Cubic Invariant Spherical Surface Harmonics in Conjunction with Diffraction Strain Pole-Figures

C. M. BRAKMAN

*Laboratory for Metallurgy, Delft University of Technology, Rotterdamseweg
137, 2628 AL Delft, The Netherlands*

(Received January 15, 1985)

Four kinds of cubic invariant spherical surface harmonics are introduced. It has been shown previously that these harmonics occur in the equations relating measured diffraction (line-shift) elastic strain and macro-stresses generating these strains for the case of textured cubic materials. As a consequence, these harmonics are important for the determination of unknown macro-stress tensor components if the o.d.f. expansion coefficients are known. On the other hand, they play a role in the determination of unknown o.d.f. expansion coefficients if the macro-stresses are known using for instance, a tensile test device on the diffractometer. Then, even the odd-order o.d.f. expansion coefficients can be obtained. In this paper, special attention is given to the mathematical construction of the cubic harmonics, the physical symmetry requirements they are subject to and some examples are given exhibiting both even and odd order harmonics.

INTRODUCTION

It has been recently shown (van Baal, 1983; Brakman, 1983; Brakman 1984a) that the “classical” $\sin^2\psi$ -law (Dölle, 1979) used for residual macro-stress determination may be adapted for the case of textured materials using relevant orientation distribution function (o.d.f.) theory. It is common practice in residual stress analysis to denote the deviation angle from the specimen’s surface normal by the angle ψ whereas the angle ϕ measures the angular distance in the specimen’s surface (Fig. 1). For only σ_{11} and $\sigma_{22} \neq 0$ and texture-free cubic materials the

FIGURE 1 Experimental arrangement.

equation relating the measured diffraction (line-shift) elastic strain $\langle \epsilon'_{zz} \rangle$ and these stresses reads:

$$\langle \epsilon'_{zz}(\psi, \phi) \rangle = s_1(hkl)[\sigma_{11} + \sigma_{22}] + \frac{1}{2}s_2(hkl)\sigma_\phi \sin^2\psi \quad (1)$$

where:

$$s_1(hkl) = s_{1122} + s_0\Gamma(hkl) \quad (1a)$$

$$\frac{1}{2}s_2(hkl) = s_{1111} - s_{1122} - 3s_0\Gamma(hkl) \quad (1b)$$

$$\Gamma(hkl) = h^2k^2 + h^2l^2 + k^2l^2 \quad (1c)$$

(in all relevant equations it has been assumed that: $h^2 + k^2 + l^2 = 1$)

$$s_0 = s_{1111} - s_{1122} - 2s_{1212} \quad (1d)$$

$$\sigma_\phi = \sigma_{11}\cos^2\phi + \sigma_{22}\sin^2\phi. \quad (1e)$$

Here the Reuss-model of poly-crystalline elastic crystal coupling has been used and s_{1111} , s_{1122} and s_{1212} are the well-known single (cubic) crystal elastic compliances. Note the predicted linear behaviour between $\langle \epsilon'_{zz} \rangle$ and $\sin^2\psi$. For the case of a specimen exhibiting crystallographic texture *and* residual macro-stresses (for instance, cold-rolled steel sheet samples with orthorhombic specimen symmetry) it has been shown

(Brakman, 1984a) that Eq. (1) may be modified using o.d.f. theory yielding:

$$\begin{aligned}
 \langle \varepsilon'_{zz}(\psi, \Phi) \rangle = & s_1(hkl)[\sigma_{11} + \sigma_{22}] + \frac{1}{2}s_2(hkl)\sigma_{\Phi}\sin^2\psi \\
 & + \frac{-s_0}{2P_{hkl}(\psi, \Phi)}\{(\sigma_{11} - \sigma_{22})\cos 2\Phi - \sigma_{\Phi}\sin^2\psi\} \\
 & \times \sum_{\substack{j=4 \\ \mu=1}} [F_1(hkl, j, \mu)B_j^{\mu}(\psi, \Phi) + F_2(hkl, j, \mu)C_j^{\mu}(\psi, \Phi)] \\
 & + \frac{+s_0}{2P_{hkl}(\psi, \Phi)}(\sigma_{11} - \sigma_{22})\sin 2\Phi \cos \psi \\
 & \times \sum_{\substack{j=4 \\ \mu=1}} [-F_1(hkl, j, \mu)C_j^{\mu}(\psi, \Phi) + F_2(hkl, j, \mu)B_j^{\mu}(\psi, \Phi)] \\
 & + \frac{+s_0}{2P_{hkl}(\psi, \Phi)}\sigma_{\Phi}\sin 2\psi \\
 & \times \sum_{\substack{j=4 \\ \mu=1}} [F_3(hkl, j, \mu)D_j^{\mu}(\psi, \Phi) + F_4(hkl, j, \mu)E_j^{\mu}(\psi, \Phi)] \\
 & + \frac{+s_0}{2P_{hkl}(\psi, \Phi)}(\sigma_{11} - \sigma_{22})\sin 2\Phi \sin \psi \\
 & \sum_{\substack{j=4 \\ \mu=1}} [F_3(hkl, j, \mu)E_j^{\mu}(\psi, \Phi) - F_4(hkl, j, \mu)D_j^{\mu}(\psi, \Phi)] \quad (2)
 \end{aligned}$$

where the series-expansion method of the o.d.f. on the rotation group in R_3 has been used cf. the theory given by Bunge (1982, pp. 47–118).

$P_{hkl}(\psi, \phi)$ = normalized (in terms of “times random”) intensity of the $\{hkl\}$ -polefigure in the ψ, ϕ -direction.

The functions $B_j^{\mu}(\psi, \phi)$, $C_j^{\mu}(\psi, \phi)$, $D_j^{\mu}(\psi, \phi)$ and $E_j^{\mu}(\psi, \phi)$ are defined in Eqs. (I–1) through (I–4) of the Appendix. They all contain the well-known o.d.f. expansion coefficients $C_j^{\mu v}$. Note that the strain $\langle \varepsilon'_{zz} \rangle$ is *not* the strain in the ψ, ϕ -direction of the specimen as a whole but rather the strain of the set of crystals having their orientation such that one of their $\{hkl\}$ lattice-plane normals, say $[hkl]$ coincides with the ψ, ϕ -direction. Hence, for the general case the measured strain depends on the $\{hkl\}$ reflection used for a given stress-state. The functions F_1

through F_4 in Eq. (2) are the spherical surface harmonics given special attention here. Their definition reads:

$$F_1(hkl, j, \mu) = (a_2^2 + b_2^2)^{\frac{1}{2}} \times \sum_{m=-j}^j \dot{A}_j^{m\mu} P_j^{m2}(\cos \phi_B) \cos[m\beta_B + 2 \arg Z_2(hkl)] \quad (3a)$$

$$F_2(hkl, j, \mu) = (a_2^2 + b_2^2)^{\frac{1}{2}} \times \sum_{m=-j}^j \dot{A}_j^{m\mu} P_j^{m2}(\cos \phi_B) \sin[m\beta_B + 2 \arg Z_2(hkl)] \quad (3b)$$

$$-F_3(hkl, j, \mu) = (a_1^2 + b_1^2)^{\frac{1}{2}} \times \sum_{m=-j}^j \dot{A}_j^{m\mu} P_j^{m1}(\cos \phi_B) \sin[m\beta_B - \arg Z_1(hkl)] \quad (3c)$$

$$F_4(hkl, j, \mu) = (a_1^2 + b_1^2)^{\frac{1}{2}} \times \sum_{m=-j}^j \dot{A}_j^{m\mu} P_j^{m1}(\cos \phi_B) \cos[m\beta_B - \arg Z_1(hkl)] \quad (3d)$$

An example of each of these functions is given in Figs. 2 through 5 where both even and odd j have been used.

The coefficients $\dot{A}_j^{m\mu}$ are the well-known cubic symmetry coefficients as introduced by Bunge (1982, pp. 384 and 501) and the functions P_j^{m1} and P_j^{m2} are defined by Bunge (1982, p. 351)

$$\phi_B = \arccos(l) \quad (4a)$$

$$\beta_B = \arccos(h(h^2 + k^2)^{-\frac{1}{2}}) \quad (4b)$$

These angles are used as given by Bunge (1982, p. 371)

$$a_1 = hk(h^2 - k^2)(h^2 + k^2)^{-\frac{1}{2}} \quad (4c)$$

$$b_1 = l(-h^4 - k^4 + h^2 l^2 + k^2 l^2)(h^2 + k^2)^{-\frac{1}{2}} \quad (4d)$$

$$a_2 = (h^4(k^2 - l^2) + k^4(h^2 - l^2))(h^2 + k^2)^{-\frac{1}{2}} \quad (4e)$$

$$b_2 = hkl(h^2 - k^2)(h^2 + k^2)^{-\frac{1}{2}} \quad (4f)$$

$$\arg Z_1(hkl) = \arctan b_1/a_1 = \arctan g(l(-h^4 - k^4 + h^2 l^2 + k^2 l^2)/hk(h^2 - k^2)) \quad (4g)$$

$$\arg Z_2(hkl) = \frac{1}{2} \arctan b_2/a_2 = \frac{1}{2} \arctan g(hkl(h^2 - k^2)/(h^4(k^2 - l^2) + k^4(h^2 - l^2))) \quad (4h)$$

FIGURE 2 Function F_1 for $j = 8$ and $\mu = 1$.

It may be shown (Penning, 1984) that:

$$a_1^2 + b_1^2 = 3h^2k^2l^2 + \Gamma(hkl) - 4\Gamma^2(hkl) \quad (4i)$$

$$a_2^2 + b_2^2 = -3h^2k^2l^2 + \Gamma^2(hkl) \quad (4j)$$

$$\arg Z_1(hkl) + \arg Z_2(hkl) = hkl\text{-permutation independent} \quad (4k)$$

Note that: $F_1 \equiv 0$ for the $\{hoo\}$ and $\{hhh\}$ reflections and $F_2 = F_3 = F_4 \equiv 0$ for the $\{hoo\}$, $\{hho\}$ and $\{hhh\}$ reflections.

Note that it follows using Eq. (2) that for the $\{hoo\}$ and $\{hhh\}$ reflec-

FIGURE 3 Function F_2 for $j = 12$ and $\mu = 1$.

tions the relevant expressions for $\langle \epsilon'_{zz} \rangle$ do *not* exhibit any texture-dependency at all if the Reuss-model is taken to be valid.

Note that Eq. (2) exhibits in principle, both even and odd j .

Note also that function F_1 and F_3 are invariant w.r.t. any permutation of h , k and l whereas F_2 and F_4 develop a negative sign for 24 of the 48 possible permutations of h , k and l . See for the latter case Figs. 3 and 5 whereas the former is demonstrated in Figs. 2 and 4.

FIGURE 4 Function F_3 for $j = 13$ and $\mu = 1$.

PHYSICAL SYMMETRY CONSIDERATIONS

Centro-symmetry of the diffraction strain pole-figure

$$\langle \epsilon'_{zz}(\psi, \phi) \rangle$$

Since the diffraction strain $\langle \epsilon'_{zz} \rangle$ is a physical quantity depending on the angles ψ and ϕ it can be represented for a given (macro) stress-

FIGURE 5 Function F_4 for $j = 9$ and $\mu = 1$.

The iso-density lines in Figures 2 thr. 5 are:

+	-0.07
×	-0.03
□	0.00
⊠	0.03
*	0.07

state in terms of a diffraction strain pole-figure as introduced by Hoffman *et al.* (1983) and also by Brakman (1984a). From Friedel’s law it follows that, similar to “conventional” diffraction intensity pole-figures, these pole-figures should exhibit centro-symmetry, that is the following should hold:

$$\langle \varepsilon'_{zz}(\pi - \psi, \pi + \phi) \rangle = \langle \varepsilon'_{zz}(\psi, \phi) \rangle \tag{5}$$

Using Eqs. (I-1) through (I-4) (see Appendix), it follows from Eq. (2) that this is *not* the case.

Analysis reveals that just like the case for the “conventional” diffraction intensity pole-figures (Bunge, 1982, p. 106) the contributions due to crystals exhibiting a $[\bar{h}kl]$ vector in the ψ , ϕ direction should be taken into account in addition to $[hkl]$. This problem has been discussed extensively elsewhere (Brakman, 1984b) where it was found that treating the 2 orientations exhibiting a $[hkl]$ and a $[\bar{h}kl]$ vector in the ψ , ϕ -direction respectively, is sufficient. Note that a $[\bar{h}kl]$ does *not* imply an inversion of cubic crystal reference axes: the choice of $[\bar{h}kl]$ as a vector parallel to the ψ , ϕ direction generates a physically different crystallite orientation within the context of this problem (Brakman, 1984a).

Then it follows, assuming equal structure factors of these two orientations, that the functions F_2 and F_4 vanish from Eq. (2).

The correct expression is immediately obtained by then omitting all terms exhibiting F_2 and F_4 in Eq. (2).

It may be inferred (see the Appendix) that centro-symmetry of $\langle \epsilon'_{zz} \rangle$ (Eq. (5)) is fulfilled then. Since $\langle \epsilon'_{zz} \rangle$ is a physical quantity it is also required that the eventual equation be invariant w.r.t. any permutation of h , k and l . Since only the functions F_1 and F_3 remain this is indeed the case. Note that functions F_2 and F_4 vanish from Eq. (2) for both even *and* odd j whereas functions F_1 and F_3 persist for both even *and* odd j values. Hence, it can be argued that the “selection-rule” obtained from the requirement cf. Eq. (5) is the vanishing of F_2 and F_4 from the eventual equation rather than imposing a restriction upon the permissible values of j as is the case with the diffraction intensity pole-figures (Bunge, 1982, p. 106).

Note that for the $\{hkk\}$ and $\{hko\}$ reflections the functions F_2 and F_4 may be shown to be equal to zero (as was also the case for the $\{hoo\}$, $\{hho\}$ and $\{hhh\}$ reflections). This may also be seen from Figs. 3 and 5. In addition to this it can be shown (Brakman, 1984b) that for the complete treatment of Eq. (2) for these reflections the consideration of the crystallite orientations associated with $[\bar{h}hk]$, or $[\bar{h}ko]$ is superfluous due to the “symmetrical” nature of these directions. It can be shown that they yield exactly the same result as follows from $[hkk]$ and $[hko]$ respectively.† Consequently, for the determination of $\langle \epsilon'_{zz} \rangle$ (if these

† In fact, it can be shown that the treatment of both orientations following from the choice of $[hkl]$ and $[\bar{h}kl]$ as vectors parallel to the ψ , ϕ direction is only necessary for those reflections where h , k , and l are all different from each other i.e. for instance, the b.c.c. $\{321\}$, $\{651\}$ reflections etc.

reflections are used) the treatment of only $[hkk]$ or $[hko]$ respectively is sufficient omitting the terms exhibiting F_2 and F_4 in Eq. (2).

Orthorhombic symmetry of the diffraction strain pole-figure cf. Eq. (2)

Using Eqs. (I-1) through (I-4) (see Appendix) it follows that Eq. (2) (minus the F_2 - and F_4 -contributions) exhibits orthorhombic symmetry cf. point-group mmm i.e.:

$$\begin{aligned}\langle \varepsilon'_{zz}(\psi, \pi - \phi) \rangle &= \langle \varepsilon'_{zz}(\psi, \pi + \phi) \rangle = \langle \varepsilon'_{zz}(\psi, 2\pi - \phi) \rangle \\ &= \langle \varepsilon'_{zz}(\pi - \psi, \phi) \rangle = \langle \varepsilon'_{zz}(\psi, \phi) \rangle\end{aligned}\quad (6)$$

Note that this can only be true for a specimen exhibiting a diffraction intensity pole-figure cf. to point group mmm where it should hold:

$$\begin{aligned}P_{hkl}(\psi, \pi - \phi) &= P_{hkl}(\psi, \pi + \phi) = P_{hkl}(\psi, 2\pi - \phi) \\ &= P_{hkl}(\pi - \psi, \phi) = P_{hkl}(\psi, \phi)\end{aligned}\quad (7)$$

Note that for the diffraction intensity pole-figure centro-symmetry is fulfilled as well:

$$P_{hkl}(\pi - \psi, \pi + \phi) = P_{hkl}(\psi, \phi). \quad (7a)$$

Cubic crystal symmetry

The cubic symmetry coefficients $\dot{A}_j^{m\mu}$ cf. Eqs. (3a) through (3d) are defined as a consequence of point-group 432:

A 4-fold rotation axis parallel to $[001]$ yields that m in Eqs. (3a) through (3d) should be equal to a multiple of 4, the 3-fold rotation axis parallel to $[111]$ leads to the well-known relationship that the coefficients $\dot{A}_j^{m\mu}$ must satisfy i.e.

$$\dot{A}_j^{s\mu} = \sum_{m=-j}^j \dot{A}_j^{m\mu} P_j^{ms} \left(\cos \frac{\pi}{2} \right) \quad (8)$$

for both even and odd j and a 2-fold rotation axis parallel to $[100]$ yields:

$$\dot{A}_j^{-m\mu} = (-1)^j \dot{A}_j^{m\mu} \quad (9)$$

The other symmetry elements of 432 do not yield additional useful relationships w.r.t. the context of this paper.

As such, rotations only are needed which comply with the series-development method of the o.d.f. on the rotation group in R_3 as has been introduced by Bunge (1982, pp. 47–118).

However, upon considering point-group $m\bar{3}m$ a centre of inversion occurs which cannot be accounted for using rotations only.

It has however, been shown (Brakman, 1984b) that due to this centre of inversion all *physically* relevant crystallite-orientations can be “reached” using rotations only. Consequently, Eq. (2) (minus the F_2 - and F_4 -contributions) should represent physical reality (the Reuss-model taken to be valid) for textured materials consisting of cubic crystals exhibiting symmetries cf. point-groups 432 or $m\bar{3}m$.

One can distinguish now between 3 cases:

- (i) crystal symmetry cf. point-group $m\bar{3}m$ and specimen symmetry cf. mmm . In this case the right-handed and left-handed o.d.f.’s are both equal and (equivalent) to *the* o.d.f. (Bunge, 1982, p. 105). The treatment given here concerns this o.d.f. and use of rotations only (as has been used in the derivation of Eq. (2)) is sufficient.

Note that specimen symmetry cf. point-group 222 can not occur if the crystals satisfy $m\bar{3}m$.

- (ii) crystal symmetry cf. point-group 432 and specimen symmetry cf. mmm . In this case the right- and left-handed o.d.f.’s are equal to each other (*the* o.d.f. does not exist here) and the o.d.f.-coefficients $C_j^{\mu\nu}$ as they occur in Eq. (2) can be regarded as:

$$C_j^{\mu\nu} = \frac{1}{2}[C_j^{L\mu\nu} + C_j^{R\mu\nu}] \text{ where } C_j^{L\mu\nu} = C_j^{R\mu\nu}$$

cf. Eq. (4.303) from Bunge (1982). Equation (2) is still adequate then.

- (iii) crystal symmetry cf. point-group 432 and specimen symmetry cf. 222. In this case the right- and left-handed o.d.f.’s are different from each other (possibly in *every* orientation g) and they have to be treated separately. However, right- and left-handedness has to be defined with respect to *some* physical property. For polycrystalline diffraction experiments and measurement of elements of 2nd order (strain) tensors (as is the case here) it can be expected that measurements obtain contributions from both right- and left-handed o.d.f.’s at *the same time*. This case is treated in Eq. (4.323) from Bunge (1982) for polycrystalline diffraction experiments. For the case of diffraction strain pole figures the o.d.f. coefficients $C_j^{\mu\nu}$ as they occur in Eq. (2) have to be substituted by: $M^R C_j^{R\mu\nu} + M^L C_j^{L\mu\nu}$ where M^R and M^L denote the fractions of the right- and left-handed crystals

respectively. The odd order $C_j^{\mu\nu}$ do not drop from Eq. (2). Consequently, the *virtual* o.d.f. giving rise to the *measured* diffraction strain pole-figure is different from the one yielding the *measured* intensity pole-figure. Eq. (2) is still adequate.

DISCUSSION

It can be seen from Figures 3 and 5 that functions F_2 and F_4 exhibit a symmetry cf. point-group 432 for both even and odd j .

In this way they resemble the "normal" cubic invariant spherical surface harmonics as defined by Bunge (1982, pp. 384 and 567):

$$\dot{K}_j^\mu(\phi_B, \beta_B) = (2\pi)^{-\frac{1}{2}} \sum_{m=-j}^j \dot{A}_j^{\mu\mu} \overline{P_j^m(\cos \phi_B)} \exp(im\beta_B) \quad (10)$$

for odd j . These functions cannot satisfy $m3m$ for odd j as analysis shows. On the other hand, functions F_1 and F_3 (Figures 2 and 4 depict examples of them for both even and odd j) satisfy $m3m$ for both even and odd j .

As such their behaviour resembles the "normal" harmonics cf. Eq. (10) for even j .

It has been shown by Bunge (1982, pp. 100–107) that for the case of diffraction intensity pole figures the treatment of the crystallite-orientations following from taking $[hkl]$ and $[\bar{h}\bar{k}\bar{l}]$ parallel to the ψ, ϕ direction leads to the occurrence in the eventual equations for the pole figure intensity of a factor equal to:

$$[1 + (-1)^j] \quad (11)$$

As a consequence, the o.d.f. expansion coefficients $C_j^{\mu\nu}$ cannot be determined for odd j from those pole-figures.

It is argued now that for the case of diffraction strain pole figures a different situation develops. It has been obtained (Brakman, 1984b) that instead of Eq. (11) the following factors then occur in the eventual equations:

$$[1 + (-1)^{2j}] \text{ for } F_1 \text{ and } F_3 \quad (12a)$$

$$[1 + (-1)^{2j+1}] \text{ for } F_2 \text{ and } F_4 \quad (12b)$$

which complies with the vanishing of F_2 and F_4 as mentioned previously. Hence, it follows using Eqs. (I-1) thr. (I-4) that the o.d.f.

expansion coefficients $C_j^{\mu\nu}$ are *not* undeterminable for odd j from diffraction (line-shift) elastic strain pole-figures.

Note that the "selection rule": $C_j^{\mu\nu}$ undeterminable for odd j for the case of diffraction intensity pole-figures is replaced here by the vanishing of functions F_2 and F_4 for both even and odd j .

Note that for *all* hkl : $F_2 = F_4 \equiv 0$ for $j = 4$ and $F_2 = 0$ for $j = 8$.

CONCLUSIONS

- (i) Four kinds of cubic invariant spherical surface harmonics have been introduced. Two of them (functions F_1 and F_3) satisfy for even *and* odd order the symmetry-requirements of point-group $m3m$ whereas the other two (functions F_2 and F_4) comply with point-group 432 for even *and* odd j . For the treatment of diffraction strain pole-figures the functions F_2 and F_4 are not necessary (except for the case of anomalous scattering).
- (ii) the functions derived may serve as a tool for the determination of unknown macro-stresses in textured cubic materials exhibiting residual or applied stress if the o.d.f. expansion coefficients are known. On the other hand, if the macro-stresses are known these functions may be used to obtain the o.d.f. expansion coefficients $C_j^{\mu\nu}$ for both even *and* odd j provided enough diffraction strain measurements are available.

References

- Baal, C. M. van. *Phys. Stat. Sol.* (a) **77**, 521–526 (1983).
 Brakman, C. M. *J. Appl. Cryst.* **16**, 325–340 (1983).
 Brakman, C. M. *Cryst. Res. Technol.*, in press (1984a).
 Brakman, C. M. *J. Appl. Cryst.*, submitted (1984b).
 Bunge, H. J. *Texture Analysis in Materials Science*, London, Butterworths (1982).
 Dölle, H. *J. Appl. Cryst.* **12**, 489–501 (1979).
 Hoffmann, J., Neff, H., Scholtes, B. and Macherauch, E. *Härterei-Tech. Mitt.* **38**, 180–183 (1983).
 Penning, P. *private communication* (1984).

APPENDIX

The functions $C_j^\mu(\psi, \phi)$ thr. $E_j^\mu(\psi, \phi)$ are defined as follows:

$$B_j^\mu(\psi, \phi) = \sum_{v=1}^{N(j)} C_j^{\mu v} (-1)^{v-1} \sqrt{2 - \delta_{v,1}} \\ \times [P_j^{2,2(v-1)}(\cos \psi) + (-1)^j P_j^{-2,2(v-1)}(\cos \psi)] \cos 2(v-1)\phi \quad (\text{I-1})$$

$$C_j^\mu(\psi, \phi) = \sum_{v=1}^{N(j)} C_j^{\mu v} (-1)^{v-1} \sqrt{2 - \delta_{v,1}} \\ \times [P_j^{2,2(v-1)}(\cos \psi) - (-1)^j P_j^{-2,2(v-1)}(\cos \psi)] \sin 2(v-1)\phi \quad (\text{I-2})$$

$$D_j^\mu(\psi, \phi) = \sum_{v=1}^{N(j)} C_j^{\mu v} (-1)^{v-1} \sqrt{2 - \delta_{v,1}} \\ \times [P_j^{1,2(v-1)}(\cos \psi) + (-1)^j P_j^{-1,2(v-1)}(\cos \psi)] \cos 2(v-1)\phi \quad (\text{I-3})$$

$$E_j^\mu(\psi, \phi) = \sum_{v=1}^{N(j)} C_j^{\mu v} (-1)^{v-1} \sqrt{2 - \delta_{v,1}} \\ \times [P_j^{1,2(v-1)}(\cos \psi) - (-1)^j P_j^{-1,2(v-1)}(\cos \psi)] \sin 2(v-1)\phi \quad (\text{I-4})$$

where $N(j) = (j+2)/2$ ("integer division").

Note that these equations have been written for orthorhombic specimen symmetry.

Note that for instance,

$$B_j^\mu(\pi - \psi, \pi + \phi) = + B_j^\mu(\psi, \phi) \quad (\text{I-5})$$

$$C_j^\mu(\pi - \psi, \pi + \phi) = - C_j^\mu(\psi, \phi) \quad (\text{I-6})$$

$$D_j^\mu(\pi - \psi, \pi + \phi) = - D_j^\mu(\psi, \phi) \quad (\text{I-7})$$

$$E_j^\mu(\pi - \psi, \pi + \phi) = + E_j^\mu(\psi, \phi) \quad (\text{I-8})$$