Thus, the internal-strain contributions to the elastic constants can be considered separately, and the $C_{ijkl}^{(0)}$... are the Brugger elastic constants in the absence of internal strains.

To illustrate the use of these equations, specific results for several structures are given below. Voigt (reduced) notation is used for all subscripts. Also, for those structures with two ions per unit cell and thus only one independent internal strain, the superscript $\alpha = 1$ is omitted.

For the zinc-blende (or diamond) structure, Eqs. (A10) and (A11) reduce to

$$C_{11} = C_{11}^{(0)}, \quad C_{12} = C_{12}^{(0)}, \quad C_{44} = C_{44}^{(0)} - U^{11}A^2 \; ;$$

$$C_{111} = C_{111}^{(0)}, \quad C_{112} = C_{112}^{(0)}, \quad C_{123} = C_{123}^{(0)} \;,$$

$$C_{144} = C_{144}^{(0)} - 2U_{14}^1 A + U_1^{11}A^2 \;,$$

$$C_{155} = C_{155}^{(0)} - 2U_{24}^1 A + U_2^{11}A^2 \;,$$

$$C_{456} = C_{456}^{(0)} - 3U_{56}^1 A + 3U_4^{23}A^2 - U^{123}A^3 \;,$$

where the internal-strain parameter, as determined from Eq. (A3) is

$$A = \frac{U_4^1}{U^{11}} = -\frac{\partial \overline{w}_1}{\partial \eta_{23}} = -\frac{\partial \overline{w}_2}{\partial \eta_{13}} = -\frac{\partial \overline{w}_3}{\partial \eta_{12}} \;.$$

The results for the hcp (or WC) structure are

$$C_{11} = C_{11}^{(0)} - U^{11}A^2, \quad C_{12} = C_{12}^{(0)} + U^{11}A^2 \;,$$

$$C_{13} = C_{13}^{(0)}, \qquad C_{33} = C_{33}^{(0)}, \qquad C_{44} = C_{44}^{(0)} \;;$$

$$C_{111} = C_{111}^{(0)} + 3U_{11}^1 A + 3U_1^{11}A^2 + U^{111}A^3 \;,$$

$$C_{112} = C_{112}^{(0)} - (2U_{11}^1 + U_{22}^1)A - (2U_1^{11} - U_2^{11})A^2 - U^{111}A^3 \;,$$

$$C_{222} = C_{222}^{(0)} - 3U_{22}^1 A + 3U_2^{11}A^2 - U^{111}A^3 \;,$$

$$C_{113} = C_{113}^{(0)} + 2U_{13}^1 A + U_3^{11}A^2 \;,$$

$$C_{123} = C_{123}^{(0)} - 2U_{13}^1 A - U_3^{11}A^2 \;,$$

$$C_{144} = C_{144}^{(0)} + U_{44}^1 A, \quad C_{155} = C_{155}^{(0)} - U_{44}^1 A \;,$$

$$C_{133} = C_{133}^{(0)}, \qquad C_{333} = C_{333}^{(0)}, \qquad C_{344} = C_{344}^{(0)} \;,$$

where

$$A = -\frac{U_1^1}{U^{11}} = \frac{\partial \overline{w}_1}{\partial \eta_{11}} = -\frac{\partial \overline{w}_1}{\partial \eta_{22}} = -\frac{\partial \overline{w}_2}{\partial \eta_{12}} \;.$$

For the wurtzite structure, which has three independent internal strains, complete results will not be given. However, we will indicate how the internal-strain parameters are obtained from Eq. (A3) for this structure. Since $U^{\alpha p \beta q}$ is nonzero only if $p = q$, Eq. (A3) becomes

$$\sum_{\alpha=1}^{3} U^{\alpha p \beta p} A_{pij}^{\alpha} = -U_{ij}^{\beta p} \;,$$

where there are no implied sums over repeated indices. Then

$$A_{pij}^{\alpha} = -\sum_{\beta=1}^{3} (\mathfrak{U}^{-1})^{\beta p \alpha p} U_{ij}^{\beta p} \;,$$

where

$$\mathfrak{U}^{\alpha p \beta p} = \begin{bmatrix} U^{1p1p} & U^{1p2p} & U^{1p3p} \\ U^{1p2p} & U^{2p2p} & U^{2p3p} \\ U^{1p3p} & U^{2p3p} & U^{3p3p} \end{bmatrix} \;.$$

APPENDIX B. METHOD OF HOMOGENEOUS DEFORMATION

For a homogeneous deformation of a lattice, i.e., a deformation where the resulting structure remains a perfect lattice, the lattice vectors and basis vectors deform according to

$$R_i'(l) = J_{ij} R_j(l) \tag{B1}$$

and

$$\tau_i'(\nu) = J_{ij} \tau_j(\nu) + w_i(\nu) \;, \tag{B2}$$

respectively. Or equivalently,

$$R_i'\binom{l}{\nu} = J_{ij} R_j\binom{l}{\nu} + w_i(\nu) \;, \tag{B3}$$

where $\vec{w}(\nu)$ is the internal strain or interlattice displacement of the νth sublattice. As is commonly done, the internal-strain vector is redefined as[17]

$$\overline{w}_i(\nu) = J_{ji} w_j(\nu) \;, \tag{B4}$$

so that the strain energy is in a form invariant with respect to rigid rotations. Then the lattice vectors $\vec{R}\binom{lk}{\nu\mu}$ deform according to

$$R_i'\binom{lk}{\nu\mu} = J_{ij} R_j\binom{lk}{\nu\mu} + (J^{-1})_{ji} \overline{w}_j(\nu\mu) \;, \tag{B5}$$

where

$$\overline{w}_j(\nu\mu) = \overline{w}_j(\nu) - \overline{w}_j(\mu) \;. \tag{B6}$$

Since the deformed reciprocal lattice is the reciprocal lattice of the deformed real lattice, the reciprocal-lattice vectors deform according to

$$G_i'(h) = (J^{-1})_{ji} G_j(h) \;. \tag{B7}$$

Volumes deform according to

$$\Omega_0'/\Omega_0 = \det|J| \;. \tag{B8}$$

In the expression for U_{es}' [Eq. (11)] the only variables which depend on deformation are $|\vec{R}'\binom{l0}{\nu\mu}|^2$, $|\vec{G}'(h)|^2$, Ω_0', and $S'(\vec{G}')$, the last of which is a function of $\vec{G}'(h) \cdot \vec{\tau}'(\nu)$. Using the definition of the Langrangian strain parameter η_{ij}, it is easily shown that

$$|\vec{R}'\binom{l0}{\nu\mu}|^2 = M_{ij} R_i\binom{l0}{\nu\mu} R_j\binom{l0}{\nu\mu} + 2\overline{w}_i(\nu\mu) R_i\binom{l0}{\nu\mu}$$
$$+ (M^{-1})_{ij} \overline{w}_i(\nu\mu) \overline{w}_j(\nu\mu) \;, \tag{B9}$$

$$|\vec{G}'(h)|^2 = (M^{-1})_{ij} G_i(h) G_j(h) \;, \tag{B10}$$

and

$$\vec{G}'(h) \cdot \vec{\tau}'(\nu) = \vec{G}(h) \cdot \vec{\tau}(\nu) + (M^{-1})_{ij} \overline{w}_i(\nu) G_j(h) \;, \tag{B11}$$

where

$$M_{ij} = 2\eta_{ij} + \delta_{ij} = J_{ki} J_{kj} \quad . \tag{B12}$$

Equations (B8)–(B11) can readily be differentiated with respect to η_{kl} by making use of the relations

$$\frac{\partial}{\partial \eta_{kl}} \left(\det|J| \right) = \det|J| (M^{-1})_{kl} , \tag{B13}$$

$$\frac{\partial}{\partial \eta_{kl}} (M_{ij}) = \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} , \tag{B14}$$

and

$$-\frac{\partial}{\partial \eta_{kl}} (M^{-1})_{ij} = (M^{-1})_{ik}(M^{-1})_{jl} + (M^{-1})_{il}(M^{-1})_{jk} . \tag{B15}$$

(Note that functions of η_{ij} have been symmetrized before differentiation.[19]) Using Eqs. (B8)–(B15) and the relations

$$\Phi_0(x) = e^{-x}/x, \quad \Phi_{-1/2}(x) = (\pi/x)^{1/2} \operatorname{erfc}(x^{1/2}) ,$$

and

$$\frac{-d\Phi_m(x)}{dx} = \Phi_{m+1}(x) = \Phi_0(x) + \frac{(m+1)\Phi_m(x)}{x} ,$$

it is straightforward to differentiate U'_{es} with respect to $\vec{\eta}$ and $\vec{w}(\nu)$.

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