

- PICHON-PESME, V., LECOMTE, C. & LACHEKAR, H. (1993). In preparation.
- PICHON-PESME, V., LECOMTE, C., WIEST, R. & BÉNARD, M. (1992). *J. Am. Chem. Soc.* **114**, 2713–2715.
- RASMUSSEN, K. (1984). In *Potential Energy Functions in Conformational Analysis. Lecture Notes in Chemistry*, Vol. 37. New York: Springer-Verlag.
- SOUHASSOU, M., LECOMTE, C., BLESSING, R. H., AUBRY, A., ROHMER, M. M., WIEST, R., BÉNARD, M. & MARRAUD, M. (1991). *Acta Cryst.* **B47**, 253–266.
- SOUHASSOU, M., LECOMTE, C., GHERMANI, N., ROHMER, M. M., WIEST, R., BÉNARD, M. & BLESSING, R. H. (1992). *J. Am. Chem. Soc.* **114**, 2371–2382.
- STONE, A. J. & PRICE, S. L. (1988). *J. Phys. Chem.* **92**, 3325–3335.

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.

Acta Cryst. (1993). **A49**, 789–790

Comment on Correlating the optical rotation of α -quartz with a skew matrix of a dielectric tensor by Szu-Lin Chen (1993). By A. M. GLAZER, *Department of Physics, Clarendon Laboratory, Parks Road, Oxford OX1 3PU, England*

(Received 2 April 1993; accepted 25 May 1993)

Abstract

A theory of optical rotation in α -quartz that was recently published by Chen [*Acta Cryst.* (1993), **A49**, 148–154] results in optically inactive directions perpendicular to the optic axis. It is pointed out here that this conclusion is not in accordance with either symmetry considerations or the observed experimental evidence.

Recently, Chen (1993) described a theoretical treatment of the optical rotation in α -quartz. The procedure involved calculations of the polarizabilities of individual SiO_4 tetrahedra within a unit cell and resulted in the conclusion that, in addition to optically inactive directions 33.83° from the optic axis, there should also be inactive directions *along the diad axes of quartz*. My purpose in writing this note is to point out that this cannot be correct and indicate some of the errors made in the theory used.

Now, it is well known that there are inactive directions at a particular azimuthal angle to the optic axis. The effect is caused by the fact that the rotation *perpendicular* to the optic axis is of opposite sign to that *along* the optic axis. Chen quotes Wahlstrom (1979) as giving this angle as 33.83° to the optic axis, but in fact this is a misunderstanding of what Wahlstrom meant by the phrase 'plate inclined at 56.17° to the optic axis' [this angle was actually determined, for example, by Szivessy & Münster (1934); it was also quoted in the well known book of Nye (1987)].

Moreover, the idea that there are additional inactive directions along the diad axes of quartz would appear to violate crystal symmetry, since the form of the gyration tensor for a trigonal crystal like quartz would require the gyration to be the same for *all* directions perpendicular to the optic axis, including the diad axes. All measurements made perpendicular to the optic axis [for example, those of Szivessy & Münster (1934), Bruhat & Grivet

(1935), Konstantinova, Ivanov & Grechushnikov (1969), Kobayashi & Uesu (1983), Kobayashi, Uesu & Takehara (1983), Horinaka, Tomii, Sonomura & Miyauchi (1985), Moxon & Renshaw (1990) and Moxon, Renshaw & Tebbutt (1991)] agree in indicating that the optical rotation perpendicular to the optic axis has a measurable value opposite in sign to that along the optic axis, so it cannot be zero for *any* direction perpendicular to the optic axis.

In addition, Chen quotes a 'prediction' of Wahlstrom (1979) that 'light travelling at right angles to the optic axis is rotated but in opposite sense to that propagated along the optic axis'. It is fair to point out that this is a misunderstanding of language, in that Wahlstrom makes no such prediction but correctly reports this as a fact, presumably on the basis of his knowledge of the well known experimental evidence already published. Wahlstrom's book, excellent though it is, is a student textbook on optical crystallography in general and is not, therefore, a primary reference for work on optical rotation. There is, in fact, a vast amount of literature, going back to the last century, in which the many theories of optical rotation in crystals are described [for a general discussion, see, for instance, Glazer & Stadnicka (1986) and Devarajan & Glazer (1986)].

So what, then, is wrong with Chen's calculation? I believe that the answer to this question lies in the oversimplification of the theory used. For instance, the calculation is made by combining together the polarizability effects of a few tetrahedra within a unit cell. This treatment, however, ignores the fact that the tetrahedra exist within a *crystal*, *i.e.* an infinitely extending structure. By restricting the calculation to a few tetrahedra within a unit cell, the author ignores the combined contributions of all the other atoms in the crystal. In any proper treatment of optical rotation in crystals, it is necessary to sum the effective electric fields throughout the whole crystal, for example *via*

an Ewald summation, since all the atoms, in principle, have an effect on all the others. It is also important to realize that the optical electric field incident on the crystal is not the same field within the crystal (Ewald, 1916; van Laar, Endeman & Bijvoet, 1968; Devarajan & Glazer, 1986). Such effects cannot be ignored in any theory of optical rotation in crystals.

References

- BRUHAT, G. & GRIVET, P. (1935). *J. Phys. Radium*, **6**, 12–26.
- CHEN, S.-L. (1993). *Acta Cryst.* **A49**, 148–154.
- DEVARAJAN, V. & GLAZER, A. M. (1986). *Acta Cryst.* **A42**, 560–569.
- EWALD, P. P. (1916). *Ann. Phys. (Leipzig)*, **49**, 117–143.
- GLAZER, A. M. & STADNICKA, K. (1986). *J. Appl. Cryst.* **19**, 108–122.
- HORINAKA, H., TOMII, K., SONOMURA, H. & MIYAUCHI, T. (1985). *Jpn. J. Appl. Phys.* **24**, 755–760.
- KOBAYASHI, J. & UESU, Y. (1983). *J. Appl. Cryst.* **16**, 204–211.
- KOBAYASHI, J., UESU, Y. & TAKEHARA, H. (1983). *J. Appl. Cryst.* **16**, 212–219.
- KONSTANTINOVA, A. F., IVANOV, N. R. & GRECHUSHNIKOV, B. N. (1969). *Sov. Phys. Crystallogr.* **14**, 222–229.
- LAAR, J. VAN, ENDEMAN, H. J. & BIJVOET, J. M. (1968). *Acta Cryst.* **A24**, 52–56.
- MOXON, J. R. L. & RENSHAW, A. R. (1990). *J. Phys. Condens. Matter*, **2**, 6807–6836.
- MOXON, J. R. L., RENSHAW, A. R. & TEBBUTT, I. J. (1991). *J. Phys. D*, **24**, 1187–1192.
- NYE, J. F. (1987). *Physical Properties of Crystals*. London: Oxford Univ. Press.
- SZIVESSY, G. & MÜNSTER, C. (1934). *Ann. Phys. (Leipzig)*, **20**, 703–736.
- WAHLSTROM, E. E. (1979). *Optical Crystallography*, 5th ed., p. 373. New York: Wiley.