A CONTINUUM THEORY OF A DIATOMIC, ELASTIC DIELECTRIC

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Abstract—The field equations and boundary conditions of the continuum theory of elastic dielectrics, including the contribution of the polarization gradient, are extended to apply to a compound material. A formula is obtained for the surface energy of deformation and polarization of a cubic crystal. The solution of a problem of plane waves leads to the identification of transverse and longitudinal optical, as well as acoustical, branches in the dispersion relation. A one-dimensional model of the NaCl-type crystal lattice of shell-model atoms is constructed and its finite difference equations of motion are shown to have the corresponding equations of the continuum theory as their long wave limit, without restriction to low frequency.

1. INTRODUCTION

THE differential equations of the classical theory of elasticity are known to be the long wave, low frequency limit of the finite difference equations of the theory of crystal lattices of mass-particles. If the lattice is a simple one of the Bravais type, with one particle per cell, there is no distinction between the long wave limit and the long wave, low frequency limit—as there are no optical branches in the dispersion relations for waves in Bravais lattices. However, in the case of a compound lattice, which has more than one particle per cell, there are high frequency optical branches as well as low frequency acoustical branches at the long wave limit. In that case, classical elasticity accounts for the long wave portions of only the acoustical branches. It has already been shown [1] how the classical equations of elasticity can be extended to include the long wave portions of the optical branches in the case of two particles per cell in a cubic crystal.

The applications now contemplated include those involving electromechanical inter-actions, so that it is appropriate to incorporate the electronic polarization, in the equations, in addition to the mechanical displacement. When this is done, the equations become the extension of the classical theory of elastic dielectrics to include the long wave, high frequency behavior of diatomic, polarizable crystals. Furthermore, even at low frequencies, wave lengths in the continuum approximation can be short enough and, at both low frequencies and in static equilibrium, dimensions can be small enough, for the effect of the polarization gradient to be significant. Consequently, the contribution of the polarization gradient is also included here. The resulting equations are then the extension, to diatomic materials, of a previous extension [2] of the classical theory of elastic dielectrics to account for the effects of the polarization gradient. At the same time, the equations are the long wave limit, not restricted to low frequencies, of the equations of a diatomic crystal lattice of polarizable atoms.

In Section 2, the potential and kinetic energy densities of the compound continuum are defined and a restriction to linearity is imposed. The field equations and boundary conditions are derived, in Section 3, by means of an extension of a linear version of Toupin's [3]

variational principle for the equations of the classical theory of elastic dielectrics. This is followed, in Section 4, by a derivation of the constitutive equations for a special case of cubic symmetry. In Section 5, a formula is derived for the surface energy of deformation and polarization. A problem of plane waves in an infinite medium is solved in Section 6 and the acoustical and optical branches of the dispersion relations for transverse and longitudinal waves are identified. A limiting form of the equations, valid at long wave lengths, is equivalent to equations, given by Born and Huang [4], leading to a dispersion formula for the dielectric constant. In the final section, a one-dimensional Cochran-type [5] lattice of Dick–Overhauser [6] shell-model atoms in an NaCl-type structure is devised and the associated finite difference equations of motion are formulated. In the long wave limit, the difference equations of the lattice become the differential equations for longitudinal optical and acoustical waves in the diatomic continuum.

2. POTENTIAL AND KINETIC ENERGIES

In a continuum theory of a crystal lattice with two atoms per cell, each material point X_i, $i = 1, 2, 3$, is the site of two atoms, say 1 and 2, as illustrated in Fig. 1. Upon deformation, the two atoms move, with separate displacements $u_i^{(1)}$ and $u_i^{(2)}$ to a single spatial point x_i at which, if the atoms are polarizable, they take on electronic polarizations $P_i^{(1)}$ and $P_i^{(2)}$. A neighboring pair of atoms, initially at $X_i + dX_i$, has displacements $u_i^{(\kappa)} + du_i^{(\kappa)}$, $\kappa = 1, 2$, and polarizations $P_i^{(\kappa)} + dP_i^{(\kappa)}$. In a linear theory, to which the present treatment is confined,

$$du_j^{(\kappa)} \approx dx_i u_{j,i}^{(\kappa)}, \qquad dP_j^{(\kappa)} \approx dx_i P_{j,i}^{(\kappa)}$$

where the summation convention for repeated indices and the comma notation for derivative (with respect to x_i) are employed.

Each point x_i may be regarded as being occupied by a point of each of two deformable and polarizable continua. The stored energy density of deformation and polarization, W^L, is assumed to be a quadratic function of the small strains, $S_{ij}^{(\kappa)}$, polarizations, $P_i^{(\kappa)}$, and
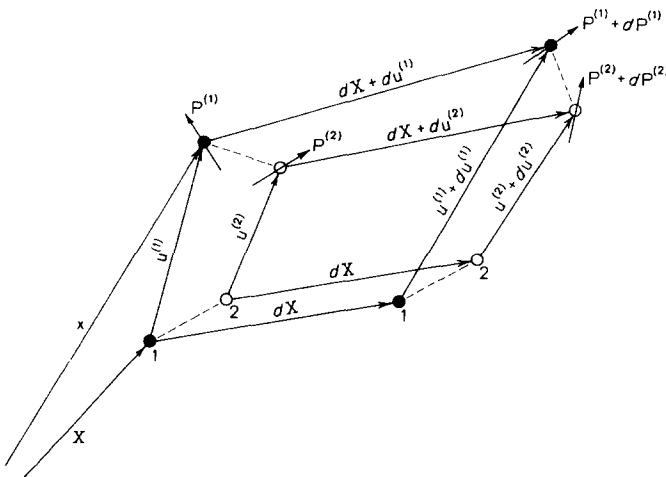

FIG. 1. Displacement and polarization in a diatomic continuum.

polarization gradients, $P_{j,i}^{(\kappa)}$, of the individual continua, and of the relative displacement, u_i^*, and relative rotation, ω_{ij}^*, of the two continua:

$$W^L = W^L(S_{ij}^{(1)}, S_{ij}^{(2)}, P_i^{(1)}, P_i^{(2)}, P_{j,i}^{(1)}, P_{j,i}^{(2)}, u_i^*, \omega_{ij}^*),\tag{1}$$

where

$$S_{ij}^{(\kappa)} = \tfrac{1}{2}(u_{j,i}^{(\kappa)} + u_{i,j}^{(\kappa)}),$$

$$u_i^* = u_i^{(2)} - u_i^{(1)},$$

$$\omega_{ij}^* = \tfrac{1}{2}(u_{j,i}^* - u_{i,j}^*).$$

With these variables, W^L is invariant in a rigid translation and rotation of the deformed and polarized body.

If the polarization and polarization gradient were omitted, W^L would be the energy density of a classical, linear, elastic body extended to accommodate a diatomic material [1]. If only the polarization gradient were omitted, W^L would be the energy density of deformation and polarization of a classical, linear, elastic dielectric extended to accommodate a diatomic material. As it stands in (1), W^L is the extension, to a diatomic material, of a previous energy function in which the inclusion of the polarization gradient has been shown to account for interesting, observed phenomena [2, 7, 8].

The total potential energy density, W, is the energy density of deformation and polarization augmented by the energy density of the Maxwell, electric self-field:

$$W = W^L + \tfrac{1}{2}\varepsilon_0\varphi_{,i}\varphi_{,i},\tag{2}$$

where ε_0 is the permittivity of a vacuum and φ is the potential of the Maxwell self-field E_i^{MS}, i.e.

$$E_i^{MS} = -\varphi_{,i}.\tag{3}$$

The associated kinetic energy density is taken as

$$T = \sum_\kappa \tfrac{1}{2}\rho^{(\kappa)}u_{j,t}^{(\kappa)}u_{j,t}^{(\kappa)}, \qquad \kappa = 1, 2; \qquad j = 1, 2, 3,\tag{4}$$

where $\rho^{(1)}$ and $\rho^{(2)}$ are the mass densities of the two continua and the "comma t" notation designates the differentiation with respect to time.

3. FIELD EQUATIONS AND BOUNDARY CONDITIONS

The field equations and boundary conditions, corresponding to the potential and kinetic energy densities formulated in the preceding section, may be derived by means of an extension of a linear version of Toupin's [3] variational principle for the classical theory of elastic dielectrics. The extension accounts for the contributions of the polarization gradients, the two continua and the kinetic energy.

First we define an electric enthalpy density:

$$H = W - (\varepsilon_0 E_i^{MS} + P_i^{(1)} + P_i^{(2)} + q^*u_i^*)E_i^{MS}\tag{5}$$

i.e. the potential energy density diminished by the product of the Maxwell self-field and the electric displacement. The inclusion of the term $q^*u_i^*$, where q^* is a charge density, was suggested by P. C. Y. Lee to accommodate applications to ionic crystals; i.e. $q^*u_i^*$ is the

ionic, or atomic, polarization as distinguished from the electronic polarizations $P_i^{(\kappa)}$. When the ionic polarization is included in what follows, the superscript $\kappa = 1$ identifies the positive ion and $\kappa = 2$ the negative ion.

Inserting (2) and (3) in (5), we find

$$H = W^L - \tfrac{1}{2}\varepsilon_0\varphi_{,i}\varphi_{,i} + \varphi_{,i}(P_i^{(1)} + P_i^{(2)} + q^*u_i^*). \tag{6}$$

In a body occupying a volume V bounded by a surface S separating V from a vacuum V', the extension of Toupin's variational principle takes the form

$$\delta \int_{t_0}^{t_1} dt \int_{V''} (T - H)\, dV + \sum_\kappa \int_{t_0}^{t_1} dt \int_V (f_i^{(\kappa)}\delta u_i^{(\kappa)} + E_i^0\delta P_i^{(\kappa)} + E_i^0 q^*\delta u_i^*)\, dV$$

$$+ \sum_\kappa \int_{t_0}^{t_1} dt \int_S t_i^{(\kappa)}\, \delta u_i^{(\kappa)}\, dS = 0, \qquad \kappa = 1, 2, \tag{7}$$

for independent variations of $u_i^{(\kappa)}$, $P_i^{(\kappa)}$ and φ between fixed limits at times t_0 and t_1. In (7), $V'' = V + V'$, $f_i^{(\kappa)}$ and $t_i^{(\kappa)}$ are the external body forces and surface tractions on the two continua and E_i^0 is the external electric field. Now,

$$\delta W^L = \sum_\kappa (T_{ij}^{(\kappa)}\, \delta S_{ij}^{(\kappa)} - E_i^{(\kappa)}\, \delta P_i^{(\kappa)} + E_{ij}^{(\kappa)}\, \delta P_{j,i}^{(\kappa)}) + T_i^*\, \delta u_i^* + T_{ij}^*\delta\omega_{ij}^*, \tag{8}$$

where

$$T_{ij}^{(\kappa)} = \frac{\partial W^L}{\partial S_{ij}^{(\kappa)}}, \quad E_i^{(\kappa)} = -\frac{\partial W^L}{\partial P_i^{(\kappa)}}, \quad E_{ij}^{(\kappa)} = \frac{\partial W^L}{\partial P_{j,i}^{(\kappa)}}, \quad T_i^* = \frac{\partial W^L}{\partial u_i^*}, \quad T_{ij}^* = \frac{\partial W^L}{\partial\omega_{ij}^*}. \tag{9}$$

With the chain rule of differentiation, (8) becomes

$$\delta W^L = -\sum_\kappa [T_{ij,i}^{(\kappa)} + (-1)^\kappa(T_{ij,i}^* - T_j^*)]\, \delta u_j^{(\kappa)} - \sum_\kappa (E_j^{(\kappa)} + E_{ij,i}^{(\kappa)})\delta P_j^{(\kappa)}$$

$$+ \sum_\kappa \{[T_{ij}^{(\kappa)} + (-1)^\kappa T_{ij}^*]\, \delta u_j^{(\kappa)}\}_{,i} + \sum_\kappa (E_{ij}^{(\kappa)}\, \delta P_j^{(\kappa)})_{,i}.$$

Treating the remaining part of H in (6) similarly, we have, in V:

$$\delta H = -\sum_\kappa [T_{ij,i}^{(\kappa)} + (-1)^\kappa(T_{ij,i}^* - T_j^* - q^*\varphi_{,i})]\, \delta u_j^{(\kappa)} - \sum_\kappa (E_j^{(\kappa)} + E_{ij,i}^{(\kappa)} - \varphi_{,i})\delta P_j^{(\kappa)}$$

$$+ \sum_\kappa [\varepsilon_0\varphi_{,ii} - P_{i,i}^{(\kappa)} - (-1)^\kappa q^*u_{i,i}^{(\kappa)}]\delta\varphi + \sum_\kappa \{[T_{ij}^{(\kappa)} + (-1)^\kappa T_{ij}^*]\, \delta u_j^{(\kappa)}\}_{,i}$$

$$+ \sum_\kappa (E_{ij}^{(\kappa)}\, \delta P_j^{(\kappa)})_{,i} - \sum_\kappa \{[\varepsilon_0\varphi_{,i} - P_i^{(\kappa)} - (-1)^\kappa q^*u_i^{(\kappa)}]\, \delta\varphi\}_{,i}; \tag{10}$$

and, in V':

$$\delta H = \varepsilon_0\varphi_{,ii}\, \delta\varphi - \varepsilon_0(\varphi_{,i}\, \delta\varphi)_{,i}. \tag{11}$$

Further, from (4),

$$\delta \int_{t_0}^{t_1} T\, dt = -\sum_\kappa \int_{t_0}^{t_1} \rho^{(\kappa)}u_{i,tt}^{(\kappa)}\, \delta u_j^{(\kappa)}\, dt. \tag{12}$$

Inserting (10)–(12) in (7) and applying the divergence theorem where appropriate, we find

$$\sum_\kappa \int_{t_0}^{t_1} dt \int_V [T_{ij,i}^{(\kappa)} + (-1)^\kappa (T_{ij,i}^* - T_j^* - q^* \varphi_{,j}) + (-1)^\kappa q^* E_j^0 + f_j^{(\kappa)} - \rho^{(\kappa)} u_{j,tt}^{(\kappa)}] \, \delta u_j^{(\kappa)} \, dV$$

$$+ \sum_\kappa \int_{t_0}^{t_1} dt \int_V \{(E_j^{(\kappa)} + E_{ij,i}^{(\kappa)} - \varphi_{,j} + E_j^0) \delta P_j^{(\kappa)} + [-\varepsilon_0 \varphi_{,ii} + P_{i,i}^{(\kappa)} + (-1)^\kappa q^* u_{i,i}^{(\kappa)}] \, \delta \varphi\} \, dV$$

$$- \sum_\kappa \int_{t_0}^{t_1} dt \int_S \{[n_i (T_{ij}^{(\kappa)} + (-1)^\kappa T_{ij}^*) - t^{(\kappa)}] \, \delta u_j^{(\kappa)} + n_i E_{ij}^{(\kappa)} \, \delta P_j^{(\kappa)} + n_i [-\varepsilon_0 [\varphi_{,i}]$$

$$+ P_i^{(\kappa)} + q^* (-1)^\kappa u_i^{(\kappa)}] \, \delta \varphi\} \, dS - \int_{t_0}^{t_1} dt \int_{V'} \varepsilon_0 \varphi_{,ii} \, dV = 0, \tag{13}$$

where n_i is the outward normal to S and $[\varphi_{,i}]$ is the jump in $\varphi_{,i}$ across S.

From (13), we have the Euler equations in V:

$$T_{ij,i}^{(\kappa)} + (-1)^\kappa (T_{ij,i}^* - T_j^* - q^* \varphi_{,i}) + f_j^{(\kappa)} + (-1)^\kappa q^* E_j^0 = \rho^{(\kappa)} u_{j,tt}^{(\kappa)},$$

$$E_j^{(\kappa)} + E_{ij,i}^{(\kappa)} - \varphi_{,j} + E_j^0 = 0, \tag{14}$$

$$-\varepsilon_0 \varphi_{,ii} + P_{i,i}^{(1)} + P_{i,i}^{(2)} + q^* u_{i,i}^* = 0;$$

and, in V':

$$\varphi_{,ii} = 0; \tag{15}$$

and also the boundary conditions on S:

$$n_i [T_{ij}^{(\kappa)} + (-1)^\kappa T_{ij}^*] = t_j^{(\kappa)},$$

$$n_i E_{ij}^{(\kappa)} = 0, \tag{16}$$

$$n_i (-\varepsilon_0 [\varphi_{,i}] + P_i^{(1)} + P_i^{(2)} + q^* u_i^*) = 0.$$

As may be seen from (13), boundary conditions alternative to (16) are the specification of $u_i^{(\kappa)}$, $P_i^{(\kappa)}$ and φ, respectively.

4. CONSTITUTIVE EQUATIONS

We consider the constitutive equations for a crystal with NaCl-type lattice structure. Such a crystal belongs to cubic class $m3m$ (International) or O_h (Schoenflies) [9] with generators [10]

$$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix} \tag{17}$$

and, as illustrated in Fig. 2, comprises two, interpenetrating, f.c.c. lattices [11] each of which has $m3m$ symmetry. Owing to the first generator in (17) (the centrosymmetry generator) there can be no coefficients of odd rank and no products of symmetric and antisymmetric variables in the quadratic function W^L. This reduces the interactions to those between variables connected by full lines in Fig. 3; whereas the dashed line segments denote excluded
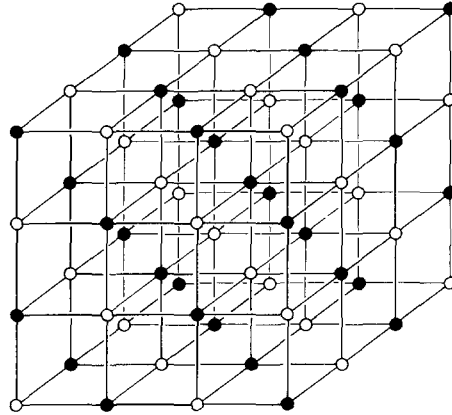
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FIG. 2. NaCl-type lattice.

interactions. The corresponding energy function is

$$W^L = \tfrac{1}{2} \sum_{\kappa,\lambda} (a_{ij}^{\kappa\lambda} P_i^{(\kappa)} P_j^{(\lambda)} + b_{ijkl}^{\kappa\lambda} P_{j,i}^{(\kappa)} P_{l,k}^{(\lambda)} + c_{ijkl}^{\kappa\lambda} S_{ij}^{(\kappa)} S_{kl}^{(\lambda)} + 2d_{ijkl}^{\kappa\lambda} P_{(j,i)}^{(\kappa)} S_{kl}^{(\lambda)})$$

$$+ \sum_{\kappa} (a^{*\kappa} u_i^* P_i^{(\kappa)} + d^{*\kappa} \omega_{ij}^* P_{[j,i]}^{(\kappa)}) + \tfrac{1}{2} a^{**} u_i^* u_i^* + c^{**} \omega_{ij}^* \omega_{ij}^*$$

$$+ \sum_{\kappa} (b^{\kappa 0} P_{i,i}^{(\kappa)} + c^{\kappa 0} S_{ii}^{(\kappa)}),$$ (18)
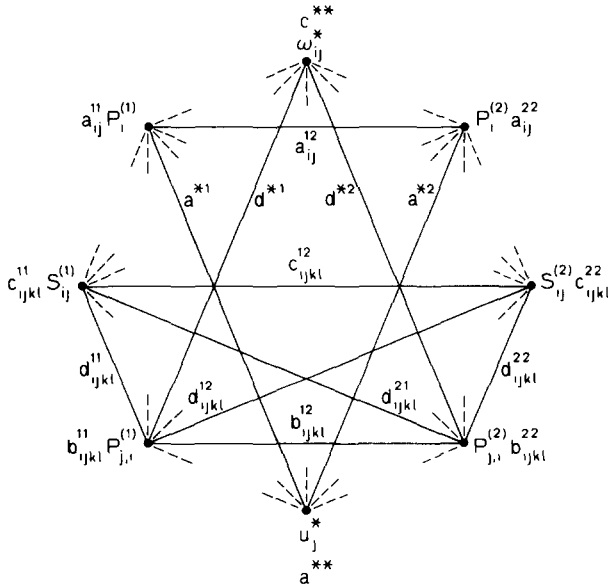

FIG. 3. Interactions among strains, polarizations, relative displacement and relative rotation in a diatomic, elastic, dielectric continuum with group $m3m$ (O_h) material symmetry.

where $P_{(j,i)}^{(\kappa)}$ and $P_{[j,i]}^{(\kappa)}$ denote the symmetric and antisymmetric parts of $P_{j,i}^{(\kappa)}$, respectively. We note that, in general,

$$a_{ij}^{\kappa\lambda} = a_{ij}^{\lambda\kappa}, \quad b_{ijkl}^{\kappa\lambda} = b_{ijkl}^{\lambda\kappa}, \quad c_{ijkl}^{\kappa\lambda} = c_{ijkl}^{\lambda\kappa} \tag{19}$$

and, from (17),

$$\begin{aligned}
a_{ij}^{\kappa\lambda} &= a_{11}^{\kappa\lambda}\delta_{ij}, \\
b_{ijkl}^{\kappa\lambda} &= b^{\kappa\lambda}\delta_{ijkl} + b_{12}^{\kappa\lambda}\delta_{ij}\delta_{kl} + b_{44}^{\kappa\lambda}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) + b_{77}^{\kappa\lambda}(\delta_{ik}\delta_{jl} - \delta_{il}\delta_{jk}), \\
c_{ijkl}^{\kappa\lambda} &= c^{\kappa\lambda}\delta_{ijkl} + c_{12}^{\kappa\lambda}\delta_{ij}\delta_{kl} + c_{44}^{\kappa\lambda}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}), \\
d_{ijkl}^{\kappa\lambda} &= d^{\kappa\lambda}\delta_{ijkl} + d_{12}^{\kappa\lambda}\delta_{ij}\delta_{kl} + d_{44}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}),
\end{aligned} \tag{20}$$

where δ_{ij} (or δ_{ijkl}) is unity when its indices are alike and zero otherwise;

$$b^{\kappa\lambda} = b_{11}^{\kappa\lambda} - b_{12}^{\kappa\lambda} - 2b_{44}^{\kappa\lambda}, \quad c^{\kappa\lambda} = c_{11}^{\kappa\lambda} - c_{12}^{\kappa\lambda} - 2c_{44}^{\kappa\lambda}, \quad d^{\kappa\lambda} = d_{11}^{\kappa\lambda} - d_{12}^{\kappa\lambda} - 2d_{44}^{\kappa\lambda}; \tag{21}$$

for $c_{ijkl}^{\kappa\lambda}$ and $d_{ijkl}^{\kappa\lambda}$ the abbreviated notation for pairs of indices, ij or kl has been used:

$$11 \to 1, \quad 22 \to 2, \quad 33 \to 3, \quad 23 \text{ or } 32 \to 4, \quad 31 \text{ or } 13 \to 5, \quad 12 \text{ or } 21 \to 6$$

and the same for $b_{ijkl}^{\kappa\lambda}$ except that

$$32 \to 7, \quad 13 \to 8, \quad 21 \to 9.$$

It may be observed that material constants with superscripts $\kappa\lambda = 11$ or 22 denote interactions within one of the two component continua whereas constants with superscripts $\kappa\lambda = 12$ or 21 denote interactions between the two component continua.

From (9) and (18)–(21), we find the constitutive equations

$$\begin{aligned}
T_{ij}^{(\kappa)} &= c^{\kappa 0}\delta_{ij} + \sum_{\lambda}(c^{\kappa\lambda}\delta_{ijkl}S_{kl}^{(\lambda)} + c_{12}^{\kappa\lambda}\delta_{ij}S_{kk}^{(\lambda)} + 2c_{44}^{\kappa\lambda}S_{ij}^{(\lambda)}) \\
&\quad + \sum_{\lambda}(d^{\lambda\kappa}\delta_{ijkl}P_{l,k}^{(\lambda)} + d_{12}^{\lambda\kappa}\delta_{ij}P_{k,k}^{(\lambda)} + 2d_{44}^{\lambda\kappa}P_{(j,i)}^{(\lambda)}), \\
-E_j^{(\kappa)} &= \sum_{\lambda}a_{11}^{\kappa\lambda}P_j^{(\lambda)} + a^{*\kappa}u_j^{*}, \\
E_{ij}^{(\kappa)} &= b^{\kappa 0}\delta_{ij} + \sum_{\lambda}(b^{\kappa\lambda}\delta_{ijkl}P_{l,k}^{(\lambda)} + b_{12}^{\kappa\lambda}\delta_{ij}P_{k,k}^{(\lambda)} + 2b_{44}^{\kappa\lambda}P_{(j,i)}^{(\lambda)} + 2b_{77}^{\kappa\lambda}P_{[j,i]}^{(\lambda)}) \\
&\quad + 2d^{*\kappa}\omega_{ij}^{*} + \sum_{\lambda}(d^{\kappa\lambda}\delta_{ijkl}S_{kl}^{(\lambda)} + d_{12}^{\kappa\lambda}\delta_{ij}S_{kk}^{(\lambda)} + 2d_{44}^{\kappa\lambda}S_{ij}^{(\lambda)}), \\
T_j^{*} &= \sum_{\lambda}a^{*\lambda}P_j^{(\lambda)} + a^{**}u_j^{*}, \\
T_{ij}^{*} &= 2\sum_{\lambda}d^{*\lambda}P_{[j,i]}^{(\lambda)} + 2c^{**}\omega_{ij}^{*}.
\end{aligned} \tag{22}$$

We shall assume that, in the initial state, i.e. when

$$P_i^{(\kappa)}, P_{j,i}^{(\kappa)}, S_{ij}^{(\kappa)}, u_i^{*}, \omega_{ij}^{*}, \varphi_{,i}, f_i^{(\kappa)}, E_i^{0} = 0, \tag{23}$$

there is no resultant force across any surface—exterior or interior. That is,

$$t_j^{(1)} + t_j^{(2)} = 0.$$

Then, from the first of (16),

$$n_i T_{ij}^{(1)} + n_i T_{ij}^{(2)} = 0;$$

so that, from the first of (22),

$$c^{10} + c^{20} = 0. \tag{24}$$

Accordingly, from (23) and (24), in the initial state:

$$E_i^{(\kappa)}, T_i^*, T_{ij}^* = 0, \qquad T_{ij}^{(1)} + T_{ij}^{(2)} = 0,$$

but there is a self-equilibrated

$$E_{ij}^{(\kappa)} = b^{\kappa 0} \delta_{ij}$$

in each component continuum.

5. SURFACE ENERGY OF DEFORMATION AND POLARIZATION

In a state of equilibrium, the total energy in V'' is, from (2),

$$\mathscr{H} = \int_V W^L \, \mathrm{d}V + \tfrac{1}{2} \int_{V''} \varepsilon_0 \varphi_{,i} \varphi_{,i} \, \mathrm{d}V. \tag{25}$$

We can write W^L in the form

$$2W^L = \sum_\kappa (T_{ij}^{(\kappa)} S_{ij}^{(\kappa)} - E_i^{(\kappa)} P_i^{(\kappa)} + E_{ij}^{(\kappa)} P_{j,i}^{(\kappa)}) + T_i^* u_i^* + T_{ij}^* \omega_{ij}^* + \sum_\kappa b^{\kappa 0} P_{i,i}^{(\kappa)} + c^{20} (S_{ii}^{(2)} - S_{ii}^{(1)}).$$

Then, by the same procedure as that employed in arriving at (13),

$$\int_V W^L \, \mathrm{d}V = -\tfrac{1}{2} \sum_\kappa \int_V \{[T_{ij,i}^{(\kappa)} + (-1)^\kappa (T_{ij,i}^* - T_j^*)] u_j^{(\kappa)} + (E_j^{(\kappa)} + E_{ij,i}^{(\kappa)}) P_j^{(\kappa)}\} \, \mathrm{d}V$$

$$+ \tfrac{1}{2} \sum_\kappa \int_S n_i \{[T_{ij}^{(\kappa)} + (-1)^\kappa T_{ij}^*] u_j^{(\kappa)} + E_{ij}^{(\kappa)} P_j^{(\kappa)}\} \, \mathrm{d}S$$

$$+ \tfrac{1}{2} \sum_\kappa \int_S n_i (b^{\kappa 0} P_i^{(\kappa)} + c^{20} u_i^*) \, \mathrm{d}S. \tag{26}$$

Also,

$$\int_{V''} \varphi_{,i} \varphi_{,i} \, \mathrm{d}V = -\int_{V''} \varphi_{,ii} \varphi \, \mathrm{d}V + \int_S n_i [\varphi_{,i}] \varphi \, \mathrm{d}S. \tag{27}$$

Inserting (26) and (27) in (25) and applying the equations of equilibrium [i.e. (14) with $u_{j,tt}^{(\kappa)} = 0$], in the absence of external forces ($f_j^{(\kappa)}, E_j^0 = 0$), we find

$$2\mathscr{H} = -\sum_\kappa \int_V [(-1)^\kappa q^* \varphi_{,i} u_i^{(\kappa)} + \varphi_{,i} P_i^{(\kappa)} + (P_{i,i}^{(\kappa)} + q^* u_{i,i}^*) \varphi] \, \mathrm{d}V$$

$$+ \sum_\kappa \int_S n_i \{[T_{ij}^{(\kappa)} + (-1)^\kappa T_{ij}^*] u_j^{(\kappa)} + E_{ij}^{(\kappa)} P_j^{(\kappa)} + \varepsilon_0 [\varphi_{,i}] \varphi\} \, \mathrm{d}S$$

$$+ \sum_\kappa \int_S n_i (b^{\kappa 0} P_i^{(\kappa)} + c^{20} u_i^*) \, \mathrm{d}S.$$

Now,

$$\int_V P_{i,i}^{(\kappa)}\varphi \, dV = -\int_V \varphi_{,i}P_i^{(\kappa)} \, dV + \int_S n_i P_i^{(\kappa)}\varphi \, dS,$$

$$\int_V q^*(u_i^*\varphi_{,i}+u_{i,i}^*\varphi) \, dV = \int_S n_i q^* u_i^* \varphi \, dS.$$

Hence,

$$2\mathscr{W} = \sum_\kappa \int_S n_i\{[T_{ij}^{(\kappa)}+(-1)^\kappa T_{ij}^*]u_j^{(\kappa)}+E_{ij}^{(\kappa)}P_j^{(\kappa)}+(\varepsilon_0[\varphi_{,i}]-P_i^{(\kappa)}-q^*u_i^*)\varphi\} \, dS$$

$$+ \sum_\kappa \int_S n_i(b^{\kappa 0}P_i^{(\kappa)}+c^{20}u_i^*) \, dS. \tag{28}$$

From (16), the first integral in (28) vanishes if the boundary is entirely free. Then

$$2\mathscr{W} = \sum_\kappa \int_S n_i(b^{\kappa 0}P_i^{(\kappa)}+c^{20}u_i^*) \, dS.$$

Accordingly, the surface energy of deformation and polarization, per unit area, is

$$W^S = \tfrac{1}{2}n_i[b^{10}P_i^{(1)}+b^{20}P_i^{(2)}+c^{20}u_i^*]_S. \tag{29}$$

6. WAVE MOTION

The equations of motion in terms of $u_i^{(\kappa)}$, $P_i^{(\kappa)}$ and φ are obtained by substituting the constitutive equations (22) into the field equations (14), with the result, for each κ,

$$\sum_\lambda [c^{\kappa\lambda}\delta_{ijkl}u_{l,ki}^{(\lambda)}+c_{12}^{\kappa\lambda}u_{i,ij}^{(\lambda)}+c_{44}^{\kappa\lambda}(u_{j,ii}^{(\lambda)}+u_{i,ij}^{(\lambda)})]$$

$$+ \sum_\lambda [d^{\lambda\kappa}\delta_{ijkl}P_{l,ki}^{(\lambda)}+d_{12}^{\lambda\kappa}P_{i,ij}^{(\lambda)}+d_{44}^{\lambda\kappa}(P_{j,ii}^{(\lambda)}+P_{i,ij}^{(\lambda)})]$$

$$+(-1)^\kappa \sum_\lambda [d^{*\lambda}(P_{j,ii}^{(\lambda)}-P_{i,ij}^{(\lambda)})-(-1)^\lambda c^{**}(u_{j,ii}^{(\lambda)}-u_{i,ij}^{(\lambda)})]$$

$$-(-1)^\kappa[a^{*1}P_j^{(1)}+a^{*2}P_j^{(2)}+a^{**}(u_j^{(2)}-u_j^{(1)})+q^*\varphi_{,j}-q^*E_j^0]+f_j^{(\kappa)} = \rho^{(\kappa)}u_{j,tt}^{(\kappa)},$$

$$\sum_\lambda [d^{\kappa\lambda}\delta_{ijkl}u_{l,ki}^{(\lambda)}+d_{12}^{\kappa\lambda}u_{i,ij}^{(\lambda)}+d_{44}^{\kappa\lambda}(u_{j,ii}^{(\lambda)}+u_{i,ij}^{(\lambda)})+(-1)^\lambda d^{*\kappa}(u_{j,ii}^{(\lambda)}-u_{i,ij}^{(\lambda)})] \tag{30}$$

$$+ \sum_\lambda [b^{\kappa\lambda}\delta_{ijkl}P_{l,ki}^{(\lambda)}+b_{12}^{\kappa\lambda}P_{i,ij}^{(\lambda)}+b_{44}^{\kappa\lambda}(P_{j,ii}^{(\lambda)}+P_{i,ij}^{(\lambda)})+b_{77}^{\kappa\lambda}(P_{j,ii}^{(\lambda)}-P_{i,ij}^{(\lambda)})]$$

$$-a_{11}^{1\kappa}P_j^{(1)}-a_{11}^{2\kappa}P_j^{(2)}-a^{**}(u_j^{(2)}-u_j^{(1)})-\varphi_{,j}+E_j^0 = 0,$$

$$-\varepsilon_0\varphi_{,ii}+P_{i,i}^{(1)}+P_{i,i}^{(2)}+q^*(u_{i,i}^{(2)}-u_{i,i}^{(1)}) = 0.$$

The essential features of wave motion are revealed by an examination of plane waves in, say, the x_1, or (100), direction:

$$u_j^{(\kappa)} = A_j^{(\kappa)} e^{i(\xi x_1-\omega t)}, \qquad P_j^{(\kappa)} = B_j^{(\kappa)} e^{i(\xi x_1-\omega t)}, \qquad \varphi = C e^{i(\xi x_1-\omega t)} \tag{31}$$

and $f_j^{(\kappa)} = E_j^0 = 0$. With these functions, the five equations (30) reduce to those for longitudinal waves if $j = 1$ and transverse waves if $j = 2$ or 3. Thus:

Longitudinal $(j = 1)$

$$c_{11}^{11}u_{1,11}^{(1)} + c_{11}^{12}u_{1,11}^{(2)} + d_{11}^{11}P_{1,11}^{(1)} + d_{11}^{21}P_{1,11}^{(2)} + a^{*1}P_1^{(1)} + a^{*2}P_1^{(2)} + a^{**}(u_1^{(2)} - u_1^{(1)}) + q^*\varphi_{,1}$$
$$= \rho^{(1)}u_{1,tt}^{(1)},$$

$$c_{11}^{21}u_{1,11}^{(1)} + c_{11}^{22}u_{1,11}^{(2)} + d_{11}^{12}P_{1,11}^{(1)} + d_{11}^{22}P_{1,11}^{(2)} - a^{*1}P_1^{(1)} - a^{*2}P_1^{(2)} - a^{**}(u_1^{(2)} - u_1^{(1)}) - q^*\varphi_{,1}$$
$$= \rho^{(2)}u_{1,tt}^{(2)},\tag{32}$$

$$d_{11}^{11}u_{1,11}^{(1)} + d_{11}^{12}u_{1,11}^{(2)} + b_{11}^{11}P_{1,11}^{(1)} + b_{11}^{12}P_{1,11}^{(2)} - a_{11}^{11}P_1^{(1)} - a_{11}^{12}P_1^{(2)} - a^{*1}(u_1^{(2)} - u_1^{(1)}) - \varphi_{,1} = 0,$$

$$d_{11}^{21}u_{1,11}^{(1)} + d_{11}^{22}u_{1,11}^{(2)} + b_{11}^{21}P_{1,11}^{(1)} + b_{11}^{22}P_{1,11}^{(2)} - a_{11}^{21}P_1^{(1)} - a_{11}^{22}P_1^{(2)} - a^{*2}(u_1^{(2)} - u_1^{(1)}) - \varphi_{,1} = 0,$$

$$P_{1,1}^{(1)} + P_{1,1}^{(2)} + q^*(u_{1,1}^{(2)} - u_{1,1}^{(1)}) - \varepsilon_0\varphi_{,11} = 0.$$

Transverse $(j = 2)$

$$(c_{44}^{11} - c^{**})u_{2,11}^{(1)} + (c_{44}^{12} + c^{**})u_{2,11}^{(2)} + (d_{44}^{11} - d^{*1})P_{2,11}^{(2)} + (d_{44}^{21} - d^{*2})P_{2,11}^{(2)}$$
$$+ a^{*1}P_2^{(1)} + a^{*2}P_2^{(2)} + a^{**}(u_2^{(2)} - u_2^{(1)}) = \rho^{(1)}u_{2,tt}^{(1)},$$

$$(c_{44}^{21} + c^{**})u_{2,11}^{(1)} + (c_{44}^{22} - c^{**})u_{2,11}^{(2)} + (d_{44}^{12} + d^{*1})P_{2,11}^{(1)} + (d_{44}^{22} + d^{*2})P_{2,11}^{(2)}$$
$$- a^{*1}P_2^{(1)} - a^{*2}P_2^{(2)} - a^{**}(u_2^{(2)} - u_2^{(1)}) = \rho^{(2)}u_{2,tt}^{(2)},$$

$$(d_{44}^{11} - d^{*1})u_{2,11}^{(1)} + (d_{44}^{12} + d^{*1})u_{2,11}^{(2)} + (b_{44}^{11} + b_{77}^{11})P_{2,11}^{(1)} + (b_{44}^{12} + b_{77}^{12})P_{2,11}^{(2)}\tag{33}$$
$$- a_{11}^{11}P_2^{(1)} - a_{11}^{12}P_2^{(2)} - a^{*1}(u_2^{(2)} - u_1^{(1)}) = 0,$$

$$(d_{44}^{21} - d^{*2})u_{2,11}^{(1)} + (d_{44}^{22} + d^{*2})u_{2,11}^{(2)} + (b_{44}^{21} + b_{77}^{21})P_{2,11}^{(1)} + (b_{44}^{22} + b_{77}^{22})P_{2,11}^{(2)}$$
$$- a_{11}^{21}P_2^{(1)} - a_{11}^{22}P_2^{(2)} - a^{*2}(u_2^{(2)} - u_2^{(1)}) = 0.$$

It may be noted that the Maxwell self-field is coupled to the mechanical displacement in the longitudinal waves, but not in the transverse waves.

Upon substituting (31) in (33) and eliminating $A_2^{(\kappa)}$ and $B_2^{(\kappa)}$, we find the dispersion relation for transverse waves:

$$\Delta_t = \begin{vmatrix} \rho^{(1)}\omega^2 - a^{**} - (c_{44}^{11} - c^{**})\xi^2 & a^{**} - (c_{44}^{12} + c^{**})\xi^2 & a^{*1} - (d_{44}^{11} - d^{*1})\xi^2 & a^{*2} - (d_{44}^{21} - d^{*2})\xi^2 \\ a^{**} - (c_{44}^{21} + c^{**})\xi^2 & \rho^{(2)}\omega^2 - a^{**} - (c_{44}^{22} - c^{**})\xi^2 & -a^{*1} - (d_{44}^{12} + d^{*1})\xi^2 & -a^{*2} - (d_{44}^{22} + d^{*2})\xi^2 \\ a^{*1} - (d_{44}^{11} - d^{*1})\xi^2 & -a^{*1} - (d_{44}^{12} + d^{*1})\xi^2 & -a_{11}^{11} - (b_{44}^{11} + b_{77}^{11})\xi^2 & -a_{11}^{12} - (b_{44}^{12} + b_{77}^{12})\xi^2 \\ a^{*2} - (d_{44}^{21} - d^{*2})\xi^2 & -a^{*2} - (d_{44}^{22} + d^{*2})\xi^2 & -a_{11}^{21} - (b_{44}^{21} + b_{77}^{21})\xi^2 & -a_{11}^{22} - (b_{44}^{22} + b_{77}^{22})\xi^2 \end{vmatrix} = 0.\tag{34}$$

This is a quartic equation in ξ^2. Of the four branches, two are real: one acoustical and one optical, as may be verified by showing that one real branch passes through $\xi = 0$, $\omega = 0$ and one through $\xi = 0$, $\omega \neq 0$. We find, in fact,

$$\lim_{\omega,\xi \to 0} \Delta_t = \lim_{\omega,\xi \to 0} [(c_{44}^{11} + c_{44}^{22} + 2c_{44}^{12})\xi^2 - (\rho^{(1)} + \rho^{(2)})\omega^2]D,$$

where

$$D = \begin{vmatrix} a_{11}^{11} & a_{11}^{12} & a^{*1} \\ a_{11}^{21} & a_{11}^{22} & a^{*2} \\ a^{*1} & a^{*2} & a^{**} \end{vmatrix}.$$

Hence, there is a transverse acoustical branch with the limiting, low frequency behavior

$$\omega = \xi[(c_{44}^{11}+c_{44}^{22}+2c_{44}^{12})/(\rho^{(1)}+\rho^{(2)})]^{1/2}. \tag{35}$$

It may be seen, from (35), that the usual low frequency shear stiffness, c_{44}, is given by

$$c_{44} = c_{44}^{11}+c_{44}^{22}+2c_{44}^{12},$$

i.e. the sum of the shear stiffnesses of the two component continua augmented by twice the intercomponent shear stiffness. Further

$$\lim_{\xi \to 0} \Delta_t = \omega^2[\rho^{(1)}\rho^{(2)}\omega^2(a_{11}^{11}a_{11}^{22}-a_{11}^{12}a_{11}^{21})-(\rho^{(1)}+\rho^{(2)})D].$$

Thus, there is a transverse optical branch with limiting (infrared absorption) frequency

$$\omega = [D/\bar{\rho}(a_{11}^{11}a_{11}^{22}-a_{11}^{12}a_{11}^{21})]^{1/2}, \tag{36}$$

where $\bar{\rho}$ is the reduced density:

$$\bar{\rho} = \rho^{(1)}\rho^{(2)}/(\rho^{(1)}+\rho^{(2)}).$$

For the longitudinal waves, substitution of (31) in (32) and elimination of $A_1^{(\kappa)}$, $B_1^{(\kappa)}$ and C yields a dispersion relation the same as that for transverse waves except that the subscript 44 is changed to 11, the constants d^{**}, c^{**} and $b_{77}^{\kappa\lambda}$ are zero, the constants $a_{11}^{\kappa\lambda}$ are replaced by $a_{11}^{\kappa\lambda}+\varepsilon_0^{-1}$, the constants $a^{*\kappa}$ are replaced by $a^{*\kappa}+q^*\varepsilon_0^{-1}$ and a^{**} is replaced by $a^{**}+(q^*)^2\varepsilon_0^{-1}$. Subject to these changes, the low frequency behavior of the longitudinal acoustical branch and the long wave limit of the longitudinal optical branch are given by (35) and (36), respectively. Note that the constants $\varepsilon_0 a_{11}^{\kappa\lambda}$ are reciprocal dielectric susceptibilities, as may be seen from the expression for $E_j^{(\kappa)}$ in the constitutive relations (22). Note, also, that q^* is zero in a non-ionic crystal.

It should be observed that the real parts of the optical branches have no valid role in solutions, of the equations of motion, in which optical and acoustical modes are coupled, say through boundary conditions. The frequencies of the two types of mode must be the same, when they are coupled, but any frequency on a real segment of an optical branch is associated with a wave length, on an acoustical branch, that is too short to be within the range of validity of the continuum theory. In such coupled situations, there is an upper limit of frequency, set by the wave length limitation of the acoustic branches, to which the solution is restricted. Below such a frequency, the optical branches are imaginary or complex and correspond to displacements and polarizations confined essentially to the neighborhood of the boundary with exponential, or oscillating exponential, spatial decay into the interior.

The special field equations governing the behavior of the continuum at infinite wave length and high frequencies may be obtained from (30) by omitting all spatial derivative terms, after employing (3), with the result:

$$a^{*1}P_i^{(1)}+a^{*2}P_i^{(2)}+a^{**}(u_i^{(2)}-u_i^{(1)})-q^*E_i^{MS} = \rho^{(1)}u_{i,tt}^{(1)},$$

$$-a^{*1}P_i^{(1)}-a^{*2}P_i^{(2)}-a^{**}(u_i^{(2)}-u_i^{(1)})+q^*E_i^{MS} = \rho^{(2)}u_{i,tt}^{(2)},$$

$$a_{11}^{11}P_i^{(1)}+a_{11}^{12}P_i^{(2)}+a^{*1}(u_i^{(2)}-u_i^{(1)})-E_i^{MS} = 0,$$

$$a_{11}^{21}P_i^{(1)}+a_{11}^{22}P_i^{(2)}+a^{*2}(u_i^{(2)}-u_i^{(1)})-E_i^{MS} = 0.$$

These are equivalent to the equations, given by Born and Huang [4], from which a dispersion formula for the dielectric constant is obtained. Thus, the weighted difference between the first two equations gives

$$-\bar{\rho}u_{i,tt}^* = a^{*1}P_i^{(1)} + a^{*2}P_i^{(2)} + a^{**}u_i^* - q^*E_i^{MS}$$

and the second two equations yield

$$P_i^{(1)} = [(a_{11}^{22} - a_{11}^{21})E_i^{MS} - (a_{11}^{22}a^{*1} - a_{11}^{21}a^{*2})u_i^*]/(a_{11}^{11}a_{11}^{22} - a_{11}^{12}a_{11}^{21}),$$

$$P_i^{(2)} = [(a_{11}^{11} - a_{11}^{12})E_i^{MS} - (a_{11}^{11}a^{*2} - a_{11}^{12}a^{*1})u_i^*]/(a_{11}^{11}a_{11}^{22} - a_{11}^{12}a_{11}^{21}).$$

Substituting the latter two in the former and defining the total polarization density as

$$P_i = P_i^{(1)} + P_i^{(2)} + q^*u_i^*,$$

we find equations of the same form as (7.1) and (7.2) in Born and Huang [4]:

$$\bar{\rho}u_{i,tt}^* = \beta_{11}u_i^* + \beta_{12}E_i^{MS},$$

$$P_i = \beta_{21}u_i^* + \beta_{22}E_i^{MS},$$

where

$$\beta_{11} = -D/(a_{11}^{11}a_{11}^{22} - a_{11}^{12}a_{11}^{21}), \qquad \beta_{22} = (a_{11}^{11} + a_{11}^{22} - 2a_{11}^{12})/(a_{11}^{11}a_{11}^{22} - a_{11}^{12}a_{11}^{21}),$$

$$\beta_{12} = \beta_{21} = -[a_{11}^{11}a^{*2} + a_{11}^{22}a^{*1} - (a^{*1} + a^{*2})a_{11}^{12} - q^*(a_{11}^{11}a_{11}^{22} - a_{11}^{22}a_{11}^{21})]/(a_{11}^{11}a_{11}^{22} - a_{11}^{12}a_{11}^{21}).$$

7. ONE-DIMENSIONAL LATTICE

The purpose of this section is to show, for the one-dimensional, longitudinal case, that the equations of motion (32), exhibited in the preceding section, are the long wave limit of the equations of motion of an NaCl-type lattice of the kind devised by Cochran [5] based on the Dick–Overhauser [6] shell model of the atom: a core, comprising the nucleus and inner electrons, surrounded by a shell of outer electrons—with the electronic polarization proportional to the relative displacement of the shell with respect to the core. In addition to the intra-atomic interaction producing the electronic polarization, certain interatomic core–core, shell–shell and core–shell interactions are taken into account. The one-dimensional NaCl-type lattice is most conveniently represented by two lines of alternating atoms (positive and negative ions, in the case of an ionic crystal) with one atom of each type at each lattice site, as shown in Fig. 4, where the two types of atom are identified by the digits 1 and 2. Nearest neighbor interactions between unlike (adjacent) atoms in each line and next nearest neighbor interactions between like atoms in the two lines are those taken into account, but no interactions between the unlike atoms at the same site are considered. With each of p and q equal to 1 or 2, the force constants of the interactions are denoted by α_p for the intra-atomic core–shell interactions and $\beta_{pq}, \gamma_{pq}, \delta_{pq}$ for the core–core, core–shell, and shell–shell interatomic interactions, respectively, between like atoms for $p = q$ and unlike atoms for $p \neq q$. We note that $\beta_{pq} = \beta_{qp}$ and $\delta_{pq} = \delta_{qp}$ but $\gamma_{pq} \neq \gamma_{qp}$. The two lines of atoms are taken to be parallel to the x_1 axis with the atom sites at $x_1 = na$, where n is a positive or negative integer. The displacements of the cores and shells of the atoms at $x_1 = na$ are denoted by $u_n^{(\kappa)}$ and $s_n^{(\kappa)}$, where $\kappa = 1, 2$ to designate the atoms of types 1 and 2 (1 for the positive ion and 2 for the negative ion, in the case of an ionic crystal).
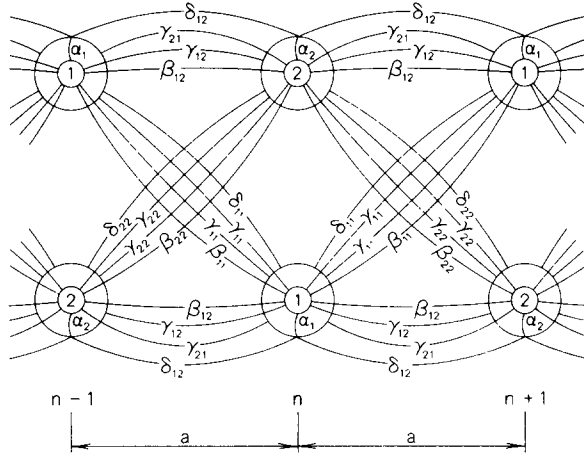
FIG. 4. One-dimensional NaCl-type lattice of shell-model atoms.

The equation of motion of the nth atom of type 1 is obtained by equating its inertia force to the sum of the forces on its core and shell exerted by the cores and shells of the two nearest neighbor (unlike) atoms, the two next nearest neighbor (like) atoms and the Maxwell, electric self-field at $x_1 = na$:

$$\beta_{11}(u_{n+1}^{(1)} - u_n^{(1)}) + \gamma_{11}(s_{n+1}^{(1)} - s_n^{(1)} + u_{n+1}^{(1)} - u_n^{(1)}) + \delta_{11}(s_{n+1}^{(1)} - s_n^{(1)})$$

$$- \beta_{11}(u_n^{(1)} - u_{n-1}^{(1)}) - \gamma_{11}(u_n^{(1)} - u_{n-1}^{(1)} + s_n^{(1)} - s_{n-1}^{(1)}) - \delta_{11}(s_n^{(1)} - s_{n-1}^{(1)})$$

$$+ \beta_{12}(u_{n+1}^{(2)} - u_n^{(1)}) + \gamma_{12}(s_{n+1}^{(2)} - u_n^{(1)}) + \gamma_{21}(u_{n+1}^{(2)} - s_n^{(1)}) + \delta_{12}(s_{n+1}^{(2)} - s_n^{(1)})$$

$$- \beta_{12}(u_n^{(1)} - u_{n-1}^{(2)}) - \gamma_{12}(u_n^{(1)} - s_{n-1}^{(2)}) - \gamma_{21}(s_n^{(1)} - u_{n-1}^{(2)}) - \delta_{12}(s_n^{(1)} - s_{n-1}^{(2)}) - q^* E_n^{MS}$$

$$= m_1 u_{n,tt}^{(1)}. \tag{37}$$

Similarly, for the shell, alone, of the type 1 atom:

$$\alpha_1(u_n^{(1)} - s_n^{(1)}) + \gamma_{11}(u_{n+1}^{(1)} - s_n^{(1)}) + \delta_{11}(s_{n+1}^{(1)} - s_n^{(1)}) - \gamma_{11}(s_n^{(1)} - u_{n-1}^{(1)}) - \delta_{11}(s_n^{(1)} - s_{n-1}^{(1)})$$

$$+ \gamma_{21}(u_{n+1}^{(2)} - s_n^{(1)}) + \delta_{12}(s_{n+1}^{(2)} - s_n^{(1)}) - \gamma_{21}(s_n^{(1)} - u_{n-1}^{(2)}) - \delta_{12}(s_n^{(1)} - s_{n-1}^{(2)}) + q E_n^{MS} = 0, \tag{38}$$

where q is the electronic charge and the mass of the shell is neglected.

We adopt the following definitions of the second central difference operation, the electronic polarization densities and the mass densities:

$$\Delta^2 f_n = (f_{n+1} + f_{n-1} - 2f_n)/a^2,$$
$$P_n^{(\kappa)} = (s_n^{(\kappa)} - u_n^{(\kappa)})q/a^3, \tag{39}$$
$$\rho^{(\kappa)} = m_\kappa/a^3, \qquad \kappa = 1, 2,$$

and also make the following identifications:

$$a_{11}^{11} = (\alpha_1 + 2\gamma_{11} + 2\gamma_{21} + 2\delta_{12})a^3 q^{-2}, \quad b_{11}^{12} = a_{11}^{12} a^2/2 = \delta_{12} a^5 q^{-2},$$

$$b_{11}^{11} = \delta_{11} a^5 q^{-2}, \qquad\qquad\qquad c_{11}^{12} = a^{**} a^2/2 = (\beta_{12} + \gamma_{12} + \gamma_{21} + \delta_{12})a^{-1},$$

$$c_{11}^{11} = (\beta_{11} + 2\gamma_{11} + \delta_{11})a^{-1}, \qquad d_{11}^{21} = a^{*2} a^2/2 = (\gamma_{12} + \delta_{12})a^2 q^{-1}, \qquad (40)$$

$$d_{11}^{11} = (\gamma_{11} + \delta_{11})a^2 q^{-1}, \qquad\qquad d_{11}^{12} = -a^{*1} a^2/2 = (\gamma_{21} + \delta_{12})a^2 q^{-1}.$$

Then (37) and (38) can be written as

$$c_{11}^{11}\Delta^2 u_n^{(1)} + c_{11}^{12}\Delta^2 u_n^{(2)} + d_{11}^{11}\Delta^2 P_n^{(1)} + d_{11}^{21}\Delta^2 P_n^{(2)} + a^{*1} P_n^{(1)}$$
$$+ a^{*2} P_n^{(2)} + a^{**}(u_n^{(2)} - u_n^{(1)}) - q^* E_n^{MS} = \rho^{(1)} u_{n,tt}^{(1)}, \qquad (41)$$

$$d_{11}^{11}\Delta^2 u_n^{(1)} + d_{11}^{12}\Delta^2 u_n^{(2)} + b_{11}^{11}\Delta^2 P_n^{(1)} + b_{11}^{12}\Delta^2 P_n^{(2)} - a_{11}^{11} P_n^{(1)}$$
$$- a_{11}^{12} P_n^{(2)} - a^{*1}(u_n^{(2)} - u_n^{(1)}) + E_n^{MS} = 0. \qquad (42)$$

In the same way, for the type 2 atom:

$$c_{11}^{21}\Delta^2 u_n^{(1)} + c_{11}^{22}\Delta^2 u_n^{(2)} + d_{11}^{12}\Delta^2 P_n^{(1)} + d_{11}^{22}\Delta^2 P_n^{(2)} - a^{*1} P_n^{(1)}$$
$$- a^{*2} P_n^{(2)} - a^{**}(u_n^{(2)} - u_n^{(1)}) + q^* E_n^{MS} = \rho^{(2)} u_{n,tt}^{(2)}. \qquad (43)$$

$$d_{11}^{21}\Delta^2 u_n^{(1)} + d_{11}^{22}\Delta^2 u_n^{(2)} + b_{11}^{21}\Delta^2 P_n^{(1)} + b_{11}^{22}\Delta^2 P_n^{(2)} - a_{11}^{21} P_n^{(1)}$$
$$- a_{11}^{22} P_n^{(2)} - a^{*2}(u_n^{(2)} - u_n^{(1)}) + E_n^{MS} = 0, \qquad (44)$$

where, in addition to (39) and (40), we identify:

$$a_{11}^{22} = (\alpha_2 + 2\gamma_{22} + 2\gamma_{12} + 2\delta_{12})a^3 q^{-2}, \quad b_{11}^{22} = \delta_{22} a^5 q^{-2}, \qquad (45)$$
$$c_{11}^{22} = (\beta_{22} + 2\gamma_{22} + \delta_{22})a^{-1}, \qquad d_{11}^{22} = (\gamma_{22} + \delta_{22})a^2 q^{-1}.$$

Also, as in [7], the charge equation may be written as

$$-\varepsilon_0 \partial_- \partial_+ \varphi_n + \partial_- [P_n^{(1)} + P_n^{(2)} + q^*(u_n^{(2)} - u_n^{(1)})] = 0, \qquad (46)$$

where ∂_+ and ∂_- are the Taylor series expansions of the derivative $\partial/\partial x_1$ in terms of forward and backward differences, respectively.

In the long wave limit,

$$u_n^{(\kappa)} \to u_1^{(\kappa)}(x_1), \qquad P_n^{(\kappa)} \to P_1^{(\kappa)}(x_1), \qquad E_n^{MS} \to E_1^{MS}(x_1) = -\partial\varphi/\partial x_1,$$
$$\Delta^2 f_n \to \partial^2 f(x_1)/\partial x_1^2, \qquad \partial_\pm \to \partial/\partial x_1. \qquad (47)$$

Then (41), (43), (42), (44) and (46), in that order, reduce to the five equations (32) in the order given.

Alternatively, in the long wave, low frequency limit, we have, in addition to (47),

$$u_1^{(1)} = u_1^{(2)}, \qquad P_1^{(1)} = P_1^{(2)}.$$

Then, with the notations

$$u_1 = u_1^{(1)} = u_1^{(2)}, \qquad \tfrac{1}{2} P_1 = P_1^{(1)} = P_1^{(2)}, \qquad \rho = \rho^{(1)} + \rho^{(2)},$$

$$a_{11} = \tfrac{1}{4}(a_{11}^{11} + a_{11}^{22} + 2a_{11}^{12}), \qquad b_{11} = \tfrac{1}{4}(b_{11}^{11} + b_{11}^{22} + 2b_{11}^{12}),$$

$$c_{11} = c_{11}^{11} + c_{11}^{22} + 2c_{11}^{12}, \qquad d_{11} = \tfrac{1}{2}(d_{11}^{11} + d_{11}^{22} + d_{11}^{12} + d_{11}^{21}),$$

the sum of (41) and (43), the sum of (42) and (44) and, finally, (46) become, respectively,

$$c_{11}u_{1,11} + d_{11}P_{1,11} = \rho u_{1,tt},$$

$$d_{11}u_{1,11} + b_{11}P_{1,11} - a_{11}P_1 - \varphi_{,1} = 0, \qquad (48)$$

$$-\varepsilon_0\varphi_{,11} + P_{1,1} = 0.$$

These are the equations found in [2] for longitudinal waves in a simple (as opposed to compound) dielectric continuum, with symmetry $m3m$, when the polarization gradient is taken into account. Thus, the long wave limit of the equations of the one-dimensional, diatomic lattice yields the equations for longitudinal waves in the compound continuum when no restriction is placed on the frequency; whereas the long wave, low frequency limit yields the equations of the simple continuum. In a three-dimensional treatment, Askar et al. [12] showed the connection between the equations of the NaCl-type lattice of polarizable atoms and the equations in [2]. A similar investigation, not restricted to low frequencies, would, presumably, reveal the connection with the three-dimensional continuum equations of the present paper.

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Абстракт—Обобщаются уравнения поля и граничнве условия континуальной теории упругих диэлектриков, учитывающей влияние градиента поляризации, с целью применения ее к сложному материалу. Получается формула для поверхностной энергии деформации и поляризации кубического кристалла. Решение задачи плоских волн приводит к отождествлению оптических продольных и поперечных ветвей, а также акустических, для зависимости дисперсии. Строится одномерная модель кристаллической сети типа NaCl оболочечной модели атомов. Уравнения движения этой модели, выраженные в конечных разностях, соответствуют уравнениям сплошной теории, в смысле ограничения длины волны, без ограничений низкой частоты.