# CONTINUUM AND LATTICE THEORIES OF INFLUENCE OF ELECTROMECHANICAL COUPLING ON CAPACITANCE OF THIN DIELECTRIC FILMS

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**Abstract**—In this paper, it is suggested that an anomaly, observed by C. A. Mead in measurements of the capacitance of thin dielectric films, may be due to an electromechanical effect not accounted for in the classical, continuum theory of piezoelectricity. A solution of equations that include the additional effect is shown to be capable of accommodating the experimental data. It is demonstrated that the augmented equations, rather than the classical ones, are a continuum approximation to the equations of a lattice of shell-model atoms. Analogous equilibrium solutions of the lattice and continuum equations are almost identical.

## INTRODUCTION

ACCORDING to the classical theory of electrostatics, the capacitance of a metal–dielectric–metal sandwich is inversely proportional to the thickness of the dielectric, so that a graph of inverse capacitance vs. thickness is a straight line through the origin. In a series of experiments with a variety of thin, dielectric films, Mead [1, 2, 3] found a different result. His experimental data fall on straight lines which, if extended to zero thickness, have positive intercepts of inverse capacitance, as illustrated in Fig. 1. Initially [1], Mead suggested that the anomaly might be due to penetration of the electric field into the electrodes; but subsequently [3, 4] he abandoned that view, although it has been supported by Ku
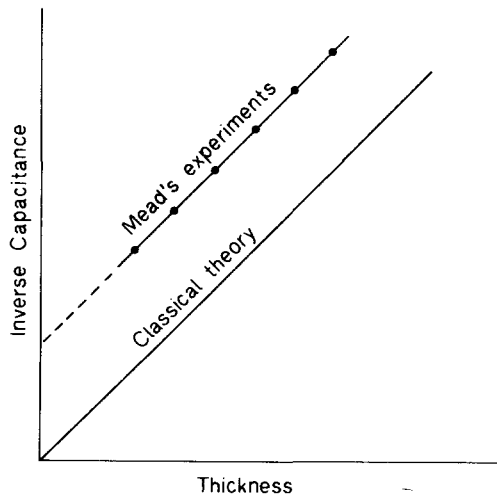


FIG. 1. Capacitance anomaly discovered by Mead [1].

and Ullman [5]. One purpose of the present paper is to show that a linear, electromechanical interaction, not accounted for in the classical, continuum theory of piezoelectricity, can produce an apparent anomaly of the same character.

The equations of classical piezoelectricity are based, in part, on the assumption that the stored energy of deformation and polarization is a function of only the strain and polarization. If the functional dependence is extended to include the polarization gradient, there can be an additional electromechanical interaction represented, in the energy, by a product of strain and polarization gradient. Since the material coefficient of such a product is a tensor of even rank, the term survives even for centrosymmetric materials—in which there is no classical piezoelectric effect. The extended equations accommodate a surface phenomenon, with a spatial exponential decay, which can become important when a dimension of the dielectric solid is small. In the first part of this paper, a solution of the extended equations, for a boundary value problem representative of Mead's experiments, is described and it is shown that the surface effect can contribute to an apparent anomaly of the type found by Mead. The appearance of the surface effect, in the solution, depends on a phenomenological constant introduced into a boundary condition to account for the influence of the properties of the metal and the metal–dielectric interface on the polarization of the dielectric at the interface.

In the second part of the paper, the same problem is treated from the point of view of a one-dimensional lattice theory, of the Cochran [6] type, based on the Dick–Overhauser [7] shell-model of the atom: a core, comprising the nucleus and inner electrons, surrounded by a shell of outer electrons. In the lattice, there are intra-atomic core–shell interactions and interatomic core–core, core–shell and shell–shell interactions. It is shown that the equations of the lattice have, as a continuum approximation, not the equations of classical piezoelectricity, but the extended equations including the contribution of the polarization gradient to the stored energy. The additional electromechanical and surface effects stem primarily from the shell–shell interaction. The solution of the difference equations of the lattice, analogous to the boundary value problem solved in the first part, yields a relation between capacitance and thickness of exactly the same form as that found in the continuum solution. The only difference in detail is in the magnitude of a length parameter characteristic of the material; and even this difference effectively disappears if the length parameter is at least as large as the distance between nearest neighbor atoms. The length parameter is the magnitude of the reciprocal wave number, at zero frequency, of the imaginary branch of the dispersion relation for longitudinal waves.

## CONTINUUM THEORY

The linear equations of an elastic, dielectric continuum, including the contribution of the polarization gradient to the stored energy, have been derived elsewhere [8] by means of a simple extension of a linear version of Toupin's [9] variational principle for the classical equations of piezoelectricity. For the special case of equilibrium of one-dimensional fields in a centrosymmetric cubic or isotropic material, in the absence of extrinsic fields, the field equations were shown to reduce to [8]

$$c_{11}\partial^2 u + d_{11}\partial^2 P = 0,$$
$$d_{11}\partial^2 u + b_{11}\partial^2 P - a_{11}P - \partial\varphi = 0, \tag{1}$$
$$-\varepsilon_0\partial^2\varphi + \partial P = 0,$$

where $\partial = d/dx$, $u$ and $P$ are the $x$-components of the mechanical displacement and electronic polarization and $\varphi$ is the potential of the Maxwell, electric self-field $E$:

$$E = -\partial\varphi. \tag{2}$$

Also, $c_{11}$ is an elastic stiffness, $\varepsilon_0$ is the permittivity of a vacuum and $\varepsilon_0 a_{11}$ is the reciprocal dielectric susceptibility ($= \eta^{-1}$). The remaining two constants ($b_{11}$ and $d_{11}$) are associated with terms, in the energy density, involving the polarization gradient: $\frac{1}{2}b_{11}$ is the coefficient of a quadratic term, $(\partial P)^2$, and $d_{11}$ is the coefficient of a product of polarization gradient and strain: $\partial P \partial u$.

If the contribution of the polarization gradient is omitted, $b_{11}$ and $d_{11}$ are zero and (1) reduce to

$$c_{11}\partial^2 u = 0,$$
$$a_{11}P + \partial\varphi = 0, \tag{3}$$
$$-\varepsilon_0\partial^2\varphi + \partial P = 0.$$

This is the simplest illustration of the fact that, in the classical theory of piezoelectricity, there is no electromechanical coupling in centrosymmetric materials. For a dielectric layer with traction-free surfaces at $x = \pm h$, on which are impressed voltages $\pm V$, the boundary conditions, according to the classical theory, are

$$(\partial u)_{x = \pm h} = 0,$$
$$(\varphi)_{x = \pm h} = \pm V; \tag{4}$$

and the solution of (3), subject to these boundary conditions, is, except for additive constants in $u$ and $\varphi$,

$$u = 0,$$
$$P = -\varepsilon_0\eta V/h, \tag{5}$$
$$\varphi = Vx/h.$$

The capacitance (per unit area) is the ratio of the surface charge (per unit area) to the voltage drop across the layer:

$$C = \frac{(\varepsilon_0\partial\varphi - P)_{x = \pm h}}{2V} = \frac{\varepsilon_0(1+\eta)}{2h} = \frac{\varepsilon}{2h}, \tag{6}$$

where $\varepsilon$ is the permittivity of the dielectric. These familar results of the classical theory are illustrated by the dashed lines in Fig. 2 and the straight line through the origin in Fig. 1.

If, again, the contribution of the polarization gradient is omitted, but the dielectric is noncentrosymmetric, a coupling term, say $f_{11}P\partial u$, where $f_{11}$ is a piezoelectric constant, appears in the energy density and the one-dimensional differential equations of the classical theory are

$$c_{11}\partial^2 u + f_{11}\partial P = 0,$$
$$f_{11}\partial u + a_{11}P + \partial\varphi = 0, \tag{7}$$
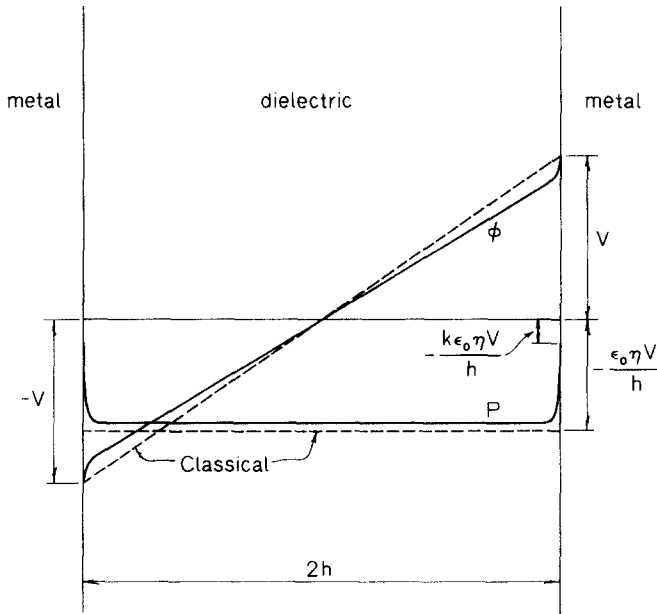$$-\varepsilon_0\partial^2\varphi + \partial P = 0.$$

FIG. 2. Distributions of potential and polarization through dielectric layer.

The boundary conditions corresponding to (4) are now

$$(c_{11}\partial u + f_{11}P)_{x=\pm h} = 0,$$

$$(\varphi)_{x=\pm h} = \pm V; \tag{8}$$

and the solution is, again except for additive constants in $u$ and $\varphi$,

$$u = -\varepsilon_0\eta' f_{11}Vx/c_{11}h,$$

$$P = -\varepsilon_0\eta'V/h,$$

$$\varphi = Vx/h, \tag{9}$$

$$C = \varepsilon_0(1+\eta')/2h,$$

where

$$\eta' = \eta/(1 - f_{11}^2\varepsilon_0\eta/c_{11}). \tag{10}$$

Thus, the only alterations introduced by the classical piezoelectric effect are the introduction of a homogeneous strain and the replacement of the susceptibility $\eta$ by $\eta'$. In view of this, the classical piezoelectric effect will be omitted in the sequel. It should be noted, however, that, for both centrosymmetric and noncentrosymmetric materials, the classical equations admit only two boundary conditions: one mechanical and one electrical.

On the other hand, solutions of (1), as shown previously [8], require an additional boundary condition—which may be taken as the specification of the surface polarization. Thus, the augmented equations permit the independent specification of the surface potential and polarization, whereas the classical equations of piezoelectricity do not. Now, the polarization at a boundary of the dielectric in a metal–dielectric–metal sandwich will

depend on the physical properties of the adjacent electrode and metal–dielectric interface; and these properties are outside the compass of the theory of dielectrics. However, since the electronic polarization in the metal is zero, it is reasonable to suppose that the surface polarization in the dielectric will lie between the classical value, given by the second of (5), and zero. Thus, assuming that the two electrodes and interfaces are the same, their influence on the surface polarization may be introduced, phenomenologically, by setting the boundary conditions

$$(P)_{x = \pm h} = -k\varepsilon_0\eta V/h, \qquad 0 \le k \le 1. \tag{11a}$$

The classical condition is $k = 1$ while $k = 0$ describes continuity of polarization across the interfaces. We suppose, also, that such mechanical forces, as may be acting across the metal–dielectric interfaces, have no resultant. This boundary condition is, as shown previously [8],

$$(c_{11} \, \partial u + d_{11} \, \partial P)_{x = \pm h} = 0. \tag{11b}$$

Finally, we suppose that the voltages applied to the dielectric at the interfaces are

$$(\varphi)_{x = \pm h} = \pm V. \tag{11c}$$

We have now to solve (1) subject to the boundary conditions (11). Let

$$\begin{aligned}
u &= B_1 \cosh(x/l), \\
P &= A_2 + B_2 \cosh(x/l), \\
\varphi &= A_3 x + B_3 \sinh(x/l),
\end{aligned} \tag{12}$$

where $l$ is a material constant, with the dimension of length, to be determined by the equations. Upon substituting (12) in (1), we find

$$A_2 = \varepsilon_0\eta A_3, \qquad B_2 = \varepsilon_0 B_3/l = -c_{11}B_1/d_{11}, \tag{13}$$

$$l = [\varepsilon_0(b_{11}c_{11} - d_{11}^2)/c_{11}(1+\eta^{-1})]^{\frac{1}{2}}. \tag{14}$$

The requirement of positive definiteness of the energy density makes $l$ real.

As for boundary conditions, (11b) is satisfied identically while (11a) and (11c) become

$$\begin{aligned}
A_2 + B_2 \cosh(h/l) &= -k\varepsilon_0\eta V/h, \\
A_3 h + B_3 \sinh(h/l) &= V,
\end{aligned} \tag{15}$$

respectively. From (13) and (15),

$$\begin{aligned}
A_3 &= (B_3/\eta l) \cosh(h/l) + kV/h, \\
B_3 &= (1-k)\eta V/[\eta \sinh(h/l) + (h/l) \cosh(h/l)].
\end{aligned} \tag{16}$$

The remaining constants, $A_2$, $B_1$ and $B_2$, are obtained easily from (16) and (13). The capacitance, ignoring any voltage drop that may occur in the electrodes, is

$$C = \frac{(\varepsilon_0 \, \partial\varphi - P)_{x = \pm h}}{2V} = \frac{\varepsilon}{2h} \frac{1 + (k\eta l/h) \tanh(h/l)}{1 + (\eta l/h) \tanh(h/l)}. \tag{17}$$

In Fig. 3 is illustrated the relation between normalized inverse capacitance and normalized thickness, described by (17), for the case $k = 0{\cdot}1$, $\eta = 10$. Calculations from Mead's data, for small $k$, indicate that $l$ is of the order of a few angstroms. Hence Mead's
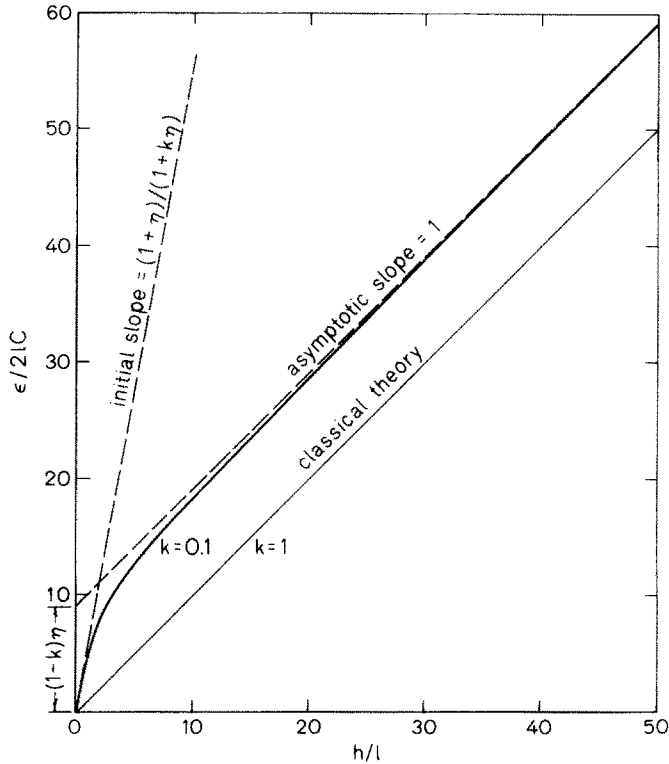
FIG. 3. Inverse capacitance vs. thickness according to augmented continuum theory; also according to
lattice theory if $l$ is replaced by $\lambda$ in both abscissa and ordinate.

data, which do not extend below a thickness of 30 Å, would be well to the right of the knee
of the curve and so, even if they did conform to (17), would give the appearance of a linear
relation which, if extended to zero thickness, would have a non-zero intercept of inverse
capacitance. This intercept, according to (17), is

$$C_0^{-1} = 2l(1-k)\eta/\varepsilon. \tag{18}$$

If $k = 1$, the intercept reduces to zero and, in fact, the whole solution reduces to the classical
one. However, it seems unlikely that the presence of the metal would not influence the
polarization of the dielectric at the metal–dielectric interface.

The variations of polarization and potential across the thickness of the dielectric are
illustrated by the curves in Fig. 2. The absolute value of the polarization is almost uniform
across the major portion of the thickness and slightly less than the uniform polarization
of the classical theory; but then drops sharply, near the interfaces, to boundary values of $k$
times the classical polarization, as specified. The potential has an almost uniform gradient,
less than the uniform gradient of the classical theory, over most of the thickness, but then
increases sharply on approaching the boundaries.

## LATTICE THEORY

We consider a single line of atoms, in a three-dimensional lattice of shell-model atoms,
as illustrated in Fig. 4. Only the intra-atomic interaction between core and shell of an atom
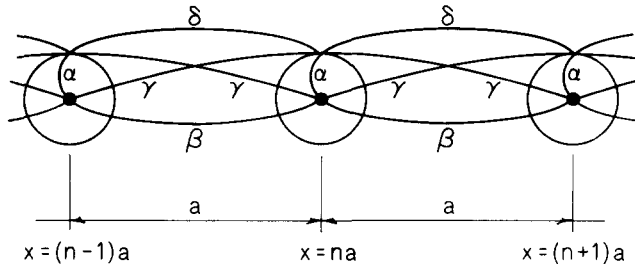
FIG. 4. Lattice of shell-model atoms.

and the interatomic interactions between nearest neighbors in the line are taken into account. The displacements of the core and shell of the atom at $x = na$ are designated by $u_n$ and $s_n$ respectively. The force constant of the intra-atomic core–shell interaction is designated by $\alpha$ and the force constants of the interatomic core–core, core–shell and shell–shell interactions are designated by $\beta$, $\gamma$ and $\delta$, respectively. All four force constants have the dimensions of force per unit length.

The equation of equilibrium of the $n$th interior atom is obtained by setting equal to zero the sum of the forces on its core and shell exerted by the cores and shells of its two nearest neighbor atoms:

$$\beta(u_{n+1} - u_n) + \gamma(s_{n+1} - u_n) + \gamma(u_{n+1} - s_n) + \delta(s_{n+1} - s_n)$$
$$- \beta(u_n - u_{n-1}) - \gamma(u_n - s_{n-1}) - \gamma(s_n - u_{n-1}) - \delta(s_n - s_{n-1}) = 0. \tag{19}$$

The equilibrium of the shell of the $n$th interior atom is expressed by

$$\alpha(u_n - s_n) + \gamma(u_{n+1} - s_n) + \delta(s_{n+1} - s_n)$$
$$- \gamma(s_n - u_{n-1}) - \delta(s_n - s_{n-1}) + qE_n = 0, \tag{20}$$

where $E_n$ is the value, at $x = na$, of the Maxwell, electric self-field and $q$ is a constant with the dimension of charge.

The polarization of the $n$th atom, per unit area of the three-dimensional lattice, is defined by

$$P_n = (s_n - u_n)q/a^3 \tag{21}$$

and we also adopt a symbol for the second central difference (divided by $a^2$):

$$\Delta^2 f_n = (f_{n+1} + f_{n-1} - 2f_n)/a^2. \tag{22}$$

Then (19) and (20) may be rewritten as

$$(\beta + 2\gamma + \delta)a^{-1}\Delta^2 u_n + (\gamma + \delta)a^2 q^{-1}\Delta^2 P_n = 0,$$
$$(\gamma + \delta)a^2 q^{-1}\Delta^2 u_n + \delta a^5 q^{-2}\Delta^2 P_n - (\alpha + 2\gamma)a^3 q^{-2}P_n + E_n = 0. \tag{23}$$

The lowest order continuum approximation to (23) is obtained by expanding the difference operator $\Delta^2$ into an infinite series of derivatives and dropping all but the first term. Then

$$\Delta^2 \rightarrow \partial^2. \tag{24}$$

Also,

$$E_n \rightarrow E = -\partial \varphi. \tag{25}$$

The resulting differential equations have exactly the same form as the first two of (1). Accordingly, if we set

$$c_{11} = (\beta + 2\gamma + \delta)a^{-1}, \qquad b_{11} = \delta a^5 q^{-2},$$

$$d_{11} = (\gamma + \delta)a^2 q^{-1}, \qquad a_{11} = (\alpha + 2\gamma)a^3 q^{-2} = \varepsilon_0^{-1}\eta^{-1}, \tag{26}$$

the first two of (1) become the lowest order continuum approximations to (23).

As may be seen from (26), the polarization gradient terms (those with coefficients $d_{11}$ and $b_{11}$) in (1) stem from shell–shell and interatomic core–shell interactions, identified by the force constants $\delta$ and $\gamma$, respectively. In fact, the form of (1) is preserved if the interatomic core–shell interaction is dropped but the shell–shell interaction is retained. If both of these interactions are omitted, the continuum approximation reduces to the classical form given by the first two of (3). Now, whereas the second of (23) is the equation of equilibrium of the shells in the lattice of shell-model atoms, the second of (3) stems, via a constitutive equation, from Toupin's [9] "equation of intramolecular force balance" based on his dumbbell model of a particle in an elastic dielectric; and the only material constant in the continuum equation is here identified as one proportional to the intra-atomic core–shell force constant, $\alpha$, in the shell-model. Thus, in the case of the classical theory for centrosymmetric materials, it is shown that the shell model and the dumbbell model are identical and the equation of equilibrium of the shell is the counterpart of Toupin's equation of intramolecular force balance. The addition of the contribution of the polarization gradient to the stored energy, in the continuum theory, converts the second of (3) to the second of (1) and extends Toupin's force balance at a point to include force balance in the neighborhood of a point. That is, balance of both intramolecular and intermolecular forces is accommodated. In relation to the lattice, the second of (1) is still a continuum approximation to the equation of equilibrium of the shell, but with the shell–shell and interatomic core–shell interactions included in the latter.

We have yet to derive the lattice counterpart of the third of (1) and establish the boundary conditions. It is illuminating to reach these results from considerations of energy.

The ratio of the potential energy of one line of atoms, of the three-dimensional lattice, to the volume $a^3$ is

$$\mathcal{W} = \sum_n \left[ \tfrac{1}{2}\varepsilon_0(\partial_+ \varphi_n)^2 + \tfrac{1}{2}\varepsilon_0^{-1}\eta^{-1}P_n^2 + \tfrac{1}{2}b_{11}(\Delta_+ P_n)^2 \right.$$

$$\left. + c_{11}(\Delta_+ u_n)^2 + d_{11}(\Delta_+ P_n)(\Delta_+ u_n) \right], \tag{27}$$

where

$$\partial_+ f_n = \sum_{m=1}^{\infty} (-1)^{m-1} m^{-1} a^{m-1} \Delta_+^m f_n \tag{28}$$

and

$$\Delta_+ f_n = (f_{n+1} - f_n)/a,$$

$$\Delta_+^2 f_n = (f_{n+2} - 2f_{n+1} + f_n)/a^2, \tag{29}$$

$$\Delta_+^3 f_n = (f_{n+3} - 3f_{n+2} + 3f_{n+1} - f_n)/a^3,$$

$$\vdots \qquad \vdots$$

i.e. $\partial_+$ is the Taylor series expansion of the derivative, $\partial$, in terms of forward differences. Thus, the first term in (27) is the contribution of the energy of the Maxwell self-field. The remaining terms constitute the contribution of the energy of the short range interactions between atoms.

As shown by Toupin [9], the equations of the classical, continuum theory of elastic dielectrics are derived from the electric enthalpy rather than the energy. An analogous procedure will be employed here. We define an electric enthalpy by

$$
\begin{aligned}
\mathcal{H} &= \mathcal{W} - \sum_n E_n(\varepsilon_0 E_n + P_n) \\
&= \sum_n \left[ -\tfrac{1}{2}\varepsilon_0(\partial_+\varphi_n)^2 + P_n\partial_+\varphi_n + \tfrac{1}{2}\varepsilon_0^{-1}\eta^{-1}P_n^2 \right. \\
&\qquad \left. + \tfrac{1}{2}b_{11}(\Delta_+ P_n)^2 + \tfrac{1}{2}c_{11}(\Delta_+ u_n)^2 + d_{11}(\Delta_+ P_n)(\Delta_+ u_n) \right].
\end{aligned}
\tag{30}
$$

Then the equations of equilibrium and the equation of electrostatics are obtained from

$$
\begin{aligned}
-\partial\mathcal{H}/\partial u_n &= c_{11}\Delta^2 u_n + d_{11}\Delta^2 P_n = 0, \\
-\partial\mathcal{H}/\partial P_n &= d_{11}\Delta^2 u_n + b_{11}\Delta^2 P_n - \varepsilon_0^{-1}\eta^{-1}P_n - \partial_+\varphi_n = 0, \\
-\partial\mathcal{H}/\partial\varphi_n &= -\varepsilon_0\partial_-\partial_+\varphi_n + \partial_- P_n = 0,
\end{aligned}
\tag{31}
$$

where

$$
\partial_- f_n = \sum_{m=1}^{\infty} m^{-1}a^{m-1}\Delta_-^m f_n
\tag{32}
$$

and

$$
\begin{aligned}
\Delta_- &= (f_n - f_{n-1})/a, \\
\Delta_-^2 &= (f_n - 2f_{n-1} + f_{n-2})/a^2, \\
\Delta_-^3 &= (f_n - 3f_{n-1} + 3f_{n-2} - f_{n-3})/a^3, \\
&\;\;\vdots \qquad \vdots
\end{aligned}
\tag{33}
$$

i.e. $\partial_-$ is the Taylor series expansion of the derivative in terms of backward differences.

It may be seen that the first two of (31) are the same as (23), which have the first two of (1) as continuum approximations, and the third of (31) has the third of (1) as its continuum form.

If the lattice is of finite thickness spanning an odd number of atoms with the end ones at $n = \pm N$, admissible boundary conditions are the specification of one member of each of the three products

$$
u_{\pm N}\frac{\partial\mathcal{H}}{\partial(\Delta_+ u_{\pm N})}, \qquad P_{\pm N}\frac{\partial\mathcal{H}}{\partial(\Delta_+ P_{\pm N})}, \qquad \varphi_{\pm N}\frac{\partial\mathcal{H}}{\partial(\partial_+\varphi_{\pm N})},
\tag{34}
$$

where

$$
\Delta_+ f_{\pm N} = (f_{\pm(N+1)} - f_N)/a, \qquad \partial_+\varphi_{\pm N} = (\partial_+\varphi_n)_{n=\pm N}.
\tag{35}
$$

We find

$$-\partial \mathcal{H}/\partial(\Delta_+ u_{\pm N}) = c_{11}\Delta_+ u_{\pm N} + d_{11}\Delta_+ P_{\pm N},$$

$$-\partial \mathcal{H}/\partial(\Delta_+ P_{\pm N}) = d_{11}\Delta_+ u_{\pm N} + b_{11}\Delta_+ P_{\pm N}, \tag{36}$$

$$-\partial \mathcal{H}/\partial(\partial_+ \varphi_{\pm N}) = \varepsilon_0 \partial_+ \varphi_{\pm N} - P_{\pm N}.$$

The problem analogous to the one solved in the preceding section is to find the solution of (31) satisfying the boundary conditions

$$c_{11}\Delta_+ u_{\pm N} + d_{11}\Delta_+ P_{\pm N} = 0,$$

$$P_{\pm N} = -k\varepsilon_0 \eta V/h, \tag{37}$$

$$\varphi_{\pm N} = \pm V,$$

where $h = Na$. We take

$$u_n = B'_1 \cosh(na/\lambda),$$

$$P_n = A'_2 + B'_2 \cosh(na/\lambda), \tag{38}$$

$$\varphi_n = [A'_3 x + B'_3 \sinh(x/\lambda)]_{x=na},$$

and note that $\partial_+ (na) = 1$ and

$$\Delta^2 \cosh(na/\lambda) = 4a^{-2} \sinh^2(a/2\lambda) \cosh(na/\lambda),$$

$$\partial_+ \sinh(na/\lambda) = \lambda^{-1} \cosh(na/\lambda),$$

$$\partial_- \cosh(na/\lambda) = \lambda^{-1} \sinh(na/\lambda), \tag{39}$$

$$\partial_- \partial_+ \sinh(na/\lambda) = \lambda^{-2} \sinh(na/\lambda).$$

Then, substituting (38) in (31), we find

$$A'_2 = \varepsilon_0 \eta A'_3, \qquad B'_2 = \varepsilon_0 B'_3/\lambda = -c_{11}B'_1/d_{11}, \tag{40}$$

$$\sinh(a/2\lambda) = a/2l, \tag{41}$$

where $l$ is the same as in (14).

Application of the boundary conditions (37) leads, by the same procedure as in the preceding section, to

$$A'_3 = (B'_3/\eta\lambda) \cosh(h/\lambda) + kV/h,$$

$$B'_3 = (1-k)\eta V/[\eta \sinh(h/\lambda) + (h/\lambda) \cosh(h/\lambda)] \tag{42}$$

and capacitance

$$C = \frac{\varepsilon}{2h} \frac{1 + (k\eta\lambda/h) \tanh(h/\lambda)}{1 + (\eta\lambda/h) \tanh(h/\lambda)}. \tag{43}$$

Thus, the entire solution is identical with the continuum one except that the displacement and polarization have significance only at the atom sites and $l$ is replaced by $\lambda$. In particular, the curve in Fig. 3 is applicable to the lattice if $l$ is replaced by $\lambda$ in both abscissa and ordinate.

If the material constant $\lambda$ is greater than the lattice constant $a$, $\lambda$ and $l$, by (41), differ by less than $4\%$ and the continuum equations are good approximations to the lattice equations. The condition $l \approx \lambda$ is all that is left, in the present case of equilibrium, of the requirements for the "long wave approximation" to be a good approximation. This statement stems from an inspection of the dispersion relations for wave solutions of (1) and (31) (after insertion of the appropriate inertia term, $\rho \ddot{u}$ or $\rho \ddot{u}_n$, in the first equation of each set). We find, for the continuum,

$$l^2 \xi^4 + \left[ 1 - \frac{b_{11}\varepsilon_0 \rho \omega^2}{c_{11}(1+\eta^{-1})} \right] \xi^2 - \frac{\rho \omega^2}{c_{11}} = 0 \tag{44}$$

and, for the lattice,

$$\frac{16 l^2}{a^4} \sin^4\left(\frac{\xi a}{2}\right) + \left[ 1 - \frac{b_{11}\varepsilon_0 \rho \omega^2}{c_{11}(1+\eta^{-1})} \right] \frac{4}{a^2} \sin^2\left(\frac{\xi a}{2}\right) - \frac{\rho \omega^2}{c_{11}} = 0, \tag{45}$$

where $\omega$ is the circular frequency and $\xi$ is the wave number. In each case, the dispersion relation ($\omega$ vs. $\xi$) has two branches: one real (acoustic) and one pure imaginary, as shown in Fig. 5. The slopes of the real branches at long wave length approach the same limit $(c_{11}/\rho)^{\frac{1}{2}}$ so that, as far as propagating waves are concerned, the single restriction to long wave length is sufficient to make the continuum theory a good approximation. At long wave lengths, the real branches correspond to low frequencies; and at zero frequency the
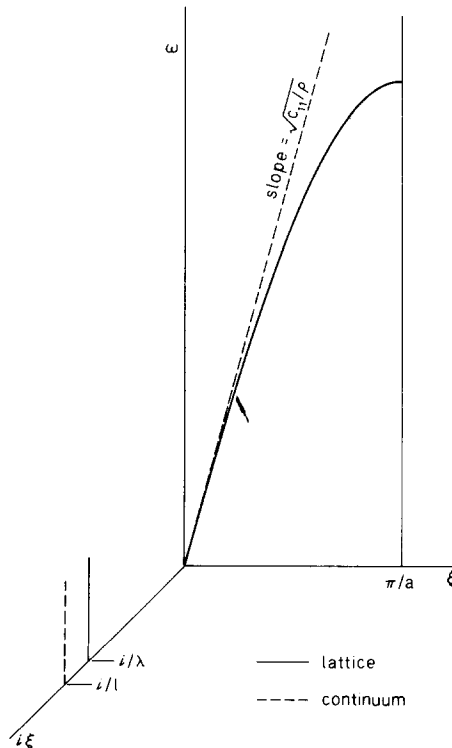


Fig. 5. Real and imaginary branches of dispersion relations for longitudinal waves according to augmented continuum theory and lattice theory.

imaginary branches have the same slope (infinite) but different intercepts: with magnitudes $l^{-1}$ for the continuum and $\lambda^{-1}$ for the lattice. If the body has a boundary at which the variables associated with the real and imaginary branches couple, amplitudes and spatial decay rates of the displacement, polarization and potential will be affected by a difference between $l$ and $\lambda$. Thus, the quality of the approximation will depend not only on the wave length but also on a property of the material: $\lambda$. In the case of a problem of equilibrium, rather than motion, the real wave length is infinite, so that the sole remaining criterion for a good approximation is a condition on a material property.

The system of difference equations (31), with or without the inertia term, is sometimes approximated by retaining only a few early terms of the infinite series expansions, (28) and (32), for $\partial_+$ and $\partial_-$. However, in many cases, as in the present one, analytic solutions of the equations are much simpler if the full infinite series are used—preserving, at the same time, the long range electrostatic action in full. Often, the third of (31) does not appear at all: the dependent variable $\varphi$ (or the Maxwell self-field) is eliminated between the second and third of (31) and only two equations (on the displacement and polarization) are employed. These are suitable for the calculation of dispersion relations for waves in an infinite lattice, which is the most frequent application; or for problems of bounded lattices with mixed ("cyclic") boundary conditions: which cannot be attained physically, but are suitable for calculations of bulk properties. For general boundary conditions, including the free boundary, the full set of three equations (seven, in three dimensions, since $\mathbf{u}$ and $\mathbf{P}$ are vectors) must be employed if surface effects are to be studied.

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Абстракт—В работе предполагается, что наблюдаемая аномалия Ц. А. Мздом в измерениях тонких диелектрических слоев, может быть вызвана электромеханическим эффектом, неучитываемым в классической, сплошной теории пьезоэлектричества. Показано, что решение уравнений, заключающих добавочный эффект, согласуется с экспериментальными данными. Показано также, что уравнения усилителя, по сравнению с классическими, правильнее отображают сплошное приближение уравнений сетки электронной оболочки атомов. Аналогические решения равновесия уравнений сетки и уравнений сплошной среды являются почти идентическими.