

$$\Omega_0^{1/3} U^{(\nu\rho)} = -\frac{Z^2 e^2}{2\Omega_0^{4/3}} \frac{2\partial_\nu}{s} \left[\sigma^{1/2} \sum_{l\mu\neq\nu} \partial_\mu (2\pi\sigma) r_\rho \Phi_{+1/2} (\sigma\pi|\vec{r}|^2) + \sum_h \text{Im}\kappa(\vec{g}, \nu) (2\pi\sigma^{-1}) g_\rho \Phi_0 (\sigma^{-1}\pi|\vec{g}|^2) \right], \quad (27)$$

$$\Omega_0^{1/3} U_{ij}^{(\nu\rho)} = \frac{Z^2 e^2}{2\Omega_0^{4/3}} \frac{2\partial_\nu}{s} \left\{ \sigma^{1/2} \sum_{l\mu\neq\nu} \partial_\mu (2\pi\sigma)^2 r_\rho r_i r_j \Phi_{+3/2} (\sigma\pi|\vec{r}|^2) + \sum_h \text{Im}\kappa(\vec{g}, \nu) [(2\pi\sigma^{-1}) g_q X_{q\rho ij} \Phi_0 (\sigma^{-1}\pi|\vec{g}|^2) - (2\pi\sigma^{-1})^2 g_\rho g_i g_j \Phi_1 (\sigma^{-1}\pi|\vec{g}|^2)] \right\}, \quad (28)$$

$$\Omega_0^{2/3} U^{(\nu\rho)(\nu q)} = \frac{Z^2 e^2}{2\Omega_0^{4/3}} \frac{2\partial_\nu}{s} \left\{ \sigma^{1/2} \sum_{l\mu\neq\nu} \partial_\mu [(2\pi\sigma)^2 r_\rho r_q \Phi_{+3/2} (\sigma\pi|\vec{r}|^2) - (2\pi\sigma) \delta_{\rho q} \Phi_{+1/2} (\sigma\pi|\vec{r}|^2)] - \sigma \sum_h \text{Re}\kappa(\vec{g}, \nu) - \partial_\nu/s \right\} (2\pi\sigma^{-1})^2 g_\rho g_q \Phi_0 (\sigma^{-1}\pi|\vec{g}|^2), \quad (29)$$

$$\Omega_0^{2/3} U^{(\nu\rho)(\mu q)} = \Omega_0^{2/3} U^{(\mu\rho)(\nu q)} = \frac{-Z^2 e^2}{2\Omega_0^{4/3}} \frac{2\partial_\nu \partial_\mu}{s} \left\{ \sigma^{1/2} \sum_l [(2\pi\sigma)^2 r_\rho r_q \Phi_{+3/2} (\sigma\pi|\vec{r}|^2) - (2\pi\sigma) \delta_{\rho q} \Phi_{+1/2} (\sigma\pi|\vec{r}|^2)] - \sigma \sum_h (1/s) \cos(2\pi\vec{g} \cdot \vec{t}) (2\pi\sigma^{-1})^2 g_\rho g_q \Phi_0 (\sigma^{-1}\pi|\vec{g}|^2) \right\}, \quad (30)$$

$$\Omega_0^{1/3} U_{ijkl}^{(\nu\rho)} = -\frac{Z^2 e^2}{2\Omega_0^{4/3}} \frac{2\partial_\nu}{s} \left\{ \sigma^{1/2} \sum_{l\mu\neq\nu} \partial_\mu (2\pi\sigma)^3 r_\rho r_i r_j r_k r_l \Phi_{+5/2} (\sigma\pi|\vec{r}|^2) + \sum_h \text{Im}\kappa(\vec{g}, \nu) [(2\pi\sigma^{-1}) g_q X_{q\rho ijkl} \Phi_0 (\sigma^{-1}\pi|\vec{g}|^2) - \frac{1}{3} (2\pi\sigma^{-1})^2 g_q (Y_{q\rho ijkl} - |\vec{g}|^2 X_{q\rho ijkl}) \Phi_1 (\sigma^{-1}\pi|\vec{g}|^2) + (2\pi\sigma^{-1})^3 g_\rho g_i g_j g_k g_l \Phi_2 (\sigma^{-1}\pi|\vec{g}|^2)] \right\}, \quad (31)$$

$$\Omega_0^{2/3} U_{ij}^{(\nu\rho)(\nu q)} = -\frac{Z^2 e^2}{2\Omega_0^{4/3}} \frac{2\partial_\nu}{s} \left\{ \sigma^{1/2} \sum_{l\mu\neq\nu} \partial_\mu [(2\pi\sigma)^3 r_\rho r_q r_i r_j \Phi_{+5/2} (\sigma\pi|\vec{r}|^2) - (2\pi\sigma)^2 \delta_{\rho q} r_i r_j \Phi_{+3/2} (\sigma\pi|\vec{r}|^2) - (2\pi\sigma) (\delta_{\rho i} \delta_{qj} + \delta_{\rho j} \delta_{qi}) \Phi_{+1/2} (\sigma\pi|\vec{r}|^2)] - \sigma \sum_h (\text{Re}\kappa(\vec{g}, \nu) - \partial_\nu/s) \times [(2\pi\sigma^{-1})^2 (Y_{\rho q ij} - \delta_{\rho q} g_i g_j) \Phi_0 (\sigma^{-1}\pi|\vec{g}|^2) - (2\pi\sigma^{-1})^3 g_\rho g_q g_i g_j \Phi_1 (\sigma^{-1}\pi|\vec{g}|^2)] \right\}, \quad (32)$$

$$\Omega_0^{2/3} U_{ij}^{(\nu\rho)(\mu q)} = \Omega_0^{2/3} U_{ij}^{(\mu\rho)(\nu q)} = \frac{Z^2 e^2}{2\Omega_0^{4/3}} \frac{2\partial_\nu \partial_\mu}{s} \left\{ \sigma^{1/2} \sum_l [(2\pi\sigma)^3 r_\rho r_q r_i r_j \Phi_{+5/2} (\sigma\pi|\vec{r}|^2) - (2\pi\sigma)^2 \delta_{\rho q} r_i r_j \Phi_{+3/2} (\sigma\pi|\vec{r}|^2) - (2\pi\sigma) (\delta_{\rho i} \delta_{qj} + \delta_{\rho j} \delta_{qi}) \Phi_{+1/2} (\sigma\pi|\vec{r}|^2)] - \sigma \sum_h (1/s) \cos(2\pi\vec{g} \cdot \vec{t}) [(2\pi\sigma^{-1})^2 (Y_{\rho q ij} - \delta_{\rho q} g_i g_j) \Phi_0 (\sigma^{-1}\pi|\vec{g}|^2) - (2\pi\sigma^{-1})^3 g_\rho g_q g_i g_j \Phi_1 (\sigma^{-1}\pi|\vec{g}|^2)] \right\}, \quad (33)$$

$$\Omega_0 U^{(\nu\rho)(\nu q)(\nu m)} = \frac{-Z^2 e^2}{2\Omega_0^{4/3}} \frac{2\partial_\nu}{s} \left\{ \sigma^{1/2} \sum_{l\mu\neq\nu} \partial_\mu [(2\pi\sigma)^3 r_\rho r_q r_m \Phi_{+5/2} (\sigma\pi|\vec{r}|^2) - (2\pi\sigma)^2 r_n X_{n\rho qm} \Phi_{+3/2} (\sigma\pi|\vec{r}|^2)] - \sigma^2 \sum_h \text{Im}\kappa(\vec{g}, \nu) (2\pi\sigma^{-1})^3 g_\rho g_q g_m \Phi_0 (\sigma^{-1}\pi|\vec{g}|^2) \right\}, \quad (34)$$

$$\Omega_0 U^{(\nu\rho)(\nu q)(\mu m)} = -\Omega_0 U^{(\mu\rho)(\mu q)(\nu m)} = \frac{Z^2 e^2}{2\Omega_0^{4/3}} \frac{2\partial_\nu \partial_\mu}{s} \left\{ \sigma^{1/2} \sum_l [(2\pi\sigma)^3 r_\rho r_q r_m \Phi_{+5/2} (\sigma\pi|\vec{r}|^2) - (2\pi\sigma)^2 r_n X_{n\rho qm} \Phi_{+3/2} (\sigma\pi|\vec{r}|^2)] - (2\pi\sigma)^2 r_n X_{n\rho qm} \Phi_{+3/2} (\sigma\pi|\vec{r}|^2) - \sigma^2 \sum_h (1/s) \sin(2\pi\vec{g} \cdot \vec{t}) (2\pi\sigma^{-1})^3 g_\rho g_q g_m \Phi_0 (\sigma^{-1}\pi|\vec{g}|^2) \right\}, \quad (35)$$

and

$$\Omega_0 U^{(\nu\rho)(\mu q)(\xi m)} = 0, \quad (36)$$

where $\nu \neq \mu \neq \xi$ and

$$\kappa(\vec{G}, \nu) = S(\vec{G}) e^{i\vec{G} \cdot \vec{r}(\nu)}. \quad (37)$$

These internal-strain derivatives are similar to elastic constants in that they transform as tensors

for any point-group operation (e.g., $U_{ij}^{(\nu\rho)*} = \mathbb{R}_{\rho q} \mathbb{R}_{ik} \mathbb{R}_{jl} U_{kl}^{(\nu q)}$, where \mathbb{R} is a point-group symmetry element). However, for those space-group operations which contain a rigid translation, e.g., screw axes or glide planes, the unit-cell label ν

also may change. An important consequence of this is that $U_{ij}^{(pp)}$, and thus the internal-strain parameter

$$A_{p,ij}(\nu) = \left(\frac{\partial \bar{w}_p(\nu)}{\partial \eta_{ij}} \right) \Big|_{\bar{\eta}=0, \bar{w}=0},$$

need not have the same symmetry as the piezoelectric tensor. An example of this is seen later when considering the wurtzite structure. Also, it is easily seen that these electrostatic derivatives obey the following relations: $U_{ij}^{(pp)}$, $U_{ij}^{(pp)(\mu q)}$, $U_{ijkl}^{(pp)}$, and $U_{ij}^{(pp)(\mu q)(\lambda m)}$ satisfy Cauchy relations in that the Cartesian indices can be arranged in any order (e.g., $U_{ij}^{(pp)} = U_{ji}^{(pp)}$); and $U_{ij}^{(pp)(\mu q)}$ is symmetric with respect to the interchanges $p \rightarrow q$ and $i \rightarrow j$.

Because the energy density depends on relative interlattice displacements, only $s-1$ of the s internal strains $\bar{w}(\nu)$ are independent.¹⁷ Thus, one may choose any independent set of internal strains \bar{w}^α ($\alpha=1, \dots, s-1$), which are linear combinations of the $\bar{w}(\nu)$,

$$\bar{w}^\alpha = \sum_{\nu=0}^{s-1} a_{\alpha\nu} \bar{w}(\nu).$$

Then, derivatives are related by

$$\frac{\partial}{\partial \bar{w}(\nu)} = \sum_{\alpha=1}^{s-1} a_{\alpha\nu} \frac{\partial}{\partial \bar{w}^\alpha}.$$

Internal strains only occur in nonprimitive lattices with ions not at centers of symmetry. Thus, of the 11 structures considered earlier, only five (diamond, zinc blende, hcp, WC, and wurtzite) can have an internal-strain contribution to the elastic constants. Because the diamond and zinc-blende lattices differ only in the sign of the ionic charges, they may be considered together. The same applies for the hcp and WC lattices. However, since the wurtzite structure consists of two interpenetrating hcp sublattices, the hcp and WC structures can be obtained from wurtzite by a suitable choice of charges. Thus, it is convenient to consider hcp and WC with wurtzite.

The zinc-blende and diamond structures have a fcc Bravais lattice with basis vectors $\vec{\tau}(0) = (0, 0, 0)$ and $\vec{\tau}(1) = (\frac{1}{4}a)(1, 1, 1)$. To form the two structures, the signs of the charges in the unit cell are chosen as $\delta_0 = +1$ and $\delta_1 = -1(+1)$ for the ionic zinc-blende (metallic diamond) structure. For structures with two ions per unit cell, there is only one independent internal strain. Here it has been chosen as

$$\bar{w} = [\vec{w}(1) - \vec{w}(0)] / (\frac{1}{4}a),$$

and thus

$$\frac{\partial}{\partial w_p} = \frac{1}{4}a \frac{\partial}{\partial w_p(1)} = -\frac{1}{4}a \frac{\partial}{\partial w_p(0)}.$$

Then, the independent electrostatic internal-strain derivatives for zinc blende with Cauchy relations are

$$\begin{aligned} U_4^1 &= -10.057668147, & U_1^{11} &= 0.819616921, \\ U^{11} &= -4.188790205, & U_2^{11} &= 10.062167052, \\ U^{123} &= 19.202879707, & U_4^{23} &= 14.250957256, \\ U_{14}^1 &= U_{24}^1 = U_{56}^1 = 16.762780245, \end{aligned}$$

in units of $Z^2 e^2 / a^4$. (The notation used here is that of Appendix A, with Voigt notation used for all subscripts.) Since the electrostatic internal-strain derivatives are proportional to $\delta_0 \delta_1$ for structures with two ions per unit cell, the results for the diamond structure are negative those of zinc blende.

The hcp, WC, and wurtzite structures have a simple hexagonal Bravais lattice with basis vectors

$$\begin{aligned} \vec{\tau}(0) &= (0, 0, 0), & \vec{\tau}(1) &= (a/\sqrt{3}, 0, \frac{1}{2}c), \\ \vec{\tau}(2) &= (0, 0, uc), & \vec{\tau}(3) &= (a/\sqrt{3}, 0, [u + \frac{1}{2}]c) \end{aligned}$$

referred to the Cartesian axes. The three structures can be formed by choosing the signs of the charges in the unit cell as follows: For metallic hcp (ionic WC) $\delta_0 = +1$, $\delta_1 = +1(-1)$, and $\delta_2 = \delta_3 = 0$; and for ionic wurtzite $\delta_0 = \delta_1 = +1$ and $\delta_2 = \delta_3 = -1$. The three independent internal strains will be taken as

$$\bar{w}^1 = [\vec{w}(1) - \vec{w}(0)] / L, \quad \bar{w}^2 = [\vec{w}(3) - \vec{w}(2)] / L,$$

and

$$\bar{w}^3 = [\vec{w}(2) - \vec{w}(0)] / L,$$

where $L = \frac{1}{2}a\sqrt{3}$. The internal strains \bar{w}^1 and \bar{w}^2 represent the interlattice displacement in the two hcp sublattices, while \bar{w}^3 is an interlattice displacement between the two hcp sublattices. Then, internal-strain derivatives are taken according to

$$\frac{\partial}{\partial w_p^1} = L \left(\frac{\partial}{\partial w_p(1)} \right), \quad \frac{\partial}{\partial w_p^2} = L \left(\frac{\partial}{\partial w_p(3)} \right)$$

and

$$\begin{aligned} \frac{\partial}{\partial w_p^3} &= L \left[\left(\frac{\partial}{\partial w_p(2)} \right) + \left(\frac{\partial}{\partial w_p(3)} \right) \right] \\ &= -L \left[\left(\frac{\partial}{\partial w_p(0)} \right) + \left(\frac{\partial}{\partial w_p(1)} \right) \right]. \end{aligned}$$

It is easily seen that derivatives with respect to \bar{w}^2 and \bar{w}^3 are zero for hcp and WC, since internal-strain derivatives with respect to $\bar{w}(\nu)$ are proportional to δ_ν . Therefore, for these two structures, the internal-strain label will be omitted and understood to be $\alpha=1$. The electrostatic internal-strain derivatives for ideal hcp with Cauchy relations are