

Short Communications

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The Debye–Waller factors of sodium fluoride. By R. C. G. KILLEAN, *School of Physical Sciences, University of St. Andrews, North Haugh, St. Andrews, Scotland*

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Errors reported by Sharma [*Acta Cryst.* (1975). A31, 157] in a previous paper [Sharma, *Acta Cryst.* (1974), A30, 299–300] are noted and commented on. It is pointed out that Sharma has given insufficient detail in his paper for an independent check to be made of his new values for the Debye–Waller factors and that these values do not support his earlier discussion.

Two recent papers by Sharma (1974*a, b*, denoted S1 and S2 respectively) in conjunction with an erratum (Sharma, 1975) are deserving of comment. As pointed out by Post (1975), it is essential that sufficient detail on calculation techniques be given in a paper in order that a reader can assess the validity of calculated results. This is even more the case when an author has been required to publish an erratum. In this case, where the erratum changes the main numerical results of S2, it is essential that independent checks on the calculations can be made so that these results can be evaluated.

Examination of S1 and S2 shows that the two papers present identical results for the Debye–Waller factors for the sodium and fluorine ions and that they list identical structure factor tables. This in itself would not be remarkable but for Sharma's statement that while no correction for TDS was made in S1, TDS corrections were made in S2. Presumably the purpose of the erratum is to give the correct Debye–Waller factors obtained from the TDS-corrected structure-factor data, data which do not appear in either S1 or S2. Sharma concluded in S2 that his Debye–Waller factors are significantly different from those of Meisalo & Merisalo (1966) but, using the latest values in Sharma's erratum, this is no longer the case. Indeed, for the fluorine ion

the hypothesis fails at even the 'possibly significant' level (Cruickshank, 1965). It must be concluded that Sharma's erratum is not just correcting typographical errors.

It would be desirable under these circumstances to make an independent check of the new calculation of the Debye–Waller factors but the data required to do this are not available. Clearly, because of the errors in S2 already admitted and the discrepancy noted above, the results reported by Sharma should be analysed with caution.

In conclusion, it is perhaps curious that no reference in S2 is made to S1 with which, ignoring the TDS issue, it is in substance identical.

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Reply to Killean's comment *The Debye–Waller factors of sodium fluoride*. By V. C. SHARMA, *Department of Physics, University of Benin, Benin City, Nigeria*

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Comments made by Killean [*Acta Cryst.* (1976). A32, 510] on papers by Sharma [*Acta Cryst.* (1974), A30, 299–300; *Acta Cryst.* (1975), A31, 157] are discussed.

Killean's (1976) comments on papers by Sharma (1974*a, b*, 1975, hereafter referred to as S1, S2 and S3 respectively) are discussed.

1. Killean (1976) points out that sufficient details on the calculation techniques were not given. A closer study of S2 should reveal that reasonable details along with the necessary references were given in that paper. The TDS correc-

tions were made by the usual analytical method developed by Cooper & Rouse (1968) which requires no such *geometrical* parameters as understood by Killean (1975). Furthermore, he has no evidence to suggest that TDS corrections in sodium fluoride using the analytical method will differ significantly from the ones using the numerical method of Cooper & Rouse (1968). In fact, this point is irrelevant, as

the major aim of S2 was neither TDS corrections nor their comparison using different methods.

2. It is stated in S1 and S2 and I confirm it again that while TDS corrections were applied in S2, no such corrections were applied in S1. In view of the published erratum in S3, S1 and S2 cannot be considered to present identical results. Furthermore, since I have more than a little doubt on the validity of TDS corrections, it was not felt desirable to give structure factors after such corrections. The structure factors in S2 were only introduced to emphasize a point on the accuracy of the observed data. The sole purpose of applying TDS corrections in S2 was to make a comparison of the root-mean-square (r.m.s.) values with those quoted by Meisalo & Merisalo (1966). Although the r.m.s. value for the fluorine ion is no longer significantly different from that of Meisalo & Merisalo, I disagree that for the sodium ion the statistical hypothesis fails at even the 'possibly significant' level (Cruickshank, 1965). Simple calculations show that $\Delta/\sigma \approx 2.50$ for the sodium ion.

3. Killean's conclusion that S1 and S2 are identical is incorrect and deserves more serious attention. To mention the major difference, S1 is devoted to the investigation of the type of extinction in a small sphere of sodium fluoride using Zachariasen's (1967) theory of extinction, as well as to the discussion of the physical significance of the extinction parameter obtained from consideration of normal crystal strain in real crystals, whereas, S2 lays major em-

phasis on the comparison of r.m.s. values of sodium and fluorine ions from a single crystal and powder data respectively after TDS corrections. It was not felt necessary to refer to S1 in S2 as each of the two papers stands alone and has a specific point to make.

In conclusion, it is abundantly clear that Killean is advocating a false 'caution' and his statement that 'Sharma's erratum is not just correcting typographical errors' is not only baseless but also erroneous.

References

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On the angular divergence of out-going beams in an asymmetric diffraction geometry. By MASAO KURIYAMA and WILLIAM J. BOETTINGER, *National Bureau of Standards, Washington, D.C. 20234, U.S.A.*

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The well-known relation for the angular divergence of beams diffracted from a perfect crystal in an asymmetric diffraction condition is derived straightforwardly from first principles.

When a divergent beam of X-rays (or neutrons or other particles) is diffracted by a perfect crystal in an asymmetric diffraction geometry, the angular divergence, $\Delta\theta_{\text{out}}$, of the outgoing beam is given by the well-known relation

$$\Delta\theta_{\text{out}} = m^{-1/2}\omega_S, \quad (1)$$

where ω_S is the rocking curve width for a symmetric reflection from the relevant diffracting planes and m is the magnification or asymmetry factor. If the incoming and outgoing beams make the angles θ_{in} and θ_{out} , respectively, with the crystal surface, the magnification factor, m , is given by

$$m = \frac{\sin \theta_{\text{out}}}{\sin \theta_{\text{in}}}. \quad (2)$$

This relation has been exploited in the measurement of rocking curve widths with double and triple crystal spectrometers (Renninger, 1961; Kohra, 1962); it has significant practical importance, since this fact facilitates the production of a highly collimated monochromatic beam, as demonstrated by Kohra & Kikuta (1968). It should be noted that this condition also provides a beam of considerably large size which may replace a scanning method in diffraction topography.

Kohra (1962) employed a sort of reciprocity law to explain relation (1). Warren (1969) obtained relation (1), using a row of atoms lying parallel to the crystal surface. This idea was motivated by Borie's (1966, 1967) work where the basic principle is Fresnel diffraction by one of the vertical atomic layers rather than by the horizontal Bragg (diffracting) planes. Recently in the International Summer School on X-ray Dynamical Theory and Topography in Limoges, France, 1975, Kohra again explained this relation virtually by a mixture of the two above-mentioned arguments. These explanations are admittedly incomplete, although appealing.

The angular divergent behavior, relation (1), can be derived in a straightforward, though very trivial, manner. The basic concept is conservation of momenta parallel to the crystal surface (Ashkin & Kuriyama, 1966) which has been known traditionally as 'the continuity condition of tangential components of wave vectors'. The incoming and outgoing momenta are denoted by \mathbf{k}_{in} and \mathbf{k}_{out} , respectively. Let \mathbf{H} be a reciprocal lattice vector. In addition to energy conservation (elastic scattering), the two-dimensional δ function in the dynamical scattering theory demands that

$$(\mathbf{k}_{\text{out}})_t = (\mathbf{k}_{\text{in}} + \mathbf{H})_t, \quad (3)$$