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

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

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. $\vec{R}(^{lk}_{\nu\mu})$ is defined as

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

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 $\vec{R}'(^{l0}_{\nu\mu})$, 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

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

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

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

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

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

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

$$\left. - 2\sigma^{1/2} \langle \mathfrak{z}^2 \rangle + \sigma^{-1} \frac{\lambda^3}{\Omega_0'} \langle \mathfrak{z} \rangle^2 D \right], \tag{8}$$

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