Supplementary data to

A. Leineweber, Anisotropic diffraction-line broadening due to anisotropic microstrain distribution; Parametrisation opportunities

In the following the complete expressions for the variance of the microstrain measured along the diffraction vector are given for the four parametrisations (with the parameters $C_{H'K'L',H''K''L''}$, E_{ijpq}, S_{HKL} and Z_{ijpq}) indicated in Table 1 in the Appendix of the main paper. This listing is done separately for the different symmetry classes with different sets of symmetry restrictions, as indicated in Table 2 in the Appendix of the main paper. For the Cartesian Z_{ijpq} parametrisation the components of the diffraction vector **g**, g_1, g_2 and g_3 are substituted by h, k, l according to Eq. (31) and Eq. (32) and (except for the triclinic case where the calculation is too tedious and does not provide additional insight), in order to emphasise the equivalency of the expressions resulting from the Z_{ijpq} parametriations with those of the S_{HKL} parametrisation using directly the crystal lattice basis.

I. Triclinic, $\bar{1}$

lattice basis

$$\left\langle \varepsilon_{hkl}^2 \right\rangle = \frac{1}{4}\left\langle d_{hkl}\right\rangle^4 \begin{bmatrix} C_{200,200}h^4 + C_{020,020}k^4 + C_{002,002}l^4 \\ +\left\{C_{110,110} + 2C_{200,020}\right\} h^2k^2 + \left\{C_{101,101} + 2C_{200,002}\right\} h^2l^2 + \left\{C_{011,011} + 2C_{020,002}\right\} k^2l^2 \\ +2\left\{C_{200,011} + C_{110,101}\right\} h^2kl + 2\left\{C_{020,101} + C_{110,011}\right\} hk^2l + 2\left\{C_{002,110} + C_{101,011}\right\} hkl^2 \\ +2C_{200,110}h^3k + 2C_{200,101}h^3l + 2C_{020,110}hk^3 + 2C_{020,011}k^3l + 2C_{002,101}hl^3 + 2C_{002,011}kl^3 \end{bmatrix}$$

$$= \frac{1}{4}\left\langle d_{hkl}\right\rangle^4 \begin{bmatrix} S_{400}h^4 + S_{040}k^4 + S_{004}l^4 \\ +S_{220}h^2k^2 + S_{202}h^2l^2 + S_{022}k^2l^2 \\ +S_{211}h^2kl + S_{121}hk^2l + S_{112}hkl^2 \\ +S_{310}h^3k + S_{301}h^3l + S_{130}hk^3 + S_{031}k^3l + hl^3S_{103} + kl^3S_{013} \end{bmatrix}$$

Cartesian basis

$$\left\langle \varepsilon_{hkl}^2 \right\rangle = \left\langle d_{hkl}\right\rangle^4 \begin{bmatrix} E_{1111}g_1^4 + E_{2222}g_2^4 + E_{3333}g_3^4 \\ +\left\{4E_{1212} + 2E_{1122}\right\} g_1^2g_2^2 + \left\{4E_{1313} + 2E_{1133}\right\} g_1^2g_3^2 + \left\{4E_{2323} + 2E_{2233}\right\} g_2^2g_3^2 \\ +\left\{8E_{1213} + 4E_{1123}\right\} g_1^2g_2g_3 + \left\{8E_{1223} + 4E_{2213}\right\} g_1g_2^2g_3 + \left\{8E_{1323} + 4E_{3312}\right\} g_1g_2g_3^2 \\ +4E_{1112}g_1^3g_2 + 4E_{1113}g_1^3g_3 + 4E_{2212}g_1g_2^3 + 4E_{2223}g_2^3g_3 + 4E_{3313}g_1g_3^3 + 4E_{3323}g_2g_3^3 \end{bmatrix}$$

$$= \left\langle d_{hkl}\right\rangle^4 \begin{bmatrix} Z_{1111}g_1^4 + Z_{2222}g_2^4 + Z_{3333}g_3^2 \\ +6Z_{1122}g_1^2g_2^2 + 6Z_{1133}g_1^2g_3^2 + 6Z_{2233}g_2^2g_3^2 \\ +12Z_{1123}g_1^2g_2g_3 + 12Z_{1223}g_1g_2^2g_3 + 12Z_{1233}g_1g_2g_3^2 \\ +4Z_{1112}g_1^3g_2 + 4Z_{1113}g_1^3g_3 + 4Z_{1222}g_1g_2^3 + 4Z_{2223}g_2^3g_3 + 4Z_{1333}g_1g_3^3 + 4Z_{2333}g_2g_3^3 \end{bmatrix}$$

II. Monoclinic, $2/m$

lattice basis

$$\left\langle \varepsilon_{hkl}^2 \right\rangle = \frac{1}{4}\left\langle d_{hkl} \right\rangle^4 \begin{bmatrix} C_{200,200}h^4 + C_{020,020}k^4 + C_{002,002}l^4 \\ +\left\{C_{110,110} + 2C_{200,020}\right\}h^2k^2 + \left\{C_{101,101} + 2C_{200,002}\right\}h^2l^2 + \left\{C_{011,011} + 2C_{020,002}\right\}k^2l^2 \\ +2\left\{C_{020,101} + C_{110,011}\right\}hk^2l + 2C_{200,101}h^3l + 2C_{002,101}hl^3 \end{bmatrix}$$

$$= \frac{1}{4}\left\langle d_{hkl} \right\rangle^4 \begin{bmatrix} S_{400}h^4 + S_{040}k^4 + S_{004}l^4 \\ +S_{220}h^2k^2 + S_{202}h^2l^2 + S_{022}k^2l^2 \\ +S_{121}hk^2l + S_{301}hk^3 + S_{103}hl^3 \end{bmatrix}$$

Cartesian basis

$$\left\langle \varepsilon_{hkl}^2 \right\rangle = \left\langle d_{hkl} \right\rangle^4 \begin{bmatrix} E_{1111}g_1^4 + E_{2222}g_2^4 + E_{3333}g_3^4 \\ +\left\{4E_{1212} + 2E_{1122}\right\}g_1^{\ 2}g_2^{\ 2} + \left\{4E_{1313} + 2E_{1133}\right\}g_1^{\ 2}g_3^{\ 2} + \left\{4E_{2323} + 2E_{2233}\right\}g_2^{\ 2}g_3^{\ 2} \\ +\left\{8E_{1223} + 4E_{2213}\right\}g_1g_2^2g_3 + 4E_{1113}g_1^{\ 3}g_3 + 4E_{3313}g_1g_3^3 \end{bmatrix}$$

$$= \left\langle d_{hkl} \right\rangle^4 \begin{bmatrix} \frac{1}{a^4}\left\{Z_{1111} - 4\cot\left\langle\beta\right\rangle Z_{1113} + 6\cot^2\left\langle\beta\right\rangle Z_{1133} - 4\cot^3\left\langle\beta\right\rangle Z_{1333} + \cot^4\left\langle\beta\right\rangle Z_{3333}\right\}h^4 \\ +\frac{1}{\left\langle b\right\rangle^4}Z_{2222}k^4 + \frac{1}{\left\langle c\right\rangle^4\sin^4\left\langle\beta\right\rangle}Z_{3333}l^4 + \frac{6}{\left\langle a\right\rangle^2\left\langle b\right\rangle^2}\left\{Z_{1122} - 2\cot\left\langle\beta\right\rangle Z_{1223} + \cot^2\left\langle\beta\right\rangle Z_{2233}\right\}h^2k^2 \\ +\frac{6}{\left\langle a\right\rangle^2\left\langle c\right\rangle^2\sin^2\left\langle\beta\right\rangle}\left\{Z_{1133} - 2\cot\left\langle\beta\right\rangle Z_{1333} + \cot^2\left\langle\beta\right\rangle Z_{3333}\right\}h^2l^2 \\ +\frac{4}{\left\langle a\right\rangle^3\left\langle c\right\rangle\sin\left\langle\beta\right\rangle}\left\{Z_{1113} - 3\cot\left\langle\beta\right\rangle Z_{1133} + 3\cot^2\left\langle\beta\right\rangle Z_{1333} - \cot^3\left\langle\beta\right\rangle Z_{3333}\right\}h^3l \\ +\frac{6}{\left\langle b\right\rangle^2\left\langle c\right\rangle^2\sin^2\left\langle\beta\right\rangle}Z_{2233}k^2l^2 + \frac{12}{\left\langle a\right\rangle\left\langle b\right\rangle^2\left\langle c\right\rangle\sin\left\langle\beta\right\rangle}\left\{Z_{1223} - \cot\left\langle\beta\right\rangle Z_{2233}\right\}hk^2l \\ +\frac{4}{\left\langle a\right\rangle\left\langle c\right\rangle^3\sin^3\left\langle\beta\right\rangle}\left\{Z_{1333} - \cot\left\langle\beta\right\rangle Z_{3333}\right\}hl^3 \end{bmatrix}$$

III. Orthorhombic, mmm

lattice basis

$$\left\langle \varepsilon_{hkl}^2 \right\rangle = \frac{1}{4}\left\langle d_{hkl} \right\rangle^4 \begin{bmatrix} C_{200,200}h^4 + C_{020,020}k^4 + C_{002,002}l^4 \\ +\left\{C_{110,110} + 2C_{200,020}\right\}h^2k^2 + \left\{C_{101,101} + 2C_{200,002}\right\}h^2l^2 + \left\{C_{011,011} + 2C_{020,002}\right\}k^2l^2 \end{bmatrix}$$

$$= \frac{1}{4}\left\langle d_{hkl} \right\rangle^4 \begin{bmatrix} S_{400}h^4 + S_{040}k^4 + S_{004}l^4 \\ +S_{220}h^2k^2 + S_{202}h^2l^2 + S_{022}k^2l^2 \end{bmatrix}$$

Cartesian basis

$$\left\langle \varepsilon_{hkl}^2 \right\rangle = \left\langle d_{hkl} \right\rangle^4 \begin{bmatrix} E_{1111}g_1^4 + E_{2222}g_2^4 + E_{3333}g_3^4 \\ +\left\{4E_{1212} + 2E_{1122}\right\}g_1^2g_2^2 + \left\{4E_{1313} + 2E_{1133}\right\}g_1^2g_3^2 + \left\{4E_{2323} + 2E_{2233}\right\}g_2^2g_3^2 \end{bmatrix}$$

$$= \left\langle d_{hkl} \right\rangle^4 \begin{bmatrix} \frac{1}{\left\langle a\right\rangle^4}Z_{1111}h^4 + \frac{1}{\left\langle b\right\rangle^4}Z_{2222}k^4 + \frac{1}{\left\langle c\right\rangle^4}Z_{3333}l^4 \\ +\frac{6}{\left\langle a\right\rangle^2\left\langle b\right\rangle^2}Z_{1122}h^2k^2 + \frac{6}{\left\langle a\right\rangle^2\left\langle c\right\rangle^2}Z_{1133}h^2l^2 + \frac{6}{\left\langle b\right\rangle^2\left\langle c\right\rangle^2}Z_{2233}k^2l^2 \end{bmatrix}$$

IV. Tetragonal, 4/*m*
lattice basis

$$\left\langle \varepsilon_{hkl}^2 \right\rangle = \frac{1}{4}\left\langle d_{hkl}\right\rangle^4 \begin{bmatrix} C_{200,200}\left(h^4+k^4\right)+C_{002,002}l^4 \\ +\left\{C_{110,110}+2C_{200,020}\right\}h^2k^2 \\ +\left\{C_{101,101}+2C_{200,002}\right\}\left(h^2l^2+k^2l^2\right) \\ +2C_{200,110}\left(h^3k-hk^3\right) \end{bmatrix}$$

$$= \frac{1}{4}\left\langle d_{hkl}\right\rangle^4 \begin{bmatrix} S_{400}\left(h^4+k^4\right)+S_{004}l^4 \\ +S_{220}h^2k^2+S_{202}\left(h^2l^2+k^2l^2\right) \\ +S_{310}\left(h^3k-hk^3\right) \end{bmatrix}$$

Cartesian basis

$$\left\langle \varepsilon_{hkl}^2 \right\rangle = \left\langle d_{hkl}\right\rangle^4 \begin{bmatrix} E_{1111}\left(g_1^4+g_2^4\right)+E_{3333}g_3^4 \\ +\left\{4E_{1212}+2E_{1122}\right\}g_1^2g_2^2+\left\{4E_{1313}+2E_{1133}\right\}\left(g_1^2g_3^2+g_2^2g_3^2\right) \\ +4E_{1112}\left(g_1^3g_2-g_1g_2^3\right) \end{bmatrix}$$

$$= \left\langle d_{hkl}\right\rangle^4 \begin{bmatrix} \frac{1}{\left\langle a\right\rangle^4}\left(h^4+k^4\right)Z_{1111}+\frac{1}{\left\langle c\right\rangle^4}Z_{3333}l^4 \\ +\frac{6}{\left\langle a\right\rangle^4}Z_{1122}h^2k^2+\frac{6}{\left\langle a\right\rangle^2\left\langle c\right\rangle^2}Z_{1133}\left(h^2l^2+k^2l^2\right) \\ +\frac{12}{\left\langle a\right\rangle^4}Z_{1112}\left(h^3k-hk^3\right) \end{bmatrix}$$

V. Tetragonal, 4/*mmm*

lattice basis

$$\left\langle \varepsilon_{hkl}^2 \right\rangle = \frac{1}{4}\left\langle d_{hkl}\right\rangle^4 \begin{bmatrix} C_{200,200}\left(h^4+k^4\right)+C_{002,002}l^4 \\ +\left\{C_{110,110}+2C_{200,020}\right\}h^2k^2 \\ +\left\{C_{101,101}+2C_{200,002}\right\}\left(h^2l^2+k^2l^2\right) \end{bmatrix}$$

$$= \frac{1}{4}\left\langle d_{hkl}\right\rangle^4 \begin{bmatrix} S_{400}\left(h^4+k^4\right)+S_{004}l^4 \\ +S_{220}h^2k^2+S_{202}\left(h^2l^2+k^2l^2\right) \end{bmatrix}$$

Cartesian basis

$$\left\langle \varepsilon_{hkl}^2 \right\rangle = \left\langle d_{hkl}\right\rangle^4 \begin{bmatrix} E_{1111}\left(g_1^4+g_2^4\right)+E_{3333}g_3^4 \\ +\left\{4E_{1212}+2E_{1122}\right\}g_1^2g_2^2+\left\{4E_{1313}+2E_{1133}\right\}\left(g_1^2g_3^2+g_2^2g_3^2\right) \end{bmatrix}$$

$$= \left\langle d_{hkl} \right\rangle^4 \begin{bmatrix} \frac{1}{\langle a \rangle^4}\left(h^4 + k^4\right) Z_{1111} + \frac{l^4}{\langle c \rangle^4} Z_{3333} \\ + \frac{6}{\langle a \rangle^4} Z_{1122} h^2 k^2 + \frac{6}{\langle a \rangle^2 \langle c \rangle^2} Z_{1133} \left(h^2 l^2 + k^2 l^2\right) \end{bmatrix}$$

VI. Trigonal/rhombohedral $\bar{3}$

a) hexagonal setting

lattice basis

$$\left\langle \varepsilon_{hkl}^2 \right\rangle = \frac{1}{4} \left\langle d_{hkl} \right\rangle^4 \begin{bmatrix} C_{200,200} \left(h^4 + 2h^3 k + 3h^2 k^2 + 2hk^3 + k^4\right) \\ + C_{002,002} l^4 + \left\{C_{101,101} + 2C_{200,002}\right\} \left(h^2 k^2 + hkl^2 + k^2 l^2\right) \\ + 2C_{200,011} \left(3h^2 kl + h^3 l - k^3 l\right) + 2C_{020,101} \left(3hk^2 l - h^3 l + k^3 l\right) \end{bmatrix}$$

$$= \frac{1}{4} \left\langle d_{hkl} \right\rangle^4 \begin{bmatrix} S_{400} \left(h^4 + 2h^3 k + 3h^2 k^2 + 2hk^3 + k^4\right) \\ + S_{004} l^4 + S_{202} \left(h^2 + k^2 + hk\right) l^2 \\ + S_{211} \left(h^2 kl + h^3 l/3 - k^3 l/3\right) \\ + S_{121} \left(hk^2 l - h^3 l/3 + k^3 l/3\right) \end{bmatrix}$$

Cartesian basis

$$\left\langle \varepsilon_{hkl}^2 \right\rangle = \left\langle d_{hkl} \right\rangle^4 \begin{bmatrix} E_{1111} \left(g_1^4 + 2g_1^2 g_2^4 + g_2^4\right) + E_{3333} g_3^4 \\ + \left\{4E_{1313} + 2E_{1133}\right\} \left(g_1^2 g_3^2 + g_2^2 g_3^2\right) \\ + E_{1123} \left(12 g_1^2 g_2 g_3 - 4 g_2^3 g_3\right) + E_{1223} \left(12 g_1 g_2^2 g_3 - 4 g_1^3 g_3\right) \end{bmatrix}$$

$$= \left\langle d_{hkl} \right\rangle^4 \begin{bmatrix} \frac{16}{9\langle a \rangle^4} Z_{1111} \left(h^4 + 2h^3 k + 3h^2 k^2 + 2hk^3 + k^4\right) \\ + \frac{1}{\langle c \rangle^4} Z_{3333} l^4 + \frac{8}{\langle a \rangle^2 \langle c \rangle^2} Z_{1133} \left(h^2 l^2 + hkl^2 + k^2 l^2\right) \\ + \frac{16}{\langle a \rangle^3 \langle c \rangle} \begin{Bmatrix} \frac{2}{3\sqrt{3}} Z_{1123} \left(h^3 l - k^3 l\right) \\ + \left[\frac{1}{\sqrt{3}} Z_{1123} + Z_{1223}\right] h^2 kl \\ + \left[Z_{1223} - Z_{1123} \frac{1}{\sqrt{3}}\right] hk^2 l \end{Bmatrix} \end{bmatrix}$$

b) rhombohedral setting

lattice basis

$$\left\langle \varepsilon_{hkl}^2 \right\rangle = \frac{1}{4}\left\langle d_{hkl} \right\rangle^4 \begin{bmatrix} C_{200,200}\left(h^4+k^4+l^4\right) \\ +\left\{C_{110,110}+2C_{200,020}\right\}\left(h^2k^2+h^2l^2+k^2l^2\right) \\ +2\left\{C_{200,011}+C_{110,101}\right\}\left(h^2kl+hk^2l+hkl^2\right) \\ +2C_{200,110}\left(h^3k+k^3l+hl^3\right)+2C_{200,101}\left(h^3l+hk^3+kl^3\right) \end{bmatrix}$$

$$= \frac{1}{4}\left\langle d_{hkl} \right\rangle^4 \begin{bmatrix} S_{400}\left(h^4+k^4+l^4\right) \\ +S_{220}\left(h^2k^2+h^2l^2+k^2l^2\right) \\ +S_{211}\left(h^2kl+hk^2l+hkl^2\right) \\ +S_{310}\left(h^3k+k^3l+hl^3\right)+S_{301}\left(h^3l+hk^3+kl^3\right) \end{bmatrix}$$

Cartesian basis (for *r*, *s*: see Eq. (32) in the main paper)

$$\left\langle \varepsilon_{hkl}^2 \right\rangle = \left\langle d_{hkl} \right\rangle^4 \begin{bmatrix} E_{1111}\left(g_1^4+g_2^4+g_3^4\right) \\ +\left\{4E_{1212}+2E_{1122}\right\}\left(g_1^2g_2^2+g_1^2g_3^2+g_2^2g_3^2\right) \\ +\left\{8E_{1213}+4E_{1123}\right\}\left(g_1^2g_2g_3+g_1g_2^2g_3+g_1g_2g_3^2\right) \\ +4E_{1112}\left(g_1^3g_2+g_2^3g_3+g_1g_3^3\right)+4E_{1113}\left(g_1^3g_3+g_1g_2^3+g_2g_3^3\right) \end{bmatrix}$$

$$= \left\langle d_{hkl} \right\rangle^4 \begin{bmatrix} \left\{\left(2s^4+r^4\right)Z_{1111}+6\left(s^4+2r^2s^2\right)Z_{1122}+12\left(2rs^3+r^2s^2\right)Z_{1123}+4\left(s^4+rs^3+r^3s\right)\left[Z_{1112}+Z_{1113}\right]\right\}\left(h^4+k^4+l^4\right) \\ +\left\{6\left(2r^2s^2+s^4\right)Z_{1111}+6\left(r^4+6r^2s^2+8rs^3+3s^4\right)Z_{1122}+24\left(r^3s+3r^2s^2+3rs^3+2s^4\right)Z_{1123}+12\left(r^3s+r^2s^2+3rs^3+s^4\right)\left[Z_{1112}+Z_{1113}\right]\right\}\left(h^2k^2+h^2l^2+k^2l^2\right) \\ +\left\{12\left(r^2s^2+2rs^3\right)Z_{1111}+24\left(r^3s+3r^2s^2+3rs^3+2s^4\right)Z_{1122}+12\left(r^4+4r^3s+9r^2s^2+14rs^3+8s^4\right)Z_{1123}+12\left(r^3s+4r^2s^2+5rs^3+2s^4\right)\left[Z_{1112}+Z_{1113}\right]\right\}\left(h^2kl+hk^2l+hkl^2\right) \\ +\left\{4\left(r^3s+rs^3+s^4\right)Z_{1111}+12\left(r^3s+r^2s^2+3rs^3+s^4\right)Z_{1122}+12\left(r^3s+4r^2s^2+5rs^3+2s^4\right)Z_{1123}+4\left(r^4+3r^2s^2+6rs^3+2s^4\right)Z_{1112}+4\left(r^3s+6r^2s^2+rs^3+4s^4\right)Z_{1113}\right\}\left(h^3k+k^3l+hl^3\right) \\ +\left\{4\left(r^3s+rs^3+s^4\right)Z_{1111}+12\left(r^3s+r^2s^2+3rs^3+s^4\right)Z_{1122}+12\left(r^3s+4r^2s^2+5rs^3+2s^4\right)Z_{1123}+4\left(r^3s+6r^2s^2+rs^3+4s^4\right)Z_{1112}+4\left(r^4+3r^2s^2+6rs^3+2s^4\right)Z_{1113}\right\}\left(h^3l+hk^3+kl^3\right) \end{bmatrix}$$

VII. Trigonal/rhombohedral $\bar{3}m1$

a) hexagonal setting

lattice basis

$$\left\langle \varepsilon_{hkl}^2 \right\rangle = \frac{1}{4}\left\langle d_{hkl} \right\rangle^4 \begin{bmatrix} C_{200,200}\left(h^4+2h^3k+3h^2k^2+2hk^3+k^4\right)+C_{002,002}l^4 \\ +\left\{C_{101,101}+2C_{200,002}\right\}\left(h^2k^2+hkl^2+k^2l^2\right) \\ +2C_{200,011}\left(3h^2kl-3hk^2l+2h^3l-2k^3l\right) \end{bmatrix}$$

$$= \frac{1}{4}\left\langle d_{hkl} \right\rangle^4 \begin{bmatrix} S_{400}\left(h^4+2h^3k+3h^2k^2+2hk^3+k^4\right)+S_{004}l^4 \\ +S_{202}\left(h^2l^2+hkl^2+k^2l^2\right) \\ +S_{211}\left(h^2kl-hk^2l+2h^3l/3-2k^3l/3\right) \end{bmatrix}$$

Cartesian basis

$$\left\langle \varepsilon_{hkl}^2 \right\rangle = \left\langle d_{hkl} \right\rangle^4 \begin{bmatrix} E_{1111}\left(g_1^4+2g_1^2g_2^4+g_2^4\right)+E_{3333}g_3^4 \\ +\left\{4E_{1313}+2E_{1133}\right\}\left(g_1^2g_3^2+g_2^2g_3^2\right) \\ +E_{1123}\left(12g_1^2g_2g_3-4g_2^3g_3\right) \end{bmatrix}$$

$$
=\left\langle d_{hkl}\right\rangle^4\left[\begin{array}{l}\frac{16}{9\langle a\rangle^4}Z_{1111}\left(h^4+2h^3k+3h^2k^2+2hk^3+k^4\right)\\+\frac{l^4}{\langle c\rangle^4}Z_{3333}l^4+\frac{8}{3a^2c^2}Z_{1133}\left(h^2l^2+hkl^2+k^2l^2\right)\\+\frac{16}{3\sqrt{3}\langle a\rangle^3\langle c\rangle}Z_{1123}\left(h^2kl-hk^2l+2h^3l/3-2k^3l/3\right)\end{array}\right]
$$

b) rhombohedral setting

lattice basis

$$
\left\langle \varepsilon_{hkl}^2\right\rangle=\frac{1}{4}\left\langle d_{hkl}\right\rangle^4\left[\begin{array}{l}C_{200,200}\left(h^4+k^4+l^4\right)\\+\left\{C_{110,110}+2C_{200,020}\right\}\left(h^2k^2+h^2l^2+k^2l^2\right)\\+2\left\{C_{200,011}+C_{110,101}\right\}\left(h^2kl+hk^2l+hkl^2\right)\\+2C_{200,110}\left(h^3k+k^3l+hl^3+h^3l+hk^3+kl^3\right)\end{array}\right]
$$

$$
=\left\langle d_{hkl}\right\rangle^4\left[\begin{array}{l}S_{400}\left(h^4+k^4+l^4\right)\\+S_{220}\left(h^2k^2+h^2l^2+k^2l^2\right)\\+S_{211}\left(h^2kl+hk^2l+hkl^2\right)\\+S_{310}\left(h^3k+k^3l+hl^3+h^3l+hk^3+kl^3\right)\end{array}\right]
$$

Cartesian basis (for r, s: see Eq. (32) in the main paper)

$$
\left\langle \varepsilon_{hkl}^2\right\rangle=\left\langle d_{hkl}\right\rangle^4\left[\begin{array}{l}E_{1111}\left(g_1^4+g_2^4+g_3^4\right)\\+\left\{4E_{1212}+2E_{1122}\right\}\left(g_1^2g_2^2+g_1^2g_3^2+g_2^2g_3^2\right)\\+\left\{8E_{1213}+4E_{1123}\right\}\left(g_1^2g_2g_3+g_1g_2^2g_3+g_1g_2g_3^2\right)\\+4E_{1112}\left(g_1^3g_2+g_1g_2^3+g_1^3g_3+g_1g_3^3+g_2^3g_3+g_2g_3^3\right)\end{array}\right]
$$

$$
=\left\langle d_{hkl}\right\rangle^4\left[\begin{array}{l}\left\{\left(2s^4+r^4\right)Z_{1111}+6\left(s^4+2r^2s^2\right)Z_{1122}+12\left(2rs^3+r^2s^2\right)Z_{1123}+8\left(s^4+rs^3+r^3s\right)Z_{1112}\right\}\left(h^4+k^4+l^4\right)\\+\left\{6\left(2r^2s^2+s^4\right)Z_{1111}+6\left(r^4+6r^2s^2+8rs^3+3s^4\right)Z_{1122}+24\left(r^3s+3r^2s^2+3rs^3+2s^4\right)Z_{1123}+24\left(r^3s+r^2s^2+3rs^3+s^4\right)Z_{1112}\right\}\left(h^2k^2+h^2l^2+k^2l^2\right)\\+\left\{12\left(r^2s^2+2rs^3\right)Z_{1111}+24\left(r^3s+3r^2s^2+3rs^3+2s^4\right)Z_{1122}+12\left(r^4+4r^3s+9r^2s^2+14rs^3+8s^4\right)Z_{1123}+24\left(r^3s+4r^2s^2+5rs^3+2s^4\right)\right\}\left(h^2kl+hk^2l+hkl^2\right)\\+\left\{4\left(r^3s+rs^3+s^4\right)Z_{1111}+12\left(r^3s+r^2s^2+3rs^3+s^4\right)Z_{1122}+12\left(r^3s+4r^2s^2+5rs^3+2s^4\right)Z_{1123}+4\left(r^4+r^3s+9r^2s^2+7rs^3+6s^4\right)Z_{1112}\right\}\left(h^3k+k^3l+hl^3+h^3l+hk^3+kl^3\right)\end{array}\right]
$$

VIII. Trigonal $\bar{3}1m$

lattice basis

$$
\left\langle \varepsilon_{hkl}^2\right\rangle=\frac{1}{4}\left\langle d_{hkl}\right\rangle^4\left[\begin{array}{l}C_{200,200}\left(h^4+2h^3k+3h^2k^2+2hk^3+k^4\right)\\+C_{002,002}l^4+6C_{200,011}\left(h^2kl+hk^2l\right)\\+\left\{C_{101,101}+2C_{200,002}\right\}\left(h^2k^2+hkl^2+k^2l^2\right)\end{array}\right]
$$

$$
=\frac{1}{4}\left\langle d_{hkl}\right\rangle^4\left[\begin{array}{l}S_{400}\left(h^4+2h^3k+3h^2k^2+2hk^3+k^4\right)\\+S_{004}l^4+S_{202}\left(h^2l^2+k^2l^2+hkl^2\right)\\+S_{211}\left(h^2kl+hk^2l\right)\end{array}\right]
$$

Cartesian basis

$$\left\langle \varepsilon_{hkl}^{2} \right\rangle = \left\langle d_{hkl} \right\rangle^{4} \begin{bmatrix} E_{1111}\left(g_1^4 + 2g_1^2 g_2^4 + g_2^4\right) + E_{3333} g_3^4 \\ + \left\{4E_{1313} + 2E_{1133}\right\}\left(g_1^2 g_3^2 + g_2^2 g_3^2\right) \\ + E_{1223}\left(12 g_1 g_2^3 g_3 - 4 g_1^3 g_3\right) \end{bmatrix}$$

$$= \left\langle d_{hkl} \right\rangle^{4} \begin{bmatrix} \dfrac{16}{9\langle a\rangle^4} Z_{1111}\left(h^4 + 2h^3k + 3h^2k^2 + 2hk^3 + k^4\right) \\ + \dfrac{1}{\langle c\rangle^4} Z_{3333} l^4 + \dfrac{8}{\langle a\rangle^2 \langle c\rangle^2} Z_{1133}\left(h^2l^2 + hkl^2 + k^2l^2\right) \\ + \dfrac{16}{\langle a\rangle^3 \langle c\rangle} Z_{1223}\left(h^2kl + hk^2l\right) \end{bmatrix}$$

IX. Hexagonal $6/m$, $6/mmm$

lattice basis

$$\left\langle \varepsilon_{hkl}^{2} \right\rangle = \frac{1}{4}\left\langle d_{hkl} \right\rangle^{4} \begin{bmatrix} C_{200,200}\left(h^4 + 2h^3k + 3h^2k^2 + 2hk^3 + k^4\right) + C_{002,002} l^4 \\ + \left\{C_{101,101} + 2C_{200,002}\right\}\left(h^2k^2 + hkl^2 + k^2l^2\right) \end{bmatrix}$$

$$= \frac{1}{4}\left\langle d_{hkl} \right\rangle^{4} \begin{bmatrix} S_{400}\left(h^4 + 2h^3k + 3h^2k^2 + 2hk^3 + k^4\right) \\ + S_{004} l^4 + S_{202}\left(h^2l^2 + k^2l^2 + hkl^2\right) \end{bmatrix}$$

Cartesian basis

$$\left\langle \varepsilon_{hkl}^{2} \right\rangle = \left\langle d_{hkl} \right\rangle^{4} \begin{bmatrix} E_{1111}\left(g_1^4 + 2g_1^2 g_2^4 + g_2^4\right) + E_{3333} g_3^4 \\ + \left\{4E_{1313} + 2E_{1133}\right\}\left(g_1^2 g_3^2 + g_2^2 g_3^2\right) \end{bmatrix}$$

$$= \left\langle d_{hkl} \right\rangle^{4} \begin{bmatrix} \dfrac{16}{9\langle a\rangle^4} Z_{1111}\left(h^4 + 2h^3k + 3h^2k^2 + 2hk^3 + k^4\right) \\ + \dfrac{1}{\langle c\rangle^4} Z_{3333} l^4 + \dfrac{8}{\langle a\rangle^2 \langle c\rangle^2} Z_{1133}\left(h^2l^2 + hkl^2 + k^2l^2\right) \end{bmatrix}$$

X. Cubic

lattice basis

$$\left\langle \varepsilon_{hkl}^{2} \right\rangle = \frac{1}{4}\left\langle d_{hkl} \right\rangle^{4} \begin{bmatrix} C_{200.200}\left(h^4 + k^4 + l^4\right) \\ + \left\{C_{110,110} + 2C_{200,020}\right\}\left(h^2k^2 + h^2l^2 + k^2l^2\right) \end{bmatrix} = \frac{1}{4}\left\langle d_{hkl} \right\rangle^{4} \begin{bmatrix} S_{400}\left(h^4 + k^4 + l^4\right) \\ + S_{220}\left(h^2k^2 + h^2l^2 + k^2l^2\right) \end{bmatrix}$$

Cartesian basis

$$\left\langle \varepsilon_{hkl}^{2} \right\rangle = \left\langle d_{hkl} \right\rangle^{4}\left[E_{1111}\left(g_1^4 + g_2^4 + g_3^4\right) + \left\{4E_{1212} + 2E_{1122}\right\}\left(g_1^2 g_2^2 + g_1^2 g_3^2 + g_2^2 g_3^2\right)\right]$$

$$= \left\langle d_{hkl} \right\rangle^{4}\left[\frac{1}{\langle a\rangle^4}\left(h^4 + k^4 + l^4\right) Z_{1111} + \frac{6}{\langle a\rangle^4}\left(h^2k^2 + h^2l^2 + k^2l^2\right) Z_{1122}\right]$$

XI. Isotropic

Cartesian basis

$\left\langle \varepsilon_{hkl}^{2} \right\rangle = E_{1111} = Z_{1111}$