[3]B. I. Halperin and M. Lax, Phys. Rev. 148, 722 (1966).

[4]E. O. Kane, Phys. Rev. 131, 79 (1963).

[5]N. F. Mott, Advan. Phys. 16, 49 (1967).

[6]M. H. Cohen, H. Fritzsche, and S. R. Ovshinsky, Phys. Rev. Letters 22, 1065 (1969).

[7]M. H. Cohen, in *Proceedings of the Tenth International Conference on the Physics of Semiconductors, Cambridge, Mass.*, 1970 (U. S. AEC, Oak Ridge, Tenn., 1970).

[8]I. M. Lifshitz, Usp. Fiz. Nauk 83, 617 (1964) [Sov. Phys. Usp. 7, 549 (1965)].

[9]P. W. Anderson, Phys. Rev. 109, 1492 (1958).

[10]E. N. Economou and M. H. Cohen, Phys. Rev. B 5, 2931 (1972).

[11]E. N. Economou, S. Kirkpatrick, M. H. Cohen, and T. P. Eggarter, Phys. Rev. Letters 25, 520 (1970).

[12]W. Kohn and J. Olson, J. Phys. (Paris) (to be published).

[13]This Hamiltonian has received wide study by several formal techniques. For recent work, see L. Schwartz and E. Siggia, Phys. Rev. B 5, 383 (1972), and references therein.

[14]S. Kirkpatrick, B. Velický, and H. Ehrenreich, Phys. Rev. B 1, 3250 (1970), Appendix B.

[15]W. Miller, Phys. Rev. 152, 70 (1966).

[16]P. G. de Gennes, P. Lafore, and J. P. Millot, J. Phys. Chem. Solids 11, 105 (1959); J. Phys. Radium 20,

624 (1959).

[17]Y. Cho and Y. Toyozawa, J. Phys. Soc. Japan Suppl. 26, 71 (1969).

[18]S. R. Broadbent and J. M. Hammersley, Proc. Cambridge Phil. Soc. 53, 642 (1957); H. L. Frisch and J. M. Hammersley, J. Soc. Ind. Appl. Math. 11, 894 (1963).

[19]V. K. S. Shante and S. Kirkpatrick, Advan. Phys. 20, 325 (1971).

[20]For conditions under which this smoothness of the density of states is a rigorous conclusion, see J. T. Edwards and D. J. Thouless, J. Phys. C 4, 453 (1971).

[21]H. Matsuda, Progr. Theoret. Phys. (Kyoto) 31, 161 (1964); R. E. Borland, Proc. Phys. Soc. (London) 83, 1027 (1964).

[22]P. Dean and M. D. Bacon, Proc. Roy. Soc. (London) A283, 64 (1964).

[23]J. E. Gubernaitis and P. L. Taylor, J. Phys. C 4, L94 (1971).

[24]J. T. Edwards and D. J. Thouless, J. Phys. C 5, 807 (1972).

[25]G. Lucovsky, M. H. Brodsky, and E. Burstein, Phys. Rev. B 2, 3295 (1970).

[26]D. W. Feldman, M. Ashkin, and J. H. Parker, Jr., Phys. Rev. Letters 17, 1209 (1966); M. A. Renucci, B. Renucci, and M. Cardona, in *Light Scattering in Solids*, edited by M. Balkanski (Plenum, New York, 1971).

Electrostatic Contributions to the Brugger-Type Elastic Constants[*]

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A general method is presented for obtaining the electrostatic contributions to the first-, second-, and third-order Brugger-type elastic constants of metallic and ionic structures. The electrostatic energy per unit initial volume of a homogeneously deformed lattice is determined by the Ewald—Fuchs method. General equations for the Brugger elastic constants are found by taking Lagrangian strain derivatives of this energy expression. Internal-strain contributions, which occur for nonprimitive structures, have been included. Results are tabulated for six metallic and five ionic structures.

I. INTRODUCTION

Electrostatic contributions can be an important part of any model calculation of elastic constants. Since these contributions are constant for a given structure, it seems appropriate to calculate and tabulate them for various ionic and metallic structures. General expressions, which are valid for any crystalline structure, are presented for the electrostatic contribution to the Brugger-type elastic constants. Also given are general expressions for electrostatic internal-strain derivatives, from which the internal-strain contribution to the Brugger-type elastic constants can be obtained. Specific results are tabulated for six metallic and five ionic structures. Whereas some

of these tabulated results have been reported elsewhere, this paper serves to increase the accuracy of earlier work, as well as unify all results.

For metallic structures, the first important results were those of Fuchs.[1,2] He calculated the two Fuchs-type second-order elastic shear constants for bcc and fcc metals. By extending Fuchs's method, Cousins[3] obtained the second- and third-order shear constants for bcc and fcc metals. More recently, Cousins[4,5] calculated the first-, second-, and third-order elastic constants of hcp metals for various c/a ratios. Instead of calculating the Fuchs-type elastic constants, which are linear combinations of the Brugger elastic constants, Suzuki *et al.*[6] directly cal-

culated the electrostatic contributions to the second- and third-order Brugger elastic constants of bcc metals. For ionic structures, Ghate[7] has calculated the electrostatic contributions to the third-order Brugger elastic constants for NaCl- and CsCl-type structures, and Blackman[8] has calculated the second-order electrostatic contributions, including internal strains, for the zinc-blende structure. In addition to a recalculation of the results cited above, the new results tabulated in this paper are the first-, second-, and third-order elastic constants of the wurtzite, WC-type, diamond, simple cubic, and simple hexagonal structures; the third-order elastic constants of zinc blende; and the internal-strain derivatives, through third order, for the zinc-blende, diamond, hcp, WC-type, and wurtzite structures.

The Ewald–Fuchs method for determining the electrostatic energy will be discussed in Sec. II. General expressions[9] for the Brugger-type elastic constants and tabular results will be presented in Sec. III. An explanation of internal strains and their contributions to the elastic constants will follow in Sec. IV.

II. EWALD-FUCHS METHOD

The electrostatic energy, per unit initial volume, of a homogeneously deformed lattice of ions is

$$U'_{11} = \left(\frac{Z^2 e^2}{2\Omega_0 \lambda}\right) \frac{1}{s} \sum_{l\nu\mu}{}' \left(\frac{\mathfrak{z}_\nu \mathfrak{z}_\mu \lambda}{|\vec{R}'\binom{l0}{\nu\mu}|}\right) \quad . \tag{1}$$

Ω_0 is the volume per ion of the undeformed state, e the electronic charge, and s the number of ions per unit cell. The summations over l and ν, μ (ν, $\mu = 0, 1, \ldots, s-1$) are sums over the Bravais lattice and unit cell, respectively. The prime on the summation means the $l = 0$, $\nu = \mu$ term is excluded from the sum. $\vec{R}\binom{lk}{\nu\mu}$ is defined as

$$\vec{R}\binom{lk}{\nu\mu} = \vec{R}\binom{l}{\nu} - \vec{R}\binom{k}{\mu} = [\vec{R}(l) + \vec{\tau}(\nu)] - [\vec{R}(k) + \vec{\tau}(\mu)] , \tag{2}$$

where $\vec{R}(l)$ is a Bravais lattice vector and $\vec{\tau}(\nu)$ is the basis vector of the νth ion in the unit cell. Throughout this paper, primed quantities, such as $\vec{R}'\binom{l0}{\nu\mu}$, will refer to the deformed state. $\mathfrak{z}_\nu$ is the sign of the ionic charge, i.e., the charge of the νth ion is $\mathfrak{z}_\nu Ze$. The parameter λ is introduced in Eq. (1) to make the summand dimensionless. Different choices for the value of λ will be discussed later.

For a given crystal structure the summation in Eq. (1) can be readily performed, but the convergence is extremely slow. A useful technique for more rapid convergence is the method originally devised by Ewald[10] for ionic lattices and extended to metals by Fuchs.[11] The following is a brief description of the Ewald–Fuchs method.

Using the definition of the Γ function, one has

$$1/x^n = [1/\Gamma(n)] \int_0^\infty dt \, t^{n-1} e^{-xt} . \tag{3}$$

By splitting the integral into two parts, one from 0 to $\pi\sigma$ and the other from $\pi\sigma$ to ∞, it follows that

$$\sum_l{}' \frac{\lambda}{|\vec{R}'\binom{l0}{\nu\mu}|} = \sum_l{}' \left(\frac{|\vec{R}'\binom{l0}{\nu\mu}|^2}{\lambda^2}\right)^{-1/2}$$

$$= \sigma^{1/2} \sum_l{}' \Phi_{-1/2}\left(\frac{\sigma\pi|\vec{R}'\binom{l0}{\nu\mu}|^2}{\lambda^2}\right)$$

$$+ \int_0^\sigma dt \, t^{-1/2}\left[\sum_l \exp\left(\frac{-\pi|\vec{R}'\binom{l0}{\nu\mu}|^2 t}{\lambda^2}\right) - \delta_{\nu\mu}\right], \tag{4}$$

where

$$\Phi_m(x) = \int_1^\infty dt \, t^m e^{-xt} . \tag{5}$$

The θ-function transformation for a (Bravais) deformed lattice is

$$\sum_l \exp\left[-\pi|\vec{R}'(l) + \vec{x}|^2 y^2\right]$$

$$= \frac{y^{-3}}{s\Omega'_0} \sum_h \exp[-i\vec{G}'(h)\cdot\vec{x}] \exp\left(\frac{-|\vec{G}'(h)|^2}{4\pi y^2}\right), \tag{6}$$

where the $\vec{G}'(h)$ vectors form the reciprocal lattice of the deformed real lattice and Ω'_0 is the volume per ion of the deformed state. Using this transformation and defining a structure factor as

$$S'(\vec{G}') = (1/s)\sum_\nu \mathfrak{z}_\nu e^{-i\vec{G}'\cdot\vec{\tau}'(\nu)} , \tag{7}$$

it can be shown that

$$U'_{11} = \frac{Z^2 e^2}{2\Omega_0 \lambda}\left[\sigma^{1/2}\frac{1}{s}\sum_{l\nu\mu}{}' \mathfrak{z}_\nu \mathfrak{z}_\mu \Phi_{-1/2}\left(\frac{\sigma\pi|\vec{R}'\binom{l0}{\nu\mu}|^2}{\lambda^2}\right)\right.$$

$$+ \sigma^{-1}\frac{\lambda^3}{\Omega'_0}\sum_h{}' |S'(\vec{G}'(h))|^2 \Phi_0\left(\frac{\lambda^2|\vec{G}'(h)|^2}{4\pi\sigma}\right)$$

$$\left. - 2\sigma^{1/2}\langle\mathfrak{z}^2\rangle + \sigma^{-1}\frac{\lambda^3}{\Omega'_0}\langle\mathfrak{z}\rangle^2 D\right] , \tag{8}$$

where

$$\langle\mathfrak{z}^2\rangle = (1/s)\sum_\nu \mathfrak{z}_\nu^2, \quad \langle\mathfrak{z}\rangle = (1/s)\sum_\nu \mathfrak{z}_\nu ,$$

and

$$D = \int_0^1 dt \, t^{-2} .$$

It should be noted that, owing to the integral D, U'_{11} diverges unless the average charge per unit cell $\langle\mathfrak{z}\rangle$ is zero. For ionic structures this is the case, and U'_{11} by itself represents the electrostatic energy density. For metallic structures $\langle\mathfrak{z}\rangle \neq 0$, and U'_{11} is divergent. However, the electrostatic energy density of metals consists not

only of U'_{ii}, but also of ion-electron and electron-electron interactions, to be denoted by U'_{ie} and U'_{ee}, respectively. For a metal, the jellium model (a lattice of positive point ions embedded in a uniform sea of electrons) will be used here. This is the model used for the electrostatic energy in the pseudopotential theory of metals.[12] Denoting the uniform electron density by n_0 $= Z \langle \mathfrak{z} \rangle / \Omega_0$, it follows that

$$U'_{ie} + U'_{ee} = - \frac{Ze^2}{\lambda \Omega_0} \frac{1}{sN_{cell}}$$

$$\times \sum_{l\nu} \mathfrak{z}_\nu \int_{\Omega'} d^3 x' \frac{n'_0 \lambda}{|\vec{x}' - \vec{R}'\binom{l}{\nu}|}$$

$$+ \frac{e^2}{2\lambda \Omega_0} \frac{1}{sN_{cell}} \int_{\Omega'} d^3 y' \int_{\Omega'} d^3 x' \frac{(n'_0)^2 \lambda}{|\vec{y}' - \vec{x}'|} ,$$

$$(9)$$

where N_{cell} is the number of unit cells. Changing variables of integration leads to $U'_{ie} = - 2U'_{ee}$, and then using the Γ-function definition, it follows that[13]

$$U'_{ie} + U'_{ee} = - U'_{ee} = - \frac{Z^2 e^2}{2\lambda \Omega_0} \sigma^{-1} \left(\frac{\lambda^3}{\Omega_0'} \right) \langle \mathfrak{z} \rangle^2 (1 + D) .$$

$$(10)$$

Thus, the electrostatic energy density U'_{es} for both metallic and ionic structures may be written

$$U'_{es} = \frac{Z^2 e^2}{2\Omega_0 \lambda} \left[\sigma^{1/2} \frac{1}{s} {\sum_{l\nu\mu}}' \mathfrak{z}_\nu \mathfrak{z}_\mu \Phi_{-1/2} \left(\frac{\sigma \pi |\vec{R}'\binom{l0}{\nu\mu}|^2}{\lambda^2} \right) \right.$$

$$+ \sigma^{-1} \frac{\lambda^3}{\Omega_0'} {\sum_h}' |S'(\vec{G}'(h))|^2 \Phi_0 \left(\frac{\lambda^2 |\vec{G}'(h)|^2}{4\pi\sigma} \right)$$

$$\left. - 2\sigma^{1/2} \langle \mathfrak{z}^2 \rangle - \sigma^{-1} \frac{\lambda^3}{\Omega_0'} \langle \mathfrak{z} \rangle^2 \right] , \quad (11)$$

remembering that $\langle \mathfrak{z} \rangle = 0$ for ionic structures. The parameter σ is a convergence parameter and is usually chosen so that the real-lattice and reciprocal-lattice sums converge at about the same rate. However, results are independent of the choice for σ.

There are two choices for the parameter λ which are of particular interest here. For $\lambda = (\Omega_0')^{1/3}$, all the strained-volume dependence of U'_{es} is contained in the $(1/\Omega_0')^{1/3}$ factor outside of the square bracket in Eq. (11), and the square bracket contains only volume-conserving shear dependence. This choice is convenient for taking Fuchs-type strain derivatives of U'_{es}. The second choice, and the one to be used throughout this paper, is $\lambda = (\Omega_0)^{1/3}$. This choice is convenient for differentiating U'_{es} with respect to the Lagrangian strain parameters,

$$\eta_{ij} = \tfrac{1}{2}(J_{ki} J_{kj} - \delta_{ij}) , \quad (12)$$

where repeated indices are to be summed and δ_{ij} is the Kronecker δ. The transformation coefficients are given by

$$J_{ij} = \frac{\partial x'_i}{\partial x_j} , \quad (13)$$

where $\vec{x}$ and $\vec{x}'$ are the position vectors of a material particle in the initial and deformed states, respectively. Derivatives of U'_{es} with respect to η_{ij} give directly the electrostatic contributions to the Brugger-type elastic constants, which will be discussed in Sec. III.

By performing the appropriate lattice and reciprocal-lattice sums in Eq. (11), the electrostatic energy for any given metallic or ionic structure can be obtained. For metallic structures, the electrostatic energy per ion is usually written in the form

$$E_{es} (\text{per ion}) = \Omega_0 U_{es} = \alpha_a \left(\frac{Z^2 e^2}{a} \right) = \alpha_0 \left(\frac{Z^2 e^2}{2r_0} \right) , \quad (14)$$

where a is the lattice constant and r_0 is the radius of the ionic sphere, given by $\tfrac{4}{3} \pi r_0^3 = \Omega_0$. Similarly for ionic structures, the electrostatic energy per molecule is written

$$E_{es} (\text{per molecule}) = 2\Omega_0 U_{es} = \alpha_a \left(\frac{Z^2 e^2}{a} \right)$$

$$= \alpha_R \left(\frac{Z^2 e^2}{R} \right) , \quad (15)$$

where R is the nearest-neighbor distance. The α coefficients entering in Eqs. (14) and (15) are known as geometric coefficients when referring to metals, and as Madelung constants when referring to ionic structures. We have evaluated these coefficients for six metallic and five ionic structures and have listed the results in Table I. For those structures involving a c/a ratio, the evaluations were performed for the case of ideal close packing of spheres, i.e., $c/a = 1$ for the simple hexagonal structure, and $c/a = \sqrt{\tfrac{8}{3}}$ for the hcp and WC-type structures. For the wurtzite structure, $c/a = \sqrt{\tfrac{8}{3}}$ and $u = \tfrac{3}{8}$, which gives equal bond lengths and bond angles.

III. GENERAL EXPRESSIONS FOR BRUGGER ELASTIC CONSTANTS

Having determined the electrostatic energy density of a deformed lattice, one can now calculate the electrostatic contributions to the elastic constants by the method of homogeneous deformation. Since internal-strain effects may be treated separately (see Appendix A), here we will only consider the case of zero internal strain, i.e., $\vec{w} = 0$. Internal-strain contributions to the elastic constants will be treated in Sec. IV. The Lagrangian strain derivatives of U'_{es} can be easily performed

(see Appendix B), thus yielding the electrostatic Brugger elastic constants

$$C_{ijkl\cdots}^{es} \equiv \left(\frac{\partial^n U_{es}'(\vec{\eta}, \vec{w}=0)}{\partial\eta_{ij}\,\partial\eta_{kl}\cdots} \right)_{\vec{\eta}=0} . \qquad (16)$$

Introducing the dimensionless parameters $\vec{r} = \vec{R}(_{\nu\mu}^{l0})/\Omega_0^{1/3}$ and $\vec{g} = \Omega_0^{1/3}\vec{G}(h)/2\pi$, the expressions for the first-, second-, and third-order elastic constants are

$$C_{ij}^{es} = -\frac{Z^2 e^2}{2\Omega_0^{4/3}} \Big\{ \sigma^{1/2}(1/s) \sum_{l\nu\mu}{}' \mathfrak{z}_\nu\mathfrak{z}_\mu (2\pi\sigma)\, r_i r_j\, \Phi_{+1/2}\,(\sigma\pi|\vec{r}|^2)$$

$$+ \sigma^{-1} \sum_h{}' |S(\vec{g})|^2 [X_{ij}\,\Phi_0\,(\sigma^{-1}\pi|\vec{g}|^2) - (2\pi\sigma^{-1})g_i g_j\,\Phi_{+1}(\sigma^{-1}\pi|\vec{g}|^2)] - \sigma^{-1}\langle\mathfrak{z}\rangle^2 X_{ij} \Big\} , \qquad (17)$$

$$C_{ijkl}^{es} = \frac{Z^2 e^2}{2\Omega_0^{4/3}} \Big\{ \sigma^{1/2}(1/s) \sum_{l\nu\mu}{}' \mathfrak{z}_\nu\mathfrak{z}_\mu (2\pi\sigma)^2\, r_i r_j r_k r_l\, \Phi_{+3/2}\,(\sigma\pi|\vec{r}|^2) + \sigma^{-1} \sum_h{}' |S(\vec{g})|^2 [X_{ijkl}\,\Phi_0(\sigma^{-1}\pi|\vec{g}|^2)$$

$$- (2\pi\sigma^{-1})\, Y_{ijkl}\,\Phi_{+1}\,(\sigma^{-1}\pi|\vec{g}|^2) + (2\pi\sigma^{-1})^2\, g_i g_j g_k g_l\,\Phi_{+2}\,(\sigma^{-1}\pi|\vec{g}|^2)] - \sigma^{-1}\langle\mathfrak{z}\rangle^2 X_{ijkl} \Big\} , \qquad (18)$$

and

$$C_{ijklmn}^{es} = \frac{-Z^2 e^2}{2\Omega_0^{4/3}} \Big\{ \sigma^{1/2}(1/s) \sum_{l\nu\mu}{}' \mathfrak{z}_\nu\mathfrak{z}_\mu (2\pi\sigma)^3\, r_i r_j r_k r_l r_m r_n\, \Phi_{+5/2}(\sigma\pi|\vec{r}|^2)$$

$$+ \sigma^{-1} \sum_h{}' |S(\vec{g})|^2 [\, X_{ijklmn}\Phi_0(\sigma^{-1}\pi|\vec{g}|^2) - (2\pi\sigma^{-1})Y_{ijklmn}\Phi_{+1}(\sigma^{-1}\pi|\vec{g}|^2) + (2\pi\sigma^{-1})^2\, Z_{ijklmn}\Phi_{+2}(\sigma^{-1}\pi|\vec{g}|^2)$$

$$- (2\pi\sigma^{-1})^3\, g_i g_j g_k g_l g_m g_n\,\Phi_{+3}\,(\sigma^{-1}\pi|\vec{g}|^2)] - \sigma^{-1}\langle\mathfrak{z}\rangle^2 X_{ijklmn} \Big\} , \qquad (19)$$

where

$$X_{ij} = \delta_{ij} , \qquad (20)$$

$$X_{ijkl} = \delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} , \qquad (21)$$

$$Y_{ijkl} = g_i g_j \delta_{kl} + g_k g_l \delta_{ij} + g_i g_k \delta_{jl}$$

$$+ g_i g_l \delta_{jk} + g_j g_k \delta_{il} + g_j g_l \delta_{ik} , \qquad (22)$$

$$X_{ijklmn} = \delta_{ij} X_{klmn} + \delta_{ik} X_{jlmn} + \delta_{il} X_{jkmn}$$

$$+ \delta_{im} X_{kljn} + \delta_{in} X_{kljm} , \qquad (23)$$

$$Y_{ijklmn} = g_i g_j X_{klmn} + g_i g_k X_{jlmn} + g_i g_l X_{jkmn} + g_i g_m X_{kljn}$$

$$+ g_i g_n X_{kljm} + g_j g_k X_{ilmn} + g_j g_l X_{ikmn} + g_j g_m X_{klin}$$

$$+ g_j g_n X_{kliim} + g_k g_l X_{ijmn} + g_k g_m X_{ijln} + g_k g_n X_{ijlm}$$

$$+ g_l g_m X_{ijkn} + g_l g_n X_{ijkm} + g_m g_n X_{ijkl} , \qquad (24)$$

and

$$Z_{ijklmn} = g_i g_j (Y_{klmn} - g_k g_l \delta_{mn}) + g_k g_l (Y_{mnij} - g_m g_n \delta_{ij})$$

$$+ g_m g_n (Y_{ijkl} - g_i g_j \delta_{kl}) . \qquad (25)$$

It is easily seen that the coefficients $X_{ij}\ldots$, $Y_{ijkl}\ldots$, and Z_{ijklmn}, and thus the elastic constants $C_{ij}^{es}\ldots$, satisfy Cauchy relations, i.e., the ordering of the subscripts is immaterial. Therefore, in general, all the elastic constants (through third order) can be obtained from only two types of first-order constants C_{II}^{es} and C_{JK}^{es}; four types of second-order constants C_{IIII}^{es}, C_{IIJJ}^{es}, C_{JJJK}^{es}, and C_{IIJK}^{es}; and seven types of third-order constants C_{IIIIII}^{es},

C_{IIIIJJ}^{es}, C_{IIJJKK}^{es}, C_{JJJJJK}^{es}, C_{JJJKKK}^{es}, C_{IIIIJK}^{es}, and C_{IIJJJK}^{es}, where the subscripts run from 1 to 3 with $I \neq J \neq K$. For these types, the elastic constants with Cauchy relations have been listed in Table II. In that table, as well as the remainder of this paper, Voigt (reduced) notation is used for the subscripts whenever referring to specific

TABLE I. Geometric coefficients for six metallic structures and Madelung constants for five ionic structures. For metals, the electrostatic energy per ion is $\alpha_a(Z^2 e^2/a) = \alpha_0(Z^2 e^2/2r_0)$, where a is the lattice constant and r_0 is the radius of the ionic sphere. For the ionic structures, the electrostatic energy per molecule is $\alpha_a(Z^2 e^2/a) = \alpha_R(Z^2 e^2/R)$, where R is the nearest-neighbor distance.

Metallic	α_a	α_0
simple cubic	−1.418 648 7397	−1.760 118 8842
fcc	−2.292 431 0371	−1.791 747 2304
bcc	−1.819 616 7248	−1.791 858 5114
diamond	−2.693 399 0221	−1.670 851 4055
simple hexagonal	−1.497 855 9763	−1.771 389 4740
hcp	−1.620 929 3075	−1.791 676 2409

Ionic	α_a	α_R
NaCl type	−3.495 129 1893	−1.747 564 5946
CsCl type	−2.035 361 5095	−1.762 674 7731
zinc blende	−3.782 926 1041	−1.638 055 0534
WC type	−1.235 585 6381	−1.235 585 6381
wurtzite	−2.680 266 9939	−1.641 321 6274

TABLE II. General Cauchy relations for first-, second-, and third-order elastic constants. Also listed are coefficients used in the general expressions for the elastic constants.

Types $ijklmn$	Elastic constants with Cauchy relations $C_{ij}...$	$X_{ij}...$	$Y_{ijkl}...$	Z_{ijklmn}
	First order			
II	C_1, C_2, C_3	1		
JK	C_4, C_5, C_6	0		
	Second order			
IIII	C_{11}, C_{22}, C_{33}	3	$6g_I^2$	
IIJJ	$C_{12}=C_{66}, C_{13}=C_{55}, C_{23}=C_{44}$	1	$g_I^2+g_J^2$	
JJJK	$C_{15}, C_{16}, C_{24}, C_{26}, C_{34}, C_{35}$	0	$3g_Jg_K$	
IIJK	$C_{14}=C_{56}, C_{25}=C_{46}, C_{36}=C_{45}$	0	g_Jg_K	
	Third order			
IIIIII	$C_{111}, C_{222}, C_{333}$	15	$45g_I^2$	$15g_I^4$
IIIIJJ	$C_{112}=C_{166}, C_{113}=C_{155}, C_{122}=C_{266}$ $C_{133}=C_{355}, C_{223}=C_{244}, C_{233}=C_{344}$	3	$6g_I^2+3g_J^2$	$g_I^4+6g_I^2g_J^2$
IIJJKK	$C_{123}=C_{144}=C_{255}=C_{366}=C_{456}$	1	$g_I^2+g_J^2+g_K^2$	$g_I^2g_J^2+g_J^2g_K^2+g_K^2g_I^2$
JJJJJK	$C_{115}, C_{116}, C_{224}, C_{226}, C_{334}, C_{335}$	0	$15g_Jg_K$	$10g_J^3g_K$
JJJKKK	$C_{126}=C_{666}, C_{135}=C_{555}, C_{234}=C_{444}$	0	$9g_Jg_K$	$3g_Jg_K(g_J^2+g_K^2)$
IIIIJK	$C_{114}=C_{156}, C_{225}=C_{246}, C_{336}=C_{345}$	0	$3g_Jg_K$	$6g_I^2g_Jg_K$
IIJJJK	$C_{125}=C_{146}=C_{566}, C_{124}=C_{256}=C_{466}$ $C_{134}=C_{356}=C_{455}, C_{136}=C_{145}=C_{556}$ $C_{235}=C_{346}=C_{445}, C_{236}=C_{245}=C_{446}$	0	$3g_Jg_K$	$g_Jg_K(3g_I^2+g_J^2)$

elastic constants. For convenience, the $X_{ij}...$, $Y_{ijkl}...$, and Z_{ijklmn} coefficients, which are used in Eqs. (17)–(19) to determine $C_{ij}^{es}...$, have also been listed.

Calculations have been completed for seven cubic structures, namely simple cubic, fcc, bcc, NaCl type, CsCl type, diamond, and zinc blende. The first-, second-, and third-order elastic constants with Cauchy relations for these structures are

$$C_1; \quad C_{11}, \quad C_{12}=C_{44};$$
and
$$C_{111}, \quad C_{112}=C_{155}, \quad C_{123}=C_{144}=C_{456}.$$

The electrostatic contributions to these constants

are listed in Table III in units of Z^2e^2/a^4, where a is the lattice parameter.

Four hexagonal structures, namely simple hexagonal, hcp, WC type, and wurtzite, have also been considered. For these structures, the elastic constants with Cauchy relations are

$$C_1, \quad C_3; \quad C_{11}, \quad C_{33}, \quad C_{12}=C_{66}=\tfrac{1}{3}C_{11}, \quad C_{13}=C_{44};$$
and
$$C_{111}, \quad C_{222}, \quad C_{112}=C_{166}=\tfrac{1}{5}(-2C_{111}+3C_{222}),$$

$$C_{122}=C_{266}=\tfrac{1}{5}(3C_{111}-2C_{222}),$$

$$C_{333}, \quad C_{113}=C_{155},$$

TABLE III. Electrostatic Brugger elastic constants for cubic structures. Entries are in units of Z^2e^2/a^4, where a is the lattice constant.

	simple cubic	fcc	bcc	NaCl type	CsCl type	diamond	zinc blende
U	−1.418 648 740	−9.169 724 148	−3.639 233 450	−13.980 516 757	−2.035 361 509	−21.547 192 177	−15.131 704 416
C_1	0.472 882 913	3.056 574 716	1.213 077 817	4.660 172 252	0.678 453 836	7.182 397 392	5.043 901 472
C_{11}	−0.143 189 083	−6.849 873 626	−2.697 885 714	−25.108 469 175	2.125 129 382	−23.345 777 443	−4.053 717 061
C_{12}	−0.637 729 828	−1.159 925 261	−0.470 673 868	5.563 976 209	−2.080 245 446	0.899 292 633	−5.538 993 678
C_{111}	−1.747 954 699	34.065 579 503	9.235 126 065	164.229 593 204	−16.226 944 863	119.055 300 863	17.207 017 149
C_{112}	1.231 950 057	0.091 894 314	2.127 151 252	−19.343 623 664	2.800 648 978	−1.163 206 824	1.530 784 079
C_{123}	0.724 749 027	5.615 837 678	−1.900 933 165	10.867 366 283	4.799 929 272	−2.170 049 518	24.633 400 230

TABLE IV. Electrostatic Brügger elastic constants for hexagonal structures with ideal structure parameters. Entries are in units of Z^2e^2/a^4, where a is the lattice constant.

	simple hexagonal $(c/a=1)$	hcp $(c/a=\sqrt{\tfrac{8}{3}})$	WC type $(c/a=\sqrt{\tfrac{8}{3}})$	wurtzite $(c/a=\sqrt{\tfrac{8}{3}}, \ u=\tfrac{3}{8})$
U	$-1.729\,575\,102$	$-2.292\,340\,210$	$-0.873\,690\,983$	$-3.790\,469\,934$
C_1	$0.533\,603\,351$	$0.764\,635\,593$	$-0.577\,163\,952$	$1.237\,266\,468$
C_3	$0.662\,368\,399$	$0.763\,069\,024$	$2.028\,018\,888$	$1.315\,936\,998$
C_{11}	$-0.605\,973\,676$	$-1.288\,353\,922$	$2.966\,252\,428$	$-2.637\,875\,499$
C_{33}	$-0.401\,414\,892$	$-1.137\,003\,974$	$-1.637\,033\,899$	$-3.558\,546\,850$
C_{12}	$-0.201\,991\,225$	$-0.429\,451\,308$	$0.988\,750\,809$	$-0.879\,291\,833$
C_{13}	$-0.792\,845\,153$	$-0.576\,101\,549$	$-2.223\,511\,382$	$-0.194\,632\,072$
C_{111}	$2.324\,128\,642$	$5.026\,701\,204$	$-15.767\,553\,741$	$12.580\,565\,280$
C_{222}	$-0.532\,222\,756$	$2.217\,541\,686$	$-19.362\,925\,160$	$2.779\,206\,544$
C_{333}	$-0.708\,777\,482$	$5.511\,268\,055$	$2.608\,789\,547$	$26.442\,451\,932$
C_{112}	$-1.248\,985\,111$	$-0.680\,155\,470$	$-5.310\,733\,599$	$-3.364\,702\,185$
C_{122}	$1.607\,366\,288$	$2.129\,004\,048$	$-1.715\,362\,181$	$6.436\,656\,550$
C_{113}	$1.954\,724\,848$	$2.095\,223\,879$	$6.247\,025\,199$	$3.973\,514\,399$
C_{123}	$0.651\,574\,949$	$0.698\,407\,960$	$2.082\,341\,733$	$1.324\,504\,800$
C_{133}	$1.357\,925\,970$	$0.086\,875\,908$	$2.788\,189\,975$	$-4.324\,858\,840$

$$C_{123} = C_{144} = C_{366} = C_{456} = \tfrac{1}{3}C_{113}, \quad C_{133} = C_{344}.$$

Electrostatic contributions to these elastic constants for ideal structure parameters are listed in Table IV in units of Z^2e^2/a^4. For all the hexagonal structures, our choice of Cartesian axes (in Miller–Bravais indices) has been 1 axis = $[10\bar{1}0]$; 2 axis = $[\bar{1}2\bar{1}0]$; and 3 axis = $[0001]$. It should be mentioned that, for the hcp structure, Cousins[5] has chosen basal axes rotated $90°$ with respect to ours. Thus, his C_{111} corresponds to our C_{222}, etc. However, our choice of axes is consistent with the only two sets of measured third-order elastic constants for hcp metals.[14,15] Also the different choice of axes eliminates the discrepancy, noted by Naimon et al.,[16] in certain Fuchs's constants calculated by Cousins.[4]

The results presented in Tables III and IV represent a higher degree of accuracy than those of earlier calculations. However, our results are essentially in agreement with those reported earlier (fcc,[1-3,9] bcc,[1-3,6,9] NaCl and CsCl,[7] zinc blende,[8] and hcp[5]). Also, all results were checked independently by doing a Fuchs-type calculation for each structure [Eq. (11) with $\lambda = (\Omega_0')^{1/3}$]. Other useful checks are the relations

$$C_{ii}^{es} = -U_{es}, \quad C_{iijj}^{es} = 3U_{es}, \quad C_{iijjkk}^{es} = -15U_{es},$$

where, as usual, repeated indices are to be summed. These can be easily derived, for example, by relating Fuchs and Brugger constants. All calculations were performed on IBM 360 and Xerox Sigma 5 computers. Convergence of all sums was such that the maximum error in the tabulated constants was $\pm 1 \times 10^{-12}$. The subroutine

for the complementary error function, necessary to generate the $\Phi_{-1/2}$ functions, was from an IBM routine with a relative error of less than 4×10^{-16}.

IV. GENERAL EXPRESSIONS FOR INTERNAL-STRAIN DERIVATIVES

In order to obtain the internal-strain contribution to the elastic constants, it is sufficient to know the energy density of the homogeneously deformed lattice as a function of both external and internal strains (see Appendix A). However, since the internal strains are determined from the total energy density, the electrostatic internal-strain contribution to the elastic constants cannot be obtained directly. It is still possible, though, to determine electrostatic internal-strain derivatives of the form

$$U^{(\nu p)(\mu q)\cdots}_{ijkl\cdots} = \left(\frac{\partial^n U'_{es}}{\partial \vec{w}_p(\nu)\,\partial \vec{w}_q(\mu)\cdots\partial \eta_{ij}\,\partial \eta_{kl}\cdots} \right)_{\vec{\eta}=0,\ \vec{w}=0}$$

(26)

where $\vec{w}(\nu)$ is the internal strain associated with the νth ion of the unit cell ($\nu = 0, 1, \cdots, s-1$). These derivatives would be combined with those arising from other terms of the energy density, thus resulting in the total internal-strain contribution to the elastic constants.

Using the method of homogeneous deformation, derivatives of $U'_{es}(\vec{\eta}, \vec{w}(\nu))$ can be easily performed (see Appendix B). Introducing the dimensionless parameter $\vec{t} = [\vec{\tau}(\nu) - \vec{\tau}(\mu)]/\Omega_0^{1/3}$, as well as $\vec{r} = \vec{R}\binom{l\,0}{\nu\,\mu}/\Omega_0^{1/3}$ and $\vec{g} = \Omega_0^{1/3}\vec{G}(h)/2\pi$, the expressions for the electrostatic internal-strain derivatives through third-order are

$$\Omega_0^{1/3} U^{(\nu p)} = -\frac{Z^2 e^2}{2\Omega_0^{4/3}} \frac{2\mathfrak{d}_\nu}{s} \left[\sigma^{1/2} \sum_{l\,\mu\neq\nu} \mathfrak{d}_\mu (2\pi\sigma) r_p \Phi_{+1/2}(\sigma\pi|\vec{r}|^2) + {\sum_h}' \operatorname{Im}\kappa(\vec{g},\nu)(2\pi\sigma^{-1})g_p \Phi_0(\sigma^{-1}\pi|\vec{g}|^2)\right] , \tag{27}$$

$$\Omega_0^{1/3} U_{ij}^{(\nu p)} = \frac{Z^2 e^2}{2\Omega_0^{4/3}} \frac{2\mathfrak{d}_\nu}{s} \left\{\sigma^{1/2} \sum_{l\,\mu\neq\nu} \mathfrak{d}_\mu (2\pi\sigma)^2 r_p r_i r_j \Phi_{+3/2}(\sigma\pi|\vec{r}|^2)\right.$$
$$\left.+ {\sum_h}' \operatorname{Im}\kappa(\vec{g},\nu)[(2\pi\sigma^{-1})g_q X_{qpij}\Phi_0(\sigma^{-1}\pi|\vec{g}|^2) - (2\pi\sigma^{-1})^2 g_p g_i g_j \Phi_1(\sigma^{-1}\pi|\vec{g}|^2)]\right\} , \tag{28}$$

$$\Omega_0^{2/3} U^{(\nu p)(\nu q)} = \frac{Z^2 e^2}{2\Omega_0^{4/3}} \frac{2\mathfrak{d}_\nu}{s} \left\{\sigma^{1/2} \sum_{l\,\mu\neq\nu} \mathfrak{d}_\mu [(2\pi\sigma)^2 r_p r_q \Phi_{+3/2}(\sigma\pi|\vec{r}|^2) - (2\pi\sigma)\delta_{pq}\Phi_{+1/2}(\sigma\pi|\vec{r}|^2)]\right.$$
$$\left.- \sigma {\sum_h}' [\operatorname{Re}\kappa(\vec{g},\nu) - \mathfrak{d}_\nu/s](2\pi\sigma^{-1})^2 g_p g_q \Phi_0(\sigma^{-1}\pi|\vec{g}|^2)\right\} , \tag{29}$$

$$\Omega_0^{2/3} U^{(\nu p)(\mu q)} = \Omega_0^{2/3} U^{(\mu p)(\nu q)} = \frac{-Z^2 e^2}{2\Omega_0^{4/3}} \frac{2\mathfrak{d}_\nu \mathfrak{d}_\mu}{s} \left\{\sigma^{1/2} \sum_l [(2\pi\sigma)^2 r_p r_q \Phi_{+3/2}(\sigma\pi|\vec{r}|^2) - (2\pi\sigma)\delta_{pq}\Phi_{+1/2}(\sigma\pi|\vec{r}|^2)]\right.$$
$$\left.- \sigma {\sum_h}' (1/s)\cos(2\pi\vec{g}\cdot\vec{t})(2\pi\sigma^{-1})^2 g_p g_q \Phi_0(\sigma^{-1}\pi|\vec{g}|^2)\right\} , \tag{30}$$

$$\Omega_0^{1/3} U_{ijkl}^{(\nu p)} = -\frac{Z^2 e^2}{2\Omega_0^{4/3}} \frac{2\mathfrak{d}_\nu}{s} \left\{\sigma^{1/2} \sum_{l\,\mu\neq\nu} \mathfrak{d}_\mu (2\pi\sigma)^3 r_p r_i r_j r_k r_l \Phi_{+5/2}(\sigma\pi|\vec{r}|^2)\right.$$
$$+ {\sum_h}' \operatorname{Im}\kappa(\vec{g},\nu)[(2\pi\sigma^{-1})g_q X_{qpijkl}\Phi_0(\sigma^{-1}\pi|\vec{g}|^2) - \tfrac{1}{3}(2\pi\sigma^{-1})^2 g_q (Y_{qpijkl} - |\vec{g}|^2 X_{qpijkl})\Phi_1(\sigma^{-1}\pi|\vec{g}|^2)$$
$$\left.+ (2\pi\sigma^{-1})^3 g_p g_i g_j g_k g_l \Phi_2(\sigma^{-1}\pi|\vec{g}|^2)]\right\} , \tag{31}$$

$$\Omega_0^{2/3} U_{ij}^{(\nu p)(\nu q)} = -\frac{Z^2 e^2}{2\Omega_0^{4/3}} \frac{2\mathfrak{d}_\nu}{s} \left\{\sigma^{1/2} \sum_{l\,\mu\neq\nu} \mathfrak{d}_\mu [(2\pi\sigma)^3 r_p r_q r_i r_j \Phi_{+5/2}(\sigma\pi|\vec{r}|^2) - (2\pi\sigma)^2 \delta_{pq} r_i r_j \Phi_{+3/2}(\sigma\pi|\vec{r}|^2)\right.$$
$$- (2\pi\sigma)(\delta_{pi}\delta_{qj} + \delta_{pj}\delta_{qi})\Phi_{+1/2}(\sigma\pi|\vec{r}|^2)] - \sigma {\sum_h}' (\operatorname{Re}\kappa(\vec{g},\nu) - \mathfrak{d}_\nu/s)$$
$$\left.\times [(2\pi\sigma^{-1})^2 (Y_{pqij} - \delta_{pq}g_i g_j)\Phi_0(\sigma^{-1}\pi|\vec{g}|^2) - (2\pi\sigma^{-1})^3 g_p g_q g_i g_j \Phi_1(\sigma^{-1}\pi|\vec{g}|^2)]\right\} , \tag{32}$$

$$\Omega_0^{2/3} U_{ij}^{(\nu p)(\mu q)} = \Omega_0^{2/3} U_{ij}^{(\mu p)(\nu q)} = \frac{Z^2 e^2}{2\Omega_0^{4/3}} \frac{2\mathfrak{d}_\nu \mathfrak{d}_\mu}{s} \left\{\sigma^{1/2} \sum_l [(2\pi\sigma)^3 r_p r_q r_i r_j \Phi_{+5/2}(\sigma\pi|\vec{r}|^2)\right.$$
$$- (2\pi\sigma)^2 \delta_{pq} r_i r_j \Phi_{+3/2}(\sigma\pi|\vec{r}|^2) - (2\pi\sigma)(\delta_{pi}\delta_{qj} + \delta_{pj}\delta_{qi})\Phi_{+1/2}(\sigma\pi|\vec{r}|^2)]$$
$$\left.- \sigma {\sum_h}' (1/s)\cos(2\pi\vec{g}\cdot\vec{t})[(2\pi\sigma^{-1})^2 (Y_{pqij} - \delta_{pq}g_i g_j)\Phi_0(\sigma^{-1}\pi|\vec{g}|^2) - (2\pi\sigma^{-1})^3 g_p g_q g_i g_j \Phi_1(\sigma^{-1}\pi|\vec{g}|^2)]\right\} , \tag{33}$$

$$\Omega_0 U^{(\nu p)(\nu q)(\nu m)} = \frac{-Z^2 e^2}{2\Omega_0^{4/3}} \frac{2\mathfrak{d}_\nu}{s} \left\{\sigma^{1/2} \sum_{l\,\mu\neq\nu} \mathfrak{d}_\mu [(2\pi\sigma)^3 r_p r_q r_m \Phi_{+5/2}(\sigma\pi|\vec{r}|^2) - (2\pi\sigma)^2 r_n X_{npqm}\Phi_{+3/2}(\sigma\pi|\vec{r}|^2)]\right.$$
$$\left.- \sigma^2 {\sum_h}' \operatorname{Im}\kappa(\vec{g},\nu)(2\pi\sigma^{-1})^3 g_p g_q g_m \Phi_0(\sigma^{-1}\pi|\vec{g}|^2)\right\} , \tag{34}$$

$$\Omega_0 U^{(\nu p)(\nu q)(\mu m)} = -\Omega_0 U^{(\mu p)(\mu q)(\nu m)} = \frac{Z^2 e^2}{2\Omega_0^{4/3}} \frac{2\mathfrak{d}_\nu \mathfrak{d}_\mu}{s} \left\{\sigma^{1/2} \sum_l [(2\pi\sigma)^3 r_p r_q r_m \Phi_{+5/2}(\sigma\pi|\vec{r}|^2)\right.$$
$$\left.- (2\pi\sigma)^2 r_n X_{npqm}\Phi_{+3/2}(\sigma\pi|\vec{r}|^2)] - \sigma^2 {\sum_h}' (1/s)\sin(2\pi\vec{g}\cdot\vec{t})(2\pi\sigma^{-1})^3 g_p g_q g_m \Phi_0(\sigma^{-1}\pi|\vec{g}|^2)\right\} , \tag{35}$$

and

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

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

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

These internal-strain derivatives are similar to elastic constants in that they transform as tensors for any point-group operation (e.g., $U_{ij}^{(\nu p)*} = \mathfrak{R}_{pq}\mathfrak{R}_{ik}\mathfrak{R}_{jl} U_{kl}^{(\nu q)}$, where $\vec{\mathfrak{R}}$ 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 $U_{ij}^{(\nu p)}$, and thus the internal-strain parameter

$$A_{pij}(\nu) = \left(\frac{\partial \overline{w}_p(\nu)}{\partial \eta_{ij}}\right)\Bigg|_{\vec{\eta}\,=\,0,\,\vec{\overline{w}}=0} ,$$

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: $U_{ij}^{(\nu p)}$, $U^{(\nu p)(\mu q)}$, $U_{ijkl}^{(\nu p)}$, and $U^{(\nu p)(\mu q)(\ell m)}$ satisfy Cauchy relations in that the Cartesian indices can be arranged in any order (e.g., $U_{ij}^{(\nu p)} = U_{ji}^{(\nu i)}$); and $U_{ij}^{(\nu p)(\mu q)}$ is symmetric with respect to the interchanges $p \leftrightarrow q$ and $i \leftrightarrow j$.

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

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

Then, derivatives are related by

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

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 $\mathfrak{z}_0 = +1$ and $\mathfrak{z}_1 = -1(+1)$ 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

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

and thus

$$\frac{\partial}{\partial \overline{w}_p} = \tfrac{1}{4}a \frac{\partial}{\partial \overline{w}_p(1)} = -\tfrac{1}{4}a \frac{\partial}{\partial \overline{w}_p(0)} .$$

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

$$U_4^1 = -10.057668147, \quad U_1^{11} = 0.819616921,$$

$$U^{11} = -4.188790205, \quad U_2^{11} = 10.062167052,$$

$$U^{123} = 19.202879707, \quad U_4^{23} = 14.250957256,$$

$$U_{14}^1 = U_{24}^1 = U_{56}^1 = 16.762780245 ,$$

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 $\mathfrak{z}_0 \mathfrak{z}_1$ 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

$$\vec{\tau}(0) = (0, 0, 0), \qquad \vec{\tau}(1) = (a/\sqrt{3}, 0, \tfrac{1}{2}c) ,$$

$$\vec{\tau}(2) = (0, 0, uc), \qquad \vec{\tau}(3) = (a/\sqrt{3}, 0, [u + \tfrac{1}{2}]c)$$

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) $\mathfrak{z}_0 = +1$, $\mathfrak{z}_1 = +1(-1)$, and $\mathfrak{z}_2 = \mathfrak{z}_3 = 0$; and for ionic wurtzite $\mathfrak{z}_0 = \mathfrak{z}_1 = +1$ and $\mathfrak{z}_2 = \mathfrak{z}_3 = -1$. The three independent internal strains will be taken as

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

and

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

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

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

and

$$\frac{\partial}{\partial \overline{w}_p^3} = L\left[\left(\frac{\partial}{\partial \overline{w}_p(2)}\right) + \left(\frac{\partial}{\partial \overline{w}_p(3)}\right)\right]$$

$$= -L\left[\left(\frac{\partial}{\partial \overline{w}_p(0)}\right) + \left(\frac{\partial}{\partial \overline{w}_p(1)}\right)\right] .$$

It is easily seen that derivatives with respect to $\vec{\overline{w}}^2$ and $\vec{\overline{w}}^3$ are zero for hcp and WC, since internal-strain derivatives with respect to $\vec{\overline{w}}(\nu)$ are proportional to $\mathfrak{z}_\nu$. 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

$U_1^1 = 0.212757375$,

$U_2^{11} = 0.148157929$,

$U^{11} = 0.215120910$,

$U_3^{11} = -1.237994447$,

$U^{33} = 4.282147161$,

$U_1^{33} = -5.305020698$,

$U^{111} = -1.206443870$,

$U_3^{33} = -10.800694409$,

$U_1^{11} = 0.014231968$,

$U_4^{23} = -5.520141607$,

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

$U_{11}^1 = 0.010837123$,

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

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

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

in units of $Z^2 e^2/a^4$. 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, β, ... on $U_{ij\cdots}^{\alpha\beta q\cdots}$ when writing specific derivatives, it is convenient to use commas to separate differentiations with respect to the three different internal strains. Then

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

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,

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

and

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$\qquad = -U_1^{,,13} = -U_1^{3,,1} = -U_1^{1,,3} = -U_1^{,3,1} = 6.812479538$,

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

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

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

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

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

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

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

$$= U_{12}^{\cdot\cdot3} = -2U_{12}^{3\cdot\prime} = 2U_{12}^{\cdot3\cdot} = U_{66}^{\cdot\cdot3} = -2U_{66}^{3\cdot\prime}$$

$$= 2U_{66}^{\cdot3\cdot} = \tfrac{1}{3}U_{15}^{\cdot\cdot1} = -4.016750345 ,$$

$$U_{35}^{\cdot\cdot1} = -2U_{35}^{1\cdot\prime} = 2U_{35}^{\cdot1\cdot} = U_{13}^{\cdot\cdot3} = -2U_{13}^{3\cdot\prime} = 2U_{13}^{\cdot3\cdot} = U_{44}^{\cdot\cdot3}$$

$$= -2U_{44}^{3\cdot\prime} = 2U_{44}^{\cdot3\cdot} = -1.058210294 ,$$

$$U_{33}^{\cdot\cdot3} = -2U_{33}^{3\cdot\prime} = 2U_{33}^{\cdot3\cdot} = 35.638709114 ,$$

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 $\tfrac{1}{2}c$). For this symmetry element, the internal-strain tensors $U_{ij\cdots}^{(\nu p)\cdots}$ transform as

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

where $\vec{\mathfrak{R}}$ 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, $U_1^{1\cdot\prime} \equiv LU_1^{(11)}$ and $U_1^{1\cdot} \equiv LU_1^{(31)}$ are not required to vanish. However, $U_1^{\cdot\cdot1} \equiv L[U_1^{(21)} + U_1^{(31)}]$ 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

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 $\vec{w}^\alpha$, 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, $U(\vec{\eta}, \vec{w}^\alpha)$, be a minimum with respect to $\vec{w}^\alpha$, i.e.,

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

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

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

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

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

and

$$0 = \frac{\partial^2}{\partial \eta_{ij}\partial \eta_{kl}}(U^{\beta q}) = U_{ijkl}^{\beta q} + \frac{\partial \vec{w}_p^\alpha}{\partial \eta_{kl}} U_{ij}^{\alpha p \beta q} + \frac{\partial \vec{w}_p^\alpha}{\partial \eta_{ij}} U_{kl}^{\alpha p \beta q}$$

$$+ \frac{\partial \vec{w}_p^\alpha}{\partial \eta_{ij}} \frac{\partial \vec{w}_r^\gamma}{\partial \eta_{kl}} U^{\alpha p \beta q \gamma r} + \frac{\partial^2 \vec{w}_p^\alpha}{\partial \eta_{ij}\partial \eta_{kl}} U^{\alpha p \beta q} , \tag{A4}$$

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

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

$$\vec{w}_p^\alpha = A_{p ij}^\alpha \eta_{ij} + \tfrac{1}{2}B_{p ijkl}^\alpha \eta_{ij}\eta_{kl} + \cdots , \tag{A5}$$

where the coefficients

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

and

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

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

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

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

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

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

$$C_{ijkl} = C_{ijkl}^{(0)} - A_{p ij}^\alpha A_{q kl}^\beta U^{\alpha p \beta q}(\vec{\eta} = 0) , \tag{A10}$$

and

$$C_{ijklmn} = C_{ijklmn}^{(0)} + A_{p ij}^\alpha U_{klmn}^{\alpha p}(\vec{\eta} = 0) + A_{p kl}^\alpha U_{ijmn}^{\alpha p}(\vec{\eta} = 0)$$

$$+ A_{p mn}^\alpha U_{ijkl}^{\alpha p}(\vec{\eta} = 0) + A_{p kl}^\alpha A_{q mn}^\beta U_{ij}^{\alpha p \beta q}(\vec{\eta} = 0)$$

$$+ A_{p ij}^\alpha A_{q mn}^\beta U_{kl}^{\alpha p \beta q}(\vec{\eta} = 0) + A_{p ij}^\alpha A_{q kl}^\beta U_{mn}^{\alpha p \beta q}(\vec{\eta} = 0)$$

$$+ A_{p ij}^\alpha A_{q kl}^\beta A_{r mn}^\gamma U^{\alpha p \beta q \gamma r}(\vec{\eta} = 0) , \tag{A11}$$

where

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

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

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

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

and

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

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

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

and

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

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

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[1]K. Fuchs, Proc. Roy. Soc. (London) A153, 622 (1936).

[2]K. Fuchs, Proc. Roy. Soc. (London) A157, 444 (1936).

[3]C. S. G. Cousins, Proc. Phys. Soc. (London) 91, 235 (1967).

[4]C. S. G. Cousins, J. Phys. C 1, 478 (1968).

[5]C. S. G. Cousins, J. Phys. F 2, 1 (1972).

[6]T. Suzuki, A. V. Granato, and J. F. Thomas, Jr., Phys. Rev. 175, 766 (1968).

[7]P. B. Ghate, Phys. Rev. 139, A1666 (1965).

[8]M. Blackman, Phil. Mag. 3, 831 (1959).

[9]D. E. MacDonald, J. Eftis, and G. M. Arkilic, J. Appl. Phys. 43, 804 (1972). As this work was being completed, D. E. MacDonald et al. presented a method similar to ours for calculating derivatives of the electrostatic energy, and expressions for the second- and third-order elastic constants were presented. However, their results were restricted to primitive lattices. Thus, they could not consider ionic structures, nonprimitive metallic structures, or the internal strains which can occur in these structures.

[10]P. P. Ewald, Ann. Physik 64, 253 (1921).

[11]K. Fuchs, Proc. Roy. Soc. (London) A151, 585 (1935).

[12]W. A. Harrison, Pseudopotentials in the Theory of Metals (Benjamin, New York, 1966).

[13]R. A. Coldwell-Horsfall and A. A. Maradudin, J. Math. Phys. 1, 395 (1960).

[14]K. D. Swartz and C. Elbaum, Phys. Rev. B 1, 1512 (1970).

[15]E. R. Naimon, Phys. Rev. B 4, 4291 (1971).

[16]E. R. Naimon, Tetsuro Suzuki, and A. V. Granato, Phys. Rev. B 4, 4297 (1971), footnote 5.

[17]M. Born and K. Huang, Dynamical Theory of Crystal Lattices (Oxford U. P., Oxford, England, 1962).

[18]K. Brugger, Phys. Rev. 133, A1611 (1964).

[19]F. D. Murnaghan, Finite Deformation of an Elastic Solid (Wiley, New York, 1951).

Low-Energy Optical Absorption in ReO₃

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The absorptivity of polycrystalline samples of ReO₃ has been measured in the range 0.11 to 2.8 eV using a calorimetric technique. New structures have been found in the absorptivity, appearing at about 0.4 and 1.0 eV. The data have been Kramers-Kronig analyzed to obtain the optical constants. Band-calculation results of Mattheiss are presented and a tentative identification of the origin of the new structures is made. A comparison of the present data with those of Feinleib, Scouler, and Ferretti is made.

INTRODUCTION

A variety of studies have recently contributed to an understanding of the transition-metal oxide ReO₃. It has been shown that ReO₃ is a good electrical conductor, is nonmagnetic, and possesses a cubic crystal structure. Information concerning the band structure of ReO₃ at the Fermi level has been provided by the de Haas–van Alphen (dHvA) measurements of Marcus,[1] the magnetothermal