Table 1. *Bijvoet ratio,* $\alpha = [I(hkl) + I(\bar{h}\bar{k}l)]/[I(\bar{h}kl) + I(h\bar{k}l)]$, *with e.s.d.'s in parentheses, as a function of crystal displacement for reflections* 281 *and* 12,5,1 *for both macrotwins in a typical crystal specimen*

Crystal size *ca* 2·3×0·24×0·20 mm; the major twin was about three times larger than the minor one.

Displacement	Major twin		Minor twin	
(mm)	281	12,5,1	281	12,5,1
0·2	2·10 (4)	0·53 (2)	0·68 (3)	2·02 (9)
0·5	2·03 (4)	0·54 (2)	0·59 (3)	2·06 (11)
0·8	2·13 (4)	0·50 (2)	0·58 (3)	2·03 (13)
1·1	2·11 (5)	0·49 (3)	0·52 (4)	2·01 (13)
1·4	2·04 (5)	0·48 (3)	0·49 (4)	2·0 (2)
1·7	2·23 (5)	0·52 (4)	0·52 (6)	1·6 (2)
2·0	2·20 (6)	0·60 (4)	0·50 (8)	1·8 (4)
Calc.	2·07	0·51	0·48	1·95

space group were confirmed by our measurements. From calculations based on the known atomic parameters and including anomalous scattering for Se and I, we could pick out Bijvoet pairs expected to differ appreciably in intensity. We chose the reflections 281 and 12,5,1 with calculated α values of 2·07 and 0·51 for Cu $K\alpha$ radiation. The needle-like crystals (2–3 mm in length) were mounted on a Stoe Stadi-2 two-circle Weissenberg diffractometer with [001] parallel to the ω axis. The intensities of the Bijvoet pairs ($hk1$, $\bar{h}\bar{k}1$) and ($\bar{h}k1$, $h\bar{k}1$) were measured for both macrotwins, using a 0·3 mm collimator and the ω-scan technique. The crystal was then displaced by *ca* 0·3 mm along the ω axis (this is very easily done on a Weissenberg-type diffractometer) and the same reflections remeasured. Results for one typical crystal are summarized in Table 1.

Results

In all five crystal specimens studied, the macrotwins were of opposite chirality. Also, the measured α values were approximately constant over the length of the crystal and sometimes even larger than the calculated values. This is not unexpected, since it is known that in non-centrosymmetric space groups with polar axes neglect of anomalous dispersion in the structure refinement (Hilti, Mayer & Rihs, 1978) will yield atomic parameters that tend to eliminate the difference between Bijvoet pairs (Cruickshank & McDonald, 1967). In fact, it seems obvious that generally the resulting errors in atomic parameters will be approximately half of those produced by a refinement including anomalous dispersion but with the wrong chirality sense. We deduce that each macrotwin was indeed homochiral.

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Non-tensorial arrays for physical properties and the direct-inspection method.

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Abstract

It is shown that the invariance relations between the elements of a non-tensorial array for a physical property are identical to the invariance relations between the corresponding tensorial components when one is only dealing with symmetry elements of order 1, 2 or 4 and with the trigonal axis $3_{[111]}$ of the cubic groups.

It is an unfortunate common practice in crystal physics to use non-tensorial arrays to represent physical properties of crystals. A well known example is given by the non-tensorial elastic compliance constants $S_{ij} = S_{ji}[i, j = 1(\equiv xx), 2(\equiv yy), 3(\equiv zz), 4(\equiv yz), 5(\equiv zx), 6(\equiv xy)]$, related to the corresponding tensorial elastic compliance constants $S_{mnpq} = S_{nmpq} = S_{mnqp} = S_{pqmn}[m, n, p, q = 1(\equiv x), 2(\equiv y), 3(\equiv z)]$ by the following equations [see *e.g.* Nye (1985), p. 134]:

$$S_{ij} = S_{mnpq} \quad \text{when } i \text{ and } j \text{ are 1, 2 or 3,}$$
$$S_{ij} = 2S_{mnpq} \quad \text{when } i \text{ or } j \text{ are 4, 5 or 6,}$$
$$S_{ij} = 4S_{mnpq} \quad \text{when } i \text{ and } j \text{ are 4, 5 or 6.}$$

It is also commonly stated in crystal physics [see *e.g.* Nye (1985), p. 135] that to impose rotational invariance on the elements of non-tensorial arrays it is best to go through the corresponding tensorial components. An alternative procedure which has been used is to apply the cumbersome method by Love of imposing invariance on a scalar, such as the elastic energy, expressed in terms of non-tensorial arrays [*e.g.* Hearmon (1953)].

Here we should like to point out that whenever the direct-inspection method is applicable as such (Fumi,

0108-7673/87/030431-02$01.50

1952), *i.e.* when one is only dealing with symmetry elements of order 1, 2 or 4 and with the trigonal axis $3_{[111]}$ of the cubic groups, which correspond to permutational or multiplicative changes of coordinates, one can easily impose rotational invariance directly on the elements of the non-tensorial arrays. This is so because purely permutational or multiplicative changes of coordinates connect to each other only elements of a non-tensorial array which are related to the corresponding tensorial components by the same numerical coefficients. Thus the invariance relations between non-tensorial elements are identical in these cases to the invariance relations between the corresponding tensorial components.

We illustrate explicitly the point for the non-tensorial elastic compliance constants S_{ij} in the symmetry group O with generating elements $4(4_z)$ and $3_{[111]}$.

$4(4_z)\ x\to y,\ y\to -x,\ z\to z$	$3_{[111]}\ x\to y,\ y\to z,\ z\to x$
$1\equiv xx\to yy\equiv 2$	$1\equiv xx\to yy\equiv 2$
$2\equiv yy\to xx\equiv 1$	$2\equiv yy\to zz\equiv 3$
$3\equiv zz\to 3$	$3\equiv zz\to xx\equiv 1$
$4\equiv yz\to -xz\equiv -5$	$4\equiv yz\to zx\equiv 5$
$5\equiv zx\to zy\equiv 4$	$5\equiv zx\to xy\equiv 6$
$6\equiv xy\to -yx\equiv -6$	$6\equiv xy\to yz\equiv 4.$

Elements S_{ij} with *one* 4 or *one* 5 are identically zero owing to $4(4_z)$. The remaining invariance equations read as follows:

$S_{11}\to S_{22}(S_{22}\to S_{11})$	$S_{11}\to S_{22}\to S_{33}$
$S_{12}\to S_{21}\equiv S_{12}$	$S_{12}\to S_{23}\to S_{31}\equiv S_{13}$
$S_{13}\to S_{23}(S_{23}\to S_{13})$	
$S_{16}\to -S_{26}(S_{26}\to -S_{16})$	$S_{16}\to S_{24}\equiv 0,\ S_{26}\to S_{34}\equiv 0$
$S_{33}\to S_{33}$	
$S_{36}\to -S_{36}\equiv 0$	
$S_{44}\to S_{55}(S_{55}\to S_{44})$	$S_{44}\to S_{55}\to S_{66}.$
$S_{45}\to -S_{54}\equiv -S_{45}\equiv 0$	
$S_{66}\to S_{66}$	

The invariant non-tensorial array S_{ij} in group O thus reads

$$\begin{pmatrix} S_{11} & S_{12} & S_{12} & 0 & 0 & 0 \\ & S_{11} & S_{12} & 0 & 0 & 0 \\ & & S_{11} & 0 & 0 & 0 \\ & & & S_{44} & 0 & 0 \\ & & & & S_{44} & 0 \\ & & & & & S_{44} \end{pmatrix}$$

in accordance with Nye (1985), Table 9, p. 140.

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Surface spherical harmonics and intensity and strain pole figures of cubic textured materials. Erratum.

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Abstract

Expressions given in Tables 2 and 3 of Brakman [*Acta Cryst.* (1987), A**43**, 270-283] are corrected. Table 2, column 2, line 1 should read

$$[S^2_{HKL}P_{hkl}+S^2_{\bar{H}\bar{K}\bar{L}}P_{\bar{h}\bar{k}\bar{l}}+S^2_{K\bar{H}L}P_{k\bar{h}l}+S^2_{\bar{K}H\bar{L}}P_{\bar{k}h\bar{l}}]D^{-1}.$$

Table 3, column 2, line 2 should read

$$\tfrac{1}{2}[1+(-1)^{j+m/2}][S^2_{HKL}+(-1)^jS^2_{\bar{H}\bar{K}\bar{L}}]/(S^2_{HKL}+S^2_{\bar{H}\bar{K}\bar{L}}).$$

All relevant information is given in the *Abstract.*

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