Table 1. Bijvoet ratio, \( \alpha = [I(hkl) + I(\bar{h}\bar{k}\bar{l})]/[I(h\overline{k}l) + I(h\overline{k}\overline{l})] \), 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

<table>
<thead>
<tr>
<th>Displacement (mm)</th>
<th>Major twin</th>
<th>Minor twin</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2</td>
<td>2.10 (4)</td>
<td>0.53 (2)</td>
</tr>
<tr>
<td>0.5</td>
<td>2.03 (4)</td>
<td>0.54 (2)</td>
</tr>
<tr>
<td>0.8</td>
<td>2.13 (4)</td>
<td>0.50 (2)</td>
</tr>
<tr>
<td>1.1</td>
<td>2.11 (5)</td>
<td>0.49 (3)</td>
</tr>
<tr>
<td>1.4</td>
<td>2.04 (5)</td>
<td>0.48 (3)</td>
</tr>
<tr>
<td>1.7</td>
<td>2.23 (5)</td>
<td>0.52 (4)</td>
</tr>
<tr>
<td>2.0</td>
<td>2.20 (6)</td>
<td>0.60 (4)</td>
</tr>
<tr>
<td>Calc.</td>
<td>2.07</td>
<td>0.51</td>
</tr>
</tbody>
</table>

In all five crystal specimens studied, the macrotwins were of opposite chirality. Also, the measured \( \alpha \) 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.

We thank Dr H. D. Flack (Geneva) for his interest, also Mrs G Rihs and Dr B. Hilti (CIBA-GEIGY, Basel) for sending us sample crystals and a list of the atomic parameters of (TSeT)\( _2 \)I.

References


Non-tensorial arrays for physical properties and the direct-inspection method. By F. G. FUMI and C. RIPAMONTI, Dipartimento di Fisica, Università de Genova and CISM/ MPI-GNSM/CNR, Unità di Genova, Genova, Italy

(Received 15 August 1986; accepted 11 December 1986)

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 \( S_{ij} = S_{[i,j]}(i,j = 1(=x), 2(=y), 3(=z), 4(=yz), 5(=zx), 6(=xy)) \), related to the corresponding tensorial elastic compliance constants \( S_{mnq} = S_{mnp} = S_{mpn} = S_{pnm} \) with the following equations [see e.g. Nye (1985), p. 134]:

\[
S_{ij} = S_{mnpq} \quad \text{when } i \text{ and } j \text{ are } 1, 2 \text{ or } 3,
\]

\[
S_{ij} = 2S_{mnpq} \quad \text{when } i \text{ or } j \text{ are } 4, 5 \text{ or } 6,
\]

\[
S_{ij} = 4S_{mnpq} \quad \text{when } i \text{ and } j \text{ are } 4, 5 \text{ or } 6.
\]

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,
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 $3_{[111]}$.

$$4(4_z)x \rightarrow y, y \rightarrow -x, z \rightarrow z \quad 3_{[111]}x \rightarrow y, y \rightarrow z, z \rightarrow x$$

<table>
<thead>
<tr>
<th>1 = xx \rightarrow yy = 2</th>
<th>1 = xx \rightarrow yy = 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>2 = yy \rightarrow xx = 1</td>
<td>2 = yy \rightarrow zz = 3</td>
</tr>
<tr>
<td>3 = zz \rightarrow xx = 3</td>
<td>3 = zz \rightarrow xx = 1</td>
</tr>
<tr>
<td>4 = yz \rightarrow -xz = -5</td>
<td>4 = yz \rightarrow zx = 5</td>
</tr>
<tr>
<td>5 = zx \rightarrow yz = 4</td>
<td>5 = zx \rightarrow xy = 6</td>
</tr>
<tr>
<td>6 = xy \rightarrow -yx = -6</td>
<td>6 = xy \rightarrow yz = 4</td>
</tr>
</tbody>
</table>

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

$$S_{11} \rightarrow S_{22}(S_{22} \rightarrow S_{11}) \quad S_{11} \rightarrow S_{22} \rightarrow S_{13}$$

$$S_{12} \rightarrow S_{21}(S_{21} \rightarrow S_{12}) \quad S_{12} \rightarrow S_{23} \rightarrow S_{11} \rightarrow S_{13}$$

$$S_{13} \rightarrow S_{23}(S_{23} \rightarrow S_{13}) \quad S_{13} \rightarrow S_{23} \rightarrow S_{11}$$

$$S_{16} \rightarrow -S_{26}(S_{26} \rightarrow -S_{16}) \quad S_{16} \rightarrow S_{24} \rightarrow S_{14} = 0, S_{26} \rightarrow S_{44} = 0$$

$$S_{33} \rightarrow S_{33} \quad S_{35} \rightarrow S_{35} \rightarrow S_{66}$$

$$S_{36} \rightarrow -S_{16} = 0 \quad S_{36} \rightarrow S_{55}(S_{55} \rightarrow S_{44}) \quad S_{44} \rightarrow S_{55} \rightarrow S_{66}$$

$$S_{45} \rightarrow -S_{54} = -S_{45} = 0 \quad S_{46} \rightarrow S_{66}$$

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

$$S_{11} \quad S_{11} \quad S_{12} \quad 0 \quad 0 \quad 0$$

$$S_{11} \quad S_{11} \quad S_{12} \quad 0 \quad 0 \quad 0$$

$$S_{11} \quad S_{11} \quad S_{12} \quad 0 \quad 0 \quad 0$$

$$S_{44} \quad 0 \quad 0 \quad S_{44} \quad 0$$

$$S_{44} \quad 0 \quad 0 \quad S_{44} \quad 0$$

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

References


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

By C. M. BRAKMAN, Delft University of Technology, Laboratory of Metallurgy, Rotterdamseweg 137, 2628 AL Delft, The Netherlands

(Received 22 March 1987)

Abstract

Expressions given in Tables 2 and 3 of Brakman [Acta Cryst. (1987), A43, 270-283] are corrected. Table 2, column 2, line 1 should read

$$[S_{HKL}^2 P_{kkl} + S_{HKL}^2 P_{kkl} + S_{HKL}^2 P_{kkl} + S_{HKL}^2 P_{kkl}] D^{-1}.$$ 

Table 3, column 2, line 2 should read

$$\frac{1}{2} [1 + (-1)^{i+m/2}] [S_{HKL}^2 + (-1)^{i} S_{HKL}^2] (S_{HKL}^2 + S_{HKL}^2).$$

All relevant information is given in the Abstract.

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