

## Appendix 4

# Linear piezoelectric theory

### A4.1 LINEAR FIELD EQUATIONS

The field equations and boundary conditions for an elastic dielectric set out in Appendix 3 are, subject to certain assumptions, valid for arbitrary electric fields and finite deformations. The assumptions were

- (a) that the electromagnetic field could be adequately described by the quasi-static electric field equations;
- (b) that the material properties of the dielectric could be described in terms of an internal energy function; and
- (c) that dissipation of energy could be neglected.

The equations are therefore sufficiently general to be used to describe electrostrictive phenomena and other non-linear effects. What may be termed the classical theory of piezoelectricity is based on a restricted set of equations, derived from those of Appendix 3 by making a general assumption of linearity.

More specifically, the assumption of linearity amounts to the neglect of any terms in the field equations that are non-linear in either the fields themselves or their spatial and temporal derivatives. An immediate consequence of this sweeping assumption is that the electrostatic stress  $t_{kl}^M + E_k P_l$ , which involves the product of the electric field quantities, is discarded, thus making it impossible for the linear theory to include electrostrictive effects. A further consequence is that the material time derivative of a field quantity  $f$  reduces to the partial time derivative, and that the distinction between the initial and current coordinates of a material particle  $X$  is lost, so that the quantities  $f_{,K}$  and  $f_{,k}$  can no longer be distinguished. Thus in the linear theory it is unnecessary to maintain the notational conventions of using upper and lower case indices to separate quantities referred to initial and current coordinates of a point  $X$  respectively.

These assumptions can be made more precise by introducing the particle displacement  $u_k(X_K)$  such that by definition

$$u_k(X_K) = x_k(X_K) - \delta_{kK} X_K$$

Then both  $u_k$  and its derivatives are assumed to be sufficiently small that only linear terms need be retained. From the definition

$$x_{k,K} = \delta_{kK} + u_{k,K}$$

so that for any field quantity  $f$

$$f_{,K} = f_{,k} x_{k,K} = f_{,k} \delta_{kK} + f_{,k} u_{k,K} \sim f_{,k} \delta_{kK}$$

and

$$\dot{f} = \partial f / \partial t + v_k f_{,k} \sim \partial f / \partial t$$

Also from the definition of the Jacobian determinant  $J$  as  $\det\{x_{k,K}\}$  it follows that up to linear terms in the displacement gradients  $u_{k,K}$

$$J = \det\{\delta_{kK} + u_{k,K}\} \sim 1 + \delta_{kK} u_{k,K}$$

The principle of conservation of mass (Eqn (A3.21)) can be written  $(\dot{\rho}J) = 0$ , or in terms of the mass density  $\rho_0$  in the initial state,  $\rho J = \rho_0$ . Substituting for  $J$  yields to first order in the displacement gradients

$$\rho = \rho_0 (1 + \delta_{kK} u_{k,K})$$

The mechanical field equations (A3.57) and (A3.61) can now be written in the linear approximation

$$\rho_0 \dot{v}_k = \rho f_k - t_{kl,l} \quad (\text{A4.1})$$

and

$$t_k = t_{kl}^l n_l \quad (\text{A4.2})$$

where now the superimposed dot is used to denote the ordinary partial time derivative rather than the material time derivative.

The stress tensor  $t_{kl}^l$  is derived from the internal energy density  $\Sigma$  by Eqn (A3.53). As shown in Section A3.6,  $\Sigma$  can be regarded as a function of the quantities  $C_{KL}$ ,  $P_K$  and the entropy per unit mass  $\sigma$ , where

$$C_{KL} = x_{k,K} x_{k,L} \quad P_K = \pi_k x_{k,K}$$

and  $\pi_k$  is the polarization per unit mass. Introducing the displacement gradients and retaining linear terms only,

$$\begin{aligned} C_{KL} &= (\delta_{kK} + u_{k,K})(\delta_{kL} + u_{k,L}) \sim \delta_{KL} + \delta_{kK} u_{k,L} + u_{k,K} \delta_{kL} \\ P_K &= (\delta_{kK} + u_{k,K}) \pi_k \sim \delta_{kK} \pi_k \end{aligned}$$

In this approximation the Lagrangian finite strain tensor reduces to the *infinitesimal strain tensor* of classical elasticity theory

$$S_{KL} = (C_{KL} - \delta_{KL})/2 \sim (\delta_{kK} u_{k,L} + u_{k,K} \delta_{kL})/2$$

and  $\Sigma$  can then be written as a function of  $S_{KL}$ ,  $P_K$  and  $\sigma$ . Equation (A3.53) can then be replaced by

$$t_{kl}^L = \rho x_{l,k} \frac{\partial \Sigma}{\partial x_{k,K}} \sim \rho \delta_{l,K} \frac{\partial \Sigma}{\partial S_{LM}} \frac{\partial S_{LM}}{\partial u_{k,K}} = \rho \frac{\partial \Sigma}{\partial S_{KL}} \delta_{kK} \delta_{lL}$$

Writing  $U = \rho \Sigma$  for the internal energy density per unit *volume*

$$t_{kl}^L = \frac{\partial U}{\partial S_{KL}} \delta_{kK} \delta_{lL}$$

If  $U$  is regarded as a function of the strains  $S_{KL}$  and the polarization  $P_k$  and entropy  $S$  per unit *volume* rather than the polarization  $\pi_k$  and entropy  $\sigma$  per unit mass, then Eqns (A3.58) and (A3.59) can be written

$$E_k = -\frac{\partial \Sigma}{\partial \pi_k} = -\frac{\partial U}{\partial P_k}$$

$$T = -\frac{\partial \Sigma}{\partial \sigma} = -\frac{\partial U}{\partial S}$$

where  $T$  has been written for the absolute temperature rather than  $\theta$ .

Dropping the distinction between initial and current coordinates, the linear field equations can be summarized as follows. For a body  $B$  occupying a volume  $V$  bounded by a surface  $S$ , the electrostatic field equations are

$$D_{k,k} = q \quad E_k = -\phi_{,k} \quad D_k = \epsilon_0 E_k + P_k \quad (\text{A4.3})$$

in  $V$  and

$$[D_k n_k] = w \quad [\phi] = 0 \quad (\text{A4.4})$$

on  $S$ , where  $E_k$ ,  $D_k$ ,  $P_k$  and  $\phi$  are the electric field, displacement, polarization and potential, and  $q$  and  $w$  are volume and surface densities of free charge. In the space outside  $V$

$$D_{k,k} = 0 \quad E_k = -\phi_{,k} \quad D_k = \epsilon_0 E_k \quad (\text{A4.5})$$

The mechanical field equations are

$$\rho_0 \dot{v}_k = \rho f_k - t_{kl,l} \quad (\text{A4.6})$$

in  $V$  and

$$t_k = t_{kl} n_l \quad (\text{A4.7})$$

on  $S$ , where  $f_k$  are the external body forces per unit mass and  $t_k$  are the surface tractions acting across  $S$ . The stress  $t_{kl}$ , where the suffix  $L$  has been dropped, is obtained from an internal energy density  $U$  given as a function of the strain tensor  $S_{kl}$ , the polarization  $P_k$  and the entropy  $S$  via

$$t_{kl} = \partial U / \partial S_{kl} \quad (\text{A4.8})$$

with  $S_{kl} = (u_{k,l} + u_{l,k})/2$ . The electric field and polarization are related by

$$E_k = \partial U / \partial P_k \quad (\text{A4.9})$$

and the absolute temperature  $T$  is given by

$$T = \partial U / \partial S \quad (\text{A4.10})$$

## A4.2 LINEAR CONSTITUTIVE RELATIONS

The field equations given in the previous section cannot be solved unless a particular functional form is adopted for the internal energy  $U$ . The assumption that  $U$  is a function of the *deformation* of the material implies a choice of a reference which can be identified with an *undeformed* state. Of course from a purely formal point of view the choice of reference state is entirely arbitrary, but on physical grounds it is natural to require that the reference state corresponds to one of *zero stresses*, mechanical and electrical. The assumption that such a state exists is far from trivial, and amounts to excluding from consideration materials such as *ferroelectrics*, which are permanently polarized, or materials which have stresses and strains 'built-in' as a result of their previous history.

The classical theory of piezoelectricity assumes that at any given temperature  $T_0$ , a reference state exists for which the strain  $S_{kl}$ , the polarization  $P_k$ , the stress  $t_{kl}$  and the electric field  $E_k$  are all simultaneously zero. If  $U_0$  and  $S_0$  are respectively the values of the internal energy and the entropy in the reference state, then for small, reversible changes it is assumed that  $U$  can be adequately expressed as a Taylor series up to and including second order terms in the strains and polarization. (For applications to problems in waves and vibrations, it is usual to assume that the changes are taking place sufficiently rapidly for thermal conduction to be ignored, that is, that they are *adiabatic* or *isentropic*. The entropy  $S$  is thus regarded as constant.) Therefore

$$U - U_0 = U_{kl}^0 S_{kl} + U_k^0 P_k + \frac{1}{2} U_{kl,mn}^0 S_{kl} S_{mn} + U_{kl,m}^0 S_{kl} P_m + \frac{1}{2} U_{k,l}^0 P_k P_l$$

where

$$\begin{aligned} U_{kl}^0 &= \partial U / \partial S_{kl} & U_k^0 &= \partial U / \partial P_k \\ U_{kl,mn}^0 &= \partial^2 U / \partial S_{kl} \partial S_{mn} & U_{kl,m}^0 &= \partial^2 U / \partial S_{kl} \partial P_m \\ U_{k,l}^0 &= \partial^2 U / \partial P_k \partial P_l \end{aligned}$$

and all the partial derivatives are evaluated at the reference state.

From Eqns (A4.8) and (A4.9) and the assumption that both the stress and field are zero in the reference state, it follows that the first order derivatives  $U_{kl}^0$  and  $U_k^0$  vanish, so that therefore

$$U - U_0 = \frac{1}{2} U_{kl,mn}^0 S_{kl} S_{mn} + U_{kl,m}^0 S_{kl} P_m + \frac{1}{2} U_{k,l}^0 P_k P_l \quad (\text{A4.11})$$

Since all the derivatives are evaluated at the reference state, they can be

regarded as constants in the consideration of small changes from the reference. In order to distinguish these *material constants* from others to be introduced later, the following definitions are introduced:

$$\begin{aligned} c_{klmn}^P &= U_{kl,mn}^0 \\ a_{mkl} &= -U_{kl,m}^0 \\ \chi_{kl}^{-1} &= U_{k,l}^0 \end{aligned} \quad (\text{A4.12})$$

Then  $U$  can be written

$$U - U_0 = \frac{1}{2} c_{klmn}^P S_{kl} S_{mn} - a_{klm} S_{kl} P_m + \frac{1}{2} \chi_{kl}^{-1} P_k P_l \quad (\text{A4.13})$$

Equations (A4.8) and (A4.9) now become

$$\begin{aligned} t_{kl} &= c_{klmn}^P S_{mn} - a_{mkl} P_m \\ E_k &= -a_{klm} S_{lm} + \chi_{kl}^{-1} P_l \end{aligned} \quad (\text{A4.14})$$

These are the fundamental linear constitutive relations for a piezoelectric material. The  $c_{klmn}^P$  are the *elastic constants* at constant polarization, the  $a_{mkl}$  are *piezoelectric constants* and the  $\chi_{kl}^{-1}$  are the components of the *inverse susceptibility tensor* at constant strain. Under rotations of the coordinate system, the  $c$ 's,  $a$ 's, and  $\chi^{-1}$ 's transform as fourth, third and second rank tensors respectively.

Because of the form of the field equations Eqns (A4.3) to (A4.7) it is advantageous to recast the constitutive relations into a form where the independent variables are the strain and the electric field, and the dependent variables are the stress and the electric displacement. This is most easily done by forming the *electric enthalpy*  $H = U - E_k P_k$ . Then the total differential of  $H$  is

$$\begin{aligned} dH &= dU - E_k dP_k - P_k dE_k \\ &= (\partial U / \partial S_{kl}) dS_{kl} + (\partial U / \partial P_k) dP_k - E_k dP_k - P_k dE_k \end{aligned}$$

But from Eqn (A4.9),  $E_k = (\partial U / \partial P_k)$  so

$$dH = (\partial U / \partial S_{kl}) dS_{kl} - P_k dE_k$$

Therefore  $H$  can be regarded as a function of  $S_{kl}$  and  $E_k$  with

$$\begin{aligned} (\partial H / \partial S_{kl}) &= (\partial U / \partial S_{kl}) = t_{kl} \\ (\partial H / \partial E_k) &= -P_k \end{aligned} \quad (\text{A4.15})$$

Just as in the case of the internal energy  $U$ ,  $H$  is then expanded in a Taylor series, but now with independent variables  $S_{kl}$  and  $E_k$ . The linear terms drop out because of Eqns (A4.15) and the assumption of zero stress and field in the reference state, leaving

$$H - H_0 = \frac{1}{2} c_{klmn}^E S_{kl} S_{mn} - e_{klm} E_k S_{lm} - \frac{1}{2} \chi_{kl} E_k E_l \quad (\text{A4.16})$$

which is analogous to Eqn (A4.13). The material constants  $c_{klmn}^E$  are the elastic

constants at constant field, the  $e_{klm}$  are piezoelectric constants, and the  $\chi_{kl}$  are the components of the susceptibility tensor. The constants are defined in an obvious manner in terms of the second derivatives of  $H$  evaluated at the reference state. Using Eqn (A4.16) in Eqn (A4.15) leads to the constitutive relations

$$t_{kl} = c_{klmn}^E S_{mn} - e_{jkl} E_j \quad (\text{A4.17})$$

$$P_k = e_{klm} S_{lm} + \chi_{kl} E_l \quad (\text{A4.18})$$

Adding a term  $\epsilon_0 E_k$  to both sides of the second equation, Eqn (A4.18), leads to

$$D_k = e_{klm} S_{lm} + \epsilon_{kl}^S E_l \quad (\text{A4.19})$$

where  $\epsilon_{kl}^S$  are the dielectric constants at constant strain, or the ‘clamped’ dielectric constants.

Equations (A4.17) and (A4.19) are the constitutive relations in their most commonly used form. Other sets useful in special circumstances can be arrived at by defining thermodynamic functions other than the enthalpy and going through the same procedure of expanding in a Taylor series. In particular, if the function  $G = U - E_k P_k - t_{kl} S_{kl}$  is used, the resulting constitutive relations take the form

$$S_{kl} = s_{klmn}^E t_{mn} + d_{jkl} E_j$$

$$D_k = d_{klm} t_{lm} + \epsilon_{kl}^t E_l$$

where the  $s_{klmn}^E$  and  $\epsilon_{kl}^t$  are the *elastic compliances* at constant field and the dielectric constants at constant stress (or ‘free’ dielectric constants) respectively, and the  $d_{klm}$  are a further set of piezoelectric constants.

Because of their definitions in terms of the second derivatives of thermodynamic functions of state, and the rule that the order of partial differentiation can be changed provided that the functions involved are sufficiently smooth, the material constants have the following symmetries. First the dielectric constants are symmetric,  $\epsilon_{kl} = \epsilon_{lk}$ . Second, for both elastic constants and compliances,  $c_{klmn} = c_{mnkl}$ . In addition, since both stress and strain tensors are symmetrical, the elastic constants have the additional symmetries  $c_{klmn} = c_{ikmn}$ , similar relations holding for the compliances. For the same reason, the piezoelectric constants are symmetric in their second and third indices, for example,  $e_{klm} = e_{kml}$ .

### A4.3 POSITIVE-DEFINITE CHARACTER OF THE INTERNAL ENERGY $U$

Since the reference state for the material has been assumed to be one such that all fields and stresses, both electrical and mechanical are zero, it is natural to

assume that any changes from the reference state will require a definite amount of external work and a consequent increase in the internal energy  $U$ . Therefore in Eqn (A4.13),  $U - U_0$  must be positive-definite.

$U$  can be expressed as a function of the strain  $S_{kl}$  and the field  $E_k$  by using  $H(S_{kl}, E_k) = U - E_k P_k$  and substituting for  $P_k$  from Eqn (A4.18). The result is

$$U - U_0 = \frac{1}{2} c_{klmn} S_{kl} S_{mn} + \frac{1}{2} \chi_{kl} E_k E_l$$

In particular, for  $E_k = 0$  it follows that  $\frac{1}{2} c_{klmn} S_{kl} S_{mn}$  is separately positive-definite, that is, is positive for all non-zero  $S_{kl}$ . If  $S_{kl}$  is replaced by the product  $x_k y_l$  then the positive-definite character is still retained, and if  $y_k$  is then replaced by  $y_k = y n_k$  where  $n_k$  is a unit vector and  $y$  an arbitrary scalar, then  $U - U_0$  formally reduces to

$$U - U_0 = \frac{1}{2} (c_{klmn} n_l n_n x_k x_m) y^2$$

Defining  $L_{km} = c_{klmn} n_l n_n$ , and noting that  $y^2 > 0$ , it then follows that  $L_{km} x_k x_m$  is also positive definite.

This is an important result, since as shown in Chapter 2, the tensor  $L_{km}$  appears in the analysis of plane wave propagation in anisotropic materials, and its positive-definite character is essential to the existence of real phase velocities.