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 $\Delta/\sigma \simeq 2{\cdot}50$ 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 emphasis 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.

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On the angular divergence of out-going beams in an asymmetric diffraction geometry.

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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

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

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

$$m = \frac{\sin\theta_{\text{out}}}{\sin\theta_{\text{in}}} . \tag{2}$$

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 $\mathbf{k}_{\text{in}}$ and $\mathbf{k}_{\text{out}}$, 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

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

where t indicates the component of a vector projected on the crystal surface. Using the incoming and outgoing angles defined before, one can write

$$|\mathbf{k}| \cos \theta_{out} = |\mathbf{k}| \cos \theta_{in} + \mathbf{H}_t , \quad (4)$$

where $|\mathbf{k}| = |\mathbf{k}_{in}| = |\mathbf{k}_{out}|$. This relation is reduced by differentiation to

$$\Delta\theta_{out} = \frac{\sin \theta_{in}}{\sin \theta_{out}} \Delta\theta_{in} = \frac{1}{m} \Delta\theta_{in} . \quad (5)$$

The divergence of the incoming beam normally guarantees that the full range of the rocking curve width is utilized to produce the diffracted beam. Hence, from dynamical theory, $\Delta\theta_{in}$ is given by

$$\Delta\theta_{in} = m^{1/2} \omega_S . \quad (6)$$

Thus, $\Delta\theta_{out}$ is obtained by substituting (6) into (5), resulting in the identical equation to that shown in relation (1). When a crystal becomes imperfect, relation (3) is relaxed, thus resulting in a larger divergence.

These principles are applicable not only to the Bragg geometry, but also to the Laue geometry. In particular, the above results extend to the Laue geometry with parallel surfaces without any modifications.

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