$U_1^1 = 0.212757375$, $U_2^{11} = 0.148157929$,

$U^{11} = 0.215120910$, $U_3^{11} = -1.237994447$,

$U^{33} = 4.282147161$, $U_1^{33} = -5.305020698$,

$U^{111} = -1.206443870$, $U_3^{33} = -10.800694409$,

$U_1^{11} = 0.014231968$, $U_4^{23} = -5.520141607$,

$U_6^{12} = \frac{1}{2}(U_1^{11} - U_2^{11}) = -0.066962980$,

$U_{11}^1 = 0.010837123$,

$U_{22}^1 = U_{26}^2 = -\frac{3}{5} U_{11}^1 = -0.006502274$,

$U_{12}^1 = U_{16}^2 = -\frac{1}{5} U_{11}^1 = -0.002167425$,

$U_{13}^1 = -U_{44}^1 = U_{15}^3 = -1.072456573$,

in units of Z^2e^2/a^4. As was the case for the diamond and zinc-blende structures, the results for the WC-type structure are negative those of hcp.

For the wurtzite structure, all three internal strains must be considered. Instead of using the internal-strain labels α, $\beta, \ldots$ on $U_{ij\ldots}^{\alpha p \beta q \cdots}$ when writing specific derivatives, it is convenient to use commas to separate differentiations with respect to the three different internal strains. Then

$$U_{ij\cdots}^{p\cdots, q\cdots, m\cdots} = \left(\frac{\partial^n U'_{es}}{\partial \overline{w}_p^1 \cdots \partial \overline{w}_q^2 \cdots \partial \overline{w}_m^3 \cdots \partial \eta_{ij} \cdots} \right)_{\overline{\eta}=0,\ \vec{w}\alpha=0} .$$

The indices before the first comma represent derivatives with respect to Cartesian components of $\overline{w}^1$; those between commas represent derivatives with respect to components of $\overline{w}^2$; and those after the second comma represent derivatives with respect to components of $\overline{w}^3$. For example,

$$U^{1,,13} = \left(\frac{\partial^3 U'_{es}}{\partial \overline{w}_1^1 \partial \overline{w}_1^3 \partial \overline{w}_3^3} \right)_{\overline{\eta}=0,\ \vec{w}\alpha=0}$$

and

$$U^{3,1,1} = \left(\frac{\partial^3 U'_{es}}{\partial \overline{w}_3^1 \partial \overline{w}_1^2 \partial \overline{w}_1^3} \right)_{\overline{\eta}=0,\ \vec{w}\alpha=0} .$$

Then, the electrostatic internal-strain derivatives for ideal wurtzite with Cauchy relations are

$U^{,,3} = -2U^{3,,} = 2U^{,3,} = -0.048542322$,

$U_5^{,,1} = -2U_5^{1,,} = 2U_5^{,1,}$

$= U_1^{,,3} = -2U_1^{3,,} = 2U_1^{,3,} = 3.425042335$,

$U_3^{,,3} = -2U_3^{3,,} = 2U_3^{,3,} = -6.704457705$,

$U_1^{1,,} = U_1^{,1,} = -2.335388332$,

$U^{,,11} = -2U^{1,,1} = 2U^{,1,1} = -6.130547391$,

$U^{11,,} = U^{,11,} = -2.850152786$, $U^{1,1,} = -1.129619894$,

$U^{,,33} = -2U^{3,,3} = 2U^{,3,3} = -6.588461139$,

$U^{33,,} = U^{,33,} = 0.987916591$, $U^{3,3,} = 6.971628768$,

$U^{,,333} = -2U^{333,,} = 2U^{,333,} = 2U^{33,,3} = 2U^{,33,3}$

$= -2U^{3,,33} = 2U^{,3,33} = -2U^{,,113} = 4U^{113,,}$

$= -4U^{,113,} = -4U^{11,,3} = -4U^{13,,1} = -4U^{,11,3}$

$= -4U^{,13,1} = 4U^{3,,11} = 4U^{1,,13} = -4U^{,3,11}$

$= -4U^{,1,13} = 79.550922034$,

$U^{33,3,} = -U^{3,33,} = -U^{3,3,3} = -2U^{11,3,} = -2U^{13,1,}$

$= 2U^{3,11,} = 2U^{1,13,} = 2U^{1,1,3} = 2U^{3,1,1}$

$= 2U^{1,3,1} = 13.883995989$,

$U^{111,,} = U^{,111,} = 27.750835335$,

$U^{11,,1} = -U^{,11,1} = -U^{1,,11} = -U^{,1,11} = -28.957279205$,

$U_1^{11,,} = U_1^{,11,} = 14.882310616$, $U_1^{1,1,} = 0.659437674$,

$U_1^{,,11} = -2U_1^{1,,1} = 2U_1^{,1,1} = 29.736157294$,

$U_2^{11,,} = U_2^{,11,} = 3.060668348$, $U_2^{1,1,} = -0.533267371$,

$U_2^{,,11} = -2U_2^{1,,1} = 2U_2^{,1,1} = 5.825020837$,

$U_3^{11,,} = U_3^{,11,} = -3.692215035$, $U_3^{1,1,} = 5.521929167$,

$U_3^{,,11} = -2U_3^{1,,1} = 2U_3^{,1,1} = -4.908441176$,

$U_1^{33,,} = U_1^{,33,} = -7.530284412$, $U_1^{3,3,} = -2.579319495$,

$U_1^{,,33} = -2U_1^{3,,3} = 2U_1^{,3,3} = -4.450527428$,

$U_3^{33,,} = U_3^{,33,} = 10.120985868$, $U_3^{3,3,} = -29.699504851$,

$U_3^{,,33} = -2U_3^{3,,3} = 2U_3^{,3,3} = 41.843360553$,

$U_4^{23,,} = U_4^{,23,} = -4.680131626$,

$U_4^{2,3,} = U_4^{3,2,} = -1.449699601$,

$U_4^{,,23} = -2U_4^{2,,3} = -2U_4^{3,,2}$

$= 2U_4^{,2,3} = 2U_4^{,3,2} = 1.680019963$,

$U_6^{12,,} = U_6^{,12,} = \frac{1}{2}(U_1^{11,,} - U_2^{11,,}) = 5.910821134$,

$U_6^{1,2,} = U_6^{2,1,} = \frac{1}{2}(U_1^{1,1,} - U_2^{1,1,}) = 0.596352523$,

$U_6^{,,12} = -2U_6^{1,,2} = -2U_6^{2,,1} = 2U_6^{,1,2} = 2U_6^{,2,1}$

$= \frac{1}{2}(U_1^{,,11} - U_2^{,,11}) = 11.955568228$,

$U_5^{11,,} = -U_5^{,11,} = -U_5^{1,,1} = -U_5^{,1,1} = U_1^{13,,} = -U_1^{,13,}$

$= -U_1^{1,,3} = -U_1^{3,,1} = -U_1^{,1,3} = -U_1^{,3,1} = 6.812479538$,

$U_{11}^{1,,} = U_{11}^{,1,} = 13.899872705$,

$U_{22}^{1,,} = U_{22}^{,1,} = U_{26}^{2,,} = U_{26}^{,2,} = -\frac{3}{5} U_{11}^{1,,} = -8.339923623$,

$U_{12}^{1,,} = U_{12}^{,1,} = U_{16}^{2,,} = U_{16}^{,2,} = -\frac{1}{5} U_{11}^{1,,} = -2.779974541$,

$U_{13}^{1,,} = U_{13}^{,1,} = -U_{44}^{1,,} = -U_{44}^{,1,} = U_{15}^{3,,} = U_{15}^{,3,} = 0.557043495$,

$U_{15}^{,,1} = -2U_{15}^{1,,} = 2U_{15}^{,1,}$

$= U_{11}^{,,3} = -2U_{11}^{3,,} = 2U_{11}^{,3,} = -12.050251035$,

$U_{25}^{,,1} = -2U_{25}^{1,,} = 2U_{25}^{,1,} = U_{46}^{,,1} = -2U_{46}^{1,,} = 2U_{46}^{,1,}$

$$= U_{12}^{\prime\prime 3} = -2\,U_{12}^{3\prime\prime} = 2\,U_{12}^{\prime 3\prime} = U_{66}^{\prime\prime 3} = -2\,U_{66}^{3\prime\prime}$$

$$= 2\,U_{66}^{\prime 3\prime} = \tfrac{1}{3}\,U_{15}^{\prime\prime 1} = -4.016750345 \ ,$$

$$U_{35}^{\prime\prime 1} = -2U_{35}^{1\prime\prime} = 2U_{35}^{\prime 1\prime} = U_{13}^{\prime\prime 3} = -2U_{13}^{3\prime\prime} = 2U_{13}^{\prime 3\prime} = U_{44}^{\prime\prime 3}$$

$$= -2U_{44}^{3\prime\prime} = 2U_{44}^{\prime 3\prime} = -1.058210294 \ ,$$

$$U_{33}^{\prime\prime 3} = -2U_{33}^{3\prime\prime} = 2U_{33}^{\prime 3\prime} = 35.638709114 \ ,$$

in units of Z^2e^2/a^4.

The space group of wurtzite contains a screw axis (a twofold rotation about the three axis and a translation by $\frac{1}{2}c$). For this symmetry element, the internal-strain tensors $U_{ij\ldots}^{(\nu\rho)\cdots}$ transform as

$$U_{ij\ldots}^{(\nu\rho)\cdots *} = \mathcal{R}_{pq}\cdots\mathcal{R}_{ik}\mathcal{R}_{jl}\cdots U_{kl\ldots}^{(\mu q)\cdots} \ ,$$

where $\overleftrightarrow{\mathcal{R}}$ is the twofold rotation matrix. As a result of the translation, the unit-cell labels $(\mu \to \nu)$ change according to $0\to 1$, $1\to 0$, $2\to 3$, and $3\to 2$. For example, this symmetry requires that

$$U_1^{(01)} = -U_1^{(11)} \quad \text{and} \quad U_1^{(21)} = -U_1^{(31)} \ .$$

Thus, $U_1^{1\prime\prime} \equiv L\,U_1^{(11)}$ and $U_1^{\prime 1\prime} \equiv L\,U_1^{(31)}$ are not required to vanish. However, $U_1^{\prime\prime 1} \equiv L[U_1^{(21)} + U_1^{(31)}]$ is required to be zero. It should be noted that if the components of a tensor are unaffected by the translation, then any component with an odd number of 1's or 2's, but not both, is required to vanish (e.g., the 111 component of the piezoelectric tensor).

ACKNOWLEDGMENTS

The authors would like to thank Terri Berker for checking the internal-strain derivatives for the wurtzite structure, and Professor A. V. Granato for encouragement and a critical reading of the manuscript.

APPENDIX A: INTERNAL-STRAIN CONTRIBUTION TO BRUGGER-TYPE ELASTIC CONSTANTS

For nonprimitive lattices with ions not at centers of symmetry, macroscopic strains in general give rise to internal strains, i.e., interlattice displacements. With s ions per unit cell, only $s-1$ internal strains are independent.[17] For convenience, they will be labeled here as $\vec{\overline{w}}^{\alpha}$, where $\alpha = 1, 2, \ldots, s-1$. These internal strains, which are functions of the external strain η_{ij}, are determined by requiring that the total energy density of the homogeneously deformed state, $U(\overleftrightarrow{\eta}, \vec{\overline{w}}^{\alpha})$, be a minimum with respect to $\vec{\overline{w}}^{\alpha}$, i.e.,

$$\left(\frac{\partial U}{\partial \overline{w}_p^{\alpha}}\right)_{\overleftrightarrow{\eta}} = 0 \quad (p = 1, 2, 3) \ . \tag{A1}$$

Denoting derivatives of $U(\overleftrightarrow{\eta}, \vec{\overline{w}}^{\alpha})$ by

$$U_{ijkl\ldots}^{\alpha p\beta q\cdots}(\overleftrightarrow{\eta}) \equiv \left(\frac{\partial^n U}{\overline{w}_p^{\alpha}\,\overline{w}_q^{\beta}\cdots\partial\eta_{ij}\partial\eta_{kl}\cdots}\right)_{\vec{\overline{w}} = \vec{\overline{w}}(\overleftrightarrow{\eta})} \ , \tag{A2}$$

the strain dependence of $\vec{\overline{w}}^{\alpha}$ can be determined by differentiating Eq. (A1) with respect to η_{ij}. Thus,

$$0 = \frac{\partial}{\partial\eta_{ij}}\frac{\partial U}{\partial\overline{w}_q^{\beta}} = \frac{\partial}{\partial\eta_{ij}}(U^{\beta q}) = U_{ij}^{\beta q} + \frac{\partial\overline{w}_p^{\alpha}}{\partial\eta_{ij}}U^{\alpha p\beta q} \tag{A3}$$

and

$$0 = \frac{\partial^2}{\partial\eta_{ij}\partial\eta_{kl}}(U^{\beta q}) = U_{ijkl}^{\beta q} + \frac{\partial\overline{w}_p^{\alpha}}{\partial\eta_{kl}}U_{ij}^{\alpha p\beta q} + \frac{\partial\overline{w}_p^{\alpha}}{\partial\eta_{ij}}U_{kl}^{\alpha p\beta q} + \frac{\partial\overline{w}_p^{\alpha}}{\partial\eta_{ij}}\frac{\partial\overline{w}_r^{\gamma}}{\partial\eta_{kl}}U^{\alpha p\beta q\gamma r} + \frac{\partial^2\overline{w}_p^{\alpha}}{\partial\eta_{ij}\partial\eta_{kl}}U^{\alpha p\beta q} \ , \tag{A4}$$

where repeated indices (including superscripts) are to be summed.

In general, $\overline{w}_p^{\alpha}$ can be expanded in a Taylor series of η_{ij},

$$\overline{w}_p^{\alpha} = A_{pij}^{\alpha}\,\eta_{ij} + \tfrac{1}{2}B_{pijkl}^{\alpha}\,\eta_{ij}\,\eta_{kl} + \cdots \ , \tag{A5}$$

where the coefficients

$$A_{pij}^{\alpha} \equiv \left(\frac{\partial\overline{w}_p^{\alpha}}{\partial\eta_{ij}}\right)_{\overleftrightarrow{\eta}=0} \tag{A6}$$

and

$$B_{pijkl}^{\alpha} \equiv \left(\frac{\partial^2\overline{w}_p^{\alpha}}{\partial\eta_{ij}\partial\eta_{kl}}\right)_{\overleftrightarrow{\eta}=0} \tag{A7}$$

are determined from Eqs. (A3) and (A4), respectively. Higher-order coefficients are similarly obtained by successive differentiation. However, knowing U as a function of $\vec{\overline{w}}^{\alpha}$ and $\overleftrightarrow{\eta}$, only the internal-strain parameters A_{pij}^{α} are needed to obtain B_{pijkl}^{α} and all higher-order coefficients, e.g., Eq. (A4) relates B_{pijkl}^{α} to the coefficients A_{pij}^{α} and derivatives of U.

Using the definition of the Brugger elastic constants,[18]

$$C_{ijkl\ldots} \equiv \left(\frac{\partial^n U(\overleftrightarrow{\eta}, \vec{\overline{w}}^{\alpha}(\overleftrightarrow{\eta}))}{\partial\eta_{ij}\partial\eta_{kl}\cdots}\right)_{\overleftrightarrow{\eta}=0} \ , \tag{A8}$$

and Eqs. (A1), (A3), and (A4), it follows that

$$C_{ij} = C_{ij}^{(0)} \ , \tag{A9}$$

$$C_{ijkl} = C_{ijkl}^{(0)} - A_{pij}^{\alpha}A_{qkl}^{\beta}\,U^{\alpha p\beta q}(\overleftrightarrow{\eta}=0) \ , \tag{A10}$$

and

$$\begin{aligned} C_{ijklmn} = C_{ijklmn}^{(0)} &+ A_{pij}^{\alpha}\,U_{klmn}^{\alpha p}(\overleftrightarrow{\eta}=0) + A_{pkl}^{\alpha}\,U_{ijmn}^{\alpha p}(\overleftrightarrow{\eta}=0) \\ &+ A_{pmn}^{\alpha}\,U_{ijkl}^{\alpha p}(\overleftrightarrow{\eta}=0) + A_{pkl}^{\alpha}A_{qmn}^{\beta}\,U_{ij}^{\alpha p\beta q}(\overleftrightarrow{\eta}=0) \\ &+ A_{pij}^{\alpha}A_{qmn}^{\beta}\,U_{kl}^{\alpha p\beta q}(\overleftrightarrow{\eta}=0) + A_{pij}^{\alpha}A_{qkl}^{\beta}\,U_{mn}^{\alpha p\beta q}(\overleftrightarrow{\eta}=0) \\ &+ A_{pij}^{\alpha}A_{qkl}^{\beta}A_{rmn}^{\gamma}\,U^{\alpha p\beta q\gamma r}(\overleftrightarrow{\eta}=0) \ , \end{aligned} \tag{A11}$$

where

$$C_{ijkl\ldots}^{(0)} = U_{ijkl\ldots}(\overleftrightarrow{\eta}=0) = \left(\frac{\partial^n U(\overleftrightarrow{\eta}, \vec{\overline{w}}^{\alpha}=0)}{\partial\eta_{ij}\,\partial\eta_{kl}\cdots}\right)_{\overleftrightarrow{\eta}=0} \ . \tag{A12}$$