structure factors indicating extinction in the data. Extinction corrections to the observed structure factors were made by the method of Zachariasen (1967). The thermal diffuse scattering (TDS) corrections to the observed structure factors were then made by the method of Cooper & Rouse (1968). The elastic constants used for this purpose were those quoted by Cottrell (1964). The TDS-corrected observed structure factors were fitted to the calculated structure factors by allowing small variations in the temperature factors of the sodium and fluorine ions only. The final values of the temperature factors which gave the best agreement between the observed and the calculated structure factors were

$$B\text{ (sodium)} = 0{\cdot}860 \pm 0{\cdot}010\text{ Å}^2$$
$$B\text{ (fluorine)} = 0{\cdot}880 \pm 0{\cdot}050\text{ Å}^2.$$

These values are about 4% higher than those obtained by using the observed structure factors not corrected for TDS and correspond to the root-mean-square vibrational displacements of $\sqrt{\overline{U^2}}$ (sodium) $= 0{\cdot}181 \pm 0{\cdot}001$ Å and $\sqrt{\overline{U^2}}$ (fluorine) $= 0{\cdot}183 \pm 0{\cdot}005$ Å as compared to the values quoted by Meisalo & Merisalo (1966) of $\sqrt{\overline{U^2}}$ (sodium) $=$ $\sqrt{\overline{U^2}}$ (fluorine) $= 0{\cdot}202 \pm 0{\cdot}007$ Å for the two ions.

It can be seen from the above that our values of the root-mean-square vibrational displacements for the two ions are significantly different from those given by the above authors. This is possibly due to the systematic errors in their intensity data arising from extinction and preferred orientation, for which no corrections were made and which gave rise to unrealistic temperature factors. However, it may be noted that the present values agree almost exactly with the values of 0·182 Å at room temperature, deduced from the Debye–Waller factors of 0·8685 Å^2 and 0·8671 Å^2 respectively for the two ions obtained by Reid & Smith (1970), using force constants derived by fitting a shell model to the measured dispersion curves.

Table 1 shows the extinction-corrected observed structure factors $F_o(\mathbf{h})$ and the calculated structure factors $F_c(\mathbf{h})$. The R index of 0·0135 based upon an agreement between the observed and the calculated structure factors reflects the accuracy with which the diffracted intensities were measured on the four-circle diffractometer.

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An analytical method of determining cubic crystal orientation from {111} surface traces. Corrections and comments.

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Attention is drawn to printing errors and an item of oversight in an earlier paper [Fong, H. S. (1973). *Acta Cryst.* A**29**, 176–182]. An item of improvement is also put forward.

In a paper of the above title (Fong, 1973) equation (25) should correctly read:

$$y = -(b+m) \pm \sqrt{\{(b+m)^2 - c - n - 2z\}}$$

and the sentence containing equation (26) should read:

For each acceptable solution for y there may be two possible values for θ and φ:

Also in the paper the directions CP, AP, and BP of the pyramidal figure $ABCP$ were taken to be [110], [0$j_2$1], and [$j_1$0j_3] respectively. It was overlooked that this selection was, when $j_1 = -1$, a set of directions actually belonging to a left-handed crystal coordinate system so that the crystal orientations obtained in this case were in fact reflexions in the OXZ or OYZ plane of the actual orientations. Correction for this oversight is easily made by slight alteration of the rotation matrix M_j to:

$$\mathsf{M}_j = \begin{pmatrix} \dfrac{j_2v_2 - v_3}{j_1w_1} & \dfrac{-j_2v_1 - v_3}{j_1w_1} & \dfrac{v_1 + v_2}{j_1w_1} \\ \dfrac{1 + v_1w_2}{w_1} & \dfrac{-1 + v_2w_2}{w_1} & \dfrac{-j_2 + v_3w_2}{w_1} \\ jv_1 & jv_2 & jv_3 \end{pmatrix}.$$

It is however recommended that CP, AP, and BP be taken instead to be respectively the directions j_3[110], j_1[011], and j_2[101] which are always a right-handed set of directions whatever the values of j_1, j_2, and j_3 and which lead to somewhat neater expressions for (v_1, v_2, v_3) and M_j:

$$v_1 = (-j_1 \cos \sigma_1 + j_2 \cos \sigma_2 + j_3 \cos \sigma_3)/\sqrt{2}$$
$$v_2 = (j_1 \cos \sigma_1 - j_2 \cos \sigma_2 + j_3 \cos \sigma_3)/\sqrt{2}$$
$$v_3 = (j_1 \cos \sigma_1 + j_2 \cos \sigma_2 - j_3 \cos \sigma_3)/\sqrt{2}$$

$$\mathsf{M}_j = \begin{pmatrix} \dfrac{v_2 - v_3}{w_1} & \dfrac{-v_3 - v_1}{w_1} & \dfrac{v_1 + v_2}{w_1} \\ \dfrac{1 + v_1w_2}{w_1} & \dfrac{-1 + v_2w_2}{w_1} & \dfrac{-1 + v_3w_2}{w_1} \\ jv_1 & jv_2 & jv_3 \end{pmatrix}$$

where $w_1 = \sqrt{[2(1 + v_1v_2 + v_1v_3 - v_2v_3)]}$
$w_2 = v_2 + v_3 - v_1$.

Reference

Fong, H. S. (1973). *Acta Cryst.* A**29**, 176–182.