in both of the enantiomorphous classes $\bar{4}$ and $\bar{4}2m$, and the original predictions of Gibbs (1882) have been confirmed (Hobden, 1968a).

The source of the effect and the reason for the difference in the magnitudes of the effect in AgGaS_2 (522 deg. mm^{-1}) and CdGa_2S_4 are still obscure. Calculations by Ramachandran's (1951a, b, c,) method based upon the interaction of point dipoles and using reasonable values of the atomic polarizabilities give optical rotatory powers for AgGaS_2 about two orders of magnitude too low. This shows that such a model is not suitable for these covalent tetrahedrally bonded compounds.

I would like to thank Mr D. S. Robertson for growing these crystals and Mr D. W. Brown for his assistance with this work.

This paper is contributed by permission of the Director, R.R.E. Copyright Controller H.M.S.O.

References

- GIBBS, J. W. (1882). *Amer. J. Sci.* **23**, 460.
 HAHN, H., FRANK, G., KLINGER, W., STORGER, A. & STORGER, G. (1955). *Z. anorg. Chem.* **279**, 241.
 HOBDEN, M. V. (1967). *Nature, Lond.* **216**, 678.
 HOBDEN, M. V. (1968a). *Acta Cryst.* **A24**, 676.
 HOBDEN, M. V. (1968b). *Nature, Lond.* **220**, 781.
 NYE, J. F. (1964). *Physical Properties of Crystals*. London: Oxford Univ Press.
 RAMACHANDRAN, G. N. (1951a). *Proc. Indian Acad. Sci.* **33**, 217.
 RAMACHANDRAN, G. N. (1951b). *Proc. Indian Acad. Sci.* **33**, 309.
 RAMACHANDRAN, G. N. (1951c). *Proc. Indian Acad. Sci.* **34**, 127.

Short Communications

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible. Publication will be quicker if the contributions are without illustrations.

Acta Cryst. (1969). **A 25**, 638

Elastic coefficients of an isotropic solid. By T. S. G. KRISHNAMURTY and V. APPALANARASIMHAM, *Andhra University, Waltair, India*

(Received 4 February 1969)

It is shown, on the basis of Jahn's method, that the conjecture made by one of us that there should be n n th order elastic coefficients of an isotropic solid does not hold good.

It is well known that elasticity expresses the relation between the applied stress and the resulting strain, both of which can be represented by the symmetric second rank tensors. Bhagavantam & Suryanarayana (1949) have employed the character method to derive the number of the non-vanishing independent elastic coefficients of orders 2 and 3 for the 32 classes of crystals. Identical results have been obtained by Jahn (1949) using the method of reduction of a representation. Recently Jahn's (1949) method has been extended by Krishnamurty & Gopalakrishnamurty (1968) to obtain the fourth- and fifth-order elastic coefficients in crystals. When the fourth-order elastic coefficients of crystals are enumerated by the character method, one of us (Krishnamurty, 1963) conjectured that the number of the n th order elastic coefficients, symmetric in all the n suffixes, of an isotropic solid (R_{∞}^n) would be n . In this note, it is shown that deviations from such a conjecture can arise from the elastic coefficients of orders higher than five.

If V denotes the representation of a polar vector and $[V^2]$ the symmetrical product (Tisza, 1933) of V with itself, then the n th order elastic coefficients, which are symmetric in all the n indices, are represented by $[[V^2]^n]$. In the reduced form of the representation, this contains terms of the type $[D_2^n]$, where D_2 is a five-dimensional representation. Some of the values of $[D_2^n]$, for $n > 5$, may be easily derived and are given by

$$[D_2^5] = 2D_0 + 2D_2 + D_3 + 3D_4 + D_5 + 3D_6 + D_7 + 2D_8 + D_9 + D_{10} + D_{12},$$

$$[D_2^6] = D_0 + 3D_2 + D_3 + 3D_4 + 2D_5 + 3D_6 + 2D_7 + 3D_8 + D_9 + 2D_{10} + D_{11} + D_{12} + D_{14},$$

$$[D_2^7] = 2D_0 + 3D_2 + D_3 + 4D_4 + 2D_5 + 4D_6 + 2D_7 + 4D_8 + 2D_9 + 3D_{10} + D_{11} + 2D_{12} + D_{13} + D_{14} + D_{16},$$

$$[D_2^8] = 2D_0 + 3D_2 + 2D_3 + 4D_4 + 2D_5 + 5D_6 + 3D_7 + 4D_8 + 3D_9 + 4D_{10} + 2D_{11} + 3D_{12} + D_{13} + 2D_{14} + D_{15} + D_{16} + D_{18},$$

and

$$[D_2^{10}] = 2D_0 + 4D_2 + D_3 + 5D_4 + 3D_5 + 5D_6 + 3D_7 + 6D_8 + 3D_9 + 5D_{10} + 3D_{11} + 4D_{12} + 2D_{13} + 3D_{14} + D_{15} + 2D_{16} + D_{17} + D_{18} + D_{20}.$$

We observe that the coefficient of D_0 in each one of the above tabulated values is different from unity except in the case $n=7$. On the other hand, we know that the coefficient of D_0 in $[D_2^n]$ ($n=2, 3, 4$ and 5) is one (Jahn, 1949; Krishnamurty & Gopalakrishnamurty, 1968). It is these coefficients of D_0 in $[D_2^n]$ which are different from unity, that are responsible for the deviations in the conjecture referred to earlier.

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_{60}^0) in the reduced form of the representation $[[V^2]^6]$, is 7, but not 6.

The authors' thanks are due to Professor T. Venkatarayudu for his kind interest in this work.

Acta Cryst. (1969). A **25**, 639

On Zachariasen's 1967 paper on the general theory of X-ray diffraction in crystals. By S. A. WERNER, *Scientific Laboratory, Ford Motor Company, Dearborn, Michigan 48121, U.S.A.*

(Received 5 December 1968 and in revised form 4 February 1969)

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 (4a) and (4b) 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 t_1 and 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 (14a) and (14b) was written down and expressed in terms of modified Bessel functions in the references given in (2)

References

- BHAGAVANTAM, S. & SURYANARAYANA, D. (1949). *Acta Cryst.* **2**, 21.
 JAHN, H. A. (1949). *Acta Cryst.* **2**, 30.
 KRISHNAMURTY, T. S. G. (1963). *Acta Cryst.* **16**, 839.
 KRISHNAMURTY, T. S. G. & GOPALAKRISHNAMURTY, P. (1968). *Acta Cryst.* A **24**, 563.
 TISZA, L. (1933). *Z. Physik*, **82**, 48.

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.

References

- DARWIN, C. G. (1922). *Phil. Mag.* **43**, 800.
 HAMILTON, W. C. (1957). *Acta Cryst.* **10**, 629.
 KATO, N. (1952). *J. Phys. Soc. Japan*, **7**, 397, 406.
 KATO, N. (1960). *Acta Cryst.* **13**, 349.
 WERNER, S. A. (1965). *The Multiple Bragg Reflection of Neutrons in Mosaic Crystals*. Thesis, The Univ. of Michigan.
 WERNER, S. A. & ARROTT, A. (1964). *Theory of Neutron Diffraction: The Multiple Bragg Reflection of Neutrons in Mosaic Crystals*. Laboratory Report No. 64-51, Ford Scientific Laboratory, Dearborn, Michigan.
 WERNER, S. A. & ARROTT, A. (1965). *Phys. Rev.* **140**, 675.
 WERNER, S. A., ARROTT, A., KING, J. S. & KENDRICK, H. (1966). *J. Appl. Phys.* **37**, 2343.
 ZACHARIASEN, W. H. (1967). *Acta Cryst.* **23**, 558.