ANALYSIS OF HARMONIC WAVES IN A COMPOSITE MATERIAL WITH PIEZOELECTRIC EFFECT

S. Minagawa, K. Yoshihara
The University of Electro-Communications, Chofu, Tokyo, Japan

and

S. Nemat-Nasser
University of California, San Diego, La Jolla, CA 92039-0411, U.S.A.

Abstract—The authors are concerned with harmonic waves propagating in a three-dimensional composite, with periodic structure, consisting of anisotropic, elastic and piezoelectric crystals, obtaining solutions by a mixed variational method. The electric field is treated as quasi-static. The stress, displacement, electric displacement and electric scalar potential are field variables subject to variations in a general variational principle. The matrix-eigenvalue problem is solved to give approximate eigenfrequencies and the corresponding eigenstates. Numerical examples are given for harmonic waves propagating in the gallium arsenide crystal with ellipsoidal inclusions of lithium niobate.

INTRODUCTION

A mixed variational method has been proposed for the treatment of harmonic waves propagating in one-, two- and three-dimensional elastic composites with periodic structure (see Nemat-Nasser, 1972; Nemat-Nasser *et al.*, 1975; Nemat-Nasser and Minagawa, 1975; Minagawa and Nemat-Nasser, 1976, 1977; Minagawa *et al.*, 1981). In this paper, we shall extend the analysis to the case where each constituent of the composite displays piezoelectric effects.

The electric field is assumed quasi-static, so that the equations of motion are coupled with the static electric field equations. This coupling is represented by the elasto-piezoelectric constitutive equations. Since the piezoelectric effect is closely related to the anisotropic structure of crystals, the analysis must be done by means of general anisotropic constitutive equations. (On the piezoelectricity of crystals, see Cady, 1964; American National Standard Institute, 1979.)

We shall start with a mixed variational principle extended for use in this case, where the field variables subject to variations are the stress, displacement, electric displacement, and electric scalar potential. These field variables are determined from among those satisfying the conditions of continuity and quasi-periodicity, by the condition that they render a new quotient stationary with respect to their independent variations. The matrix eigenvalue problem will be solved to give approximate eigenfrequencies and their corresponding eigenstates. Numerical examples will be given for eigenfrequencies of harmonic waves in a composite with ellipsoidal inclusions.

BASIC EQUATIONS

We assume a three-dimensional Cartesian coordinate system, with respect to which the position of a material point is stated as x_i. Throughout this paper, the lower case roman indices $i, j, k, \ldots$ take 1, 2 or 3, and Einstein's summation convention is used for indices appearing twice in one expression. A comma followed by an index (or indices) means the derivative(s) with regard to the corresponding space coordinate(s).

For harmonic waves with frequency ω, we have the following set of basic field equations.

(a) Divergence equations:

$$\sigma_{jk,k} + \lambda \rho u_j = 0, \quad D_{k,k} = 0, \tag{1}$$

where $\lambda = \omega^2$, $\sigma_{jk}(\mathbf{x}) \exp[\pm i\omega t]$, $u_j(\mathbf{x}) \exp[\pm i\omega t]$ and $D_k(\mathbf{x}) \exp[\pm i\omega t]$ are the fields of stress, displacement and electric displacement, t is the time, $i = \sqrt{-1}$, and ρ the mass-density of the material. The materials are assumed to be insulated so that no free electric charges exist.

(b) Constitutive equations:

$$e_{jk} = g_{jkpq}\sigma_{pq} + g_{pjk}D_p, \quad E_j = -g_{jpq}\sigma_{pq} + g_{jk}D_k. \tag{2}$$

where $e_{jk}(\mathbf{x}) \exp[\pm i\omega t]$ and $E_j(\mathbf{x}) \exp[\pm i\omega t]$ are the strain and electric fields, and g_{jkpq}, g_{pjk}, g_{jk} are the material tensors satisfying the following symmetry conditions:

$$g_{jkpq} = g_{kjpq} = g_{jkqp} = g_{pqjk}, \quad g_{pjk} = g_{pkj}, \quad g_{jk} = g_{kj}. \tag{3}$$

(c) Gradient equations:

$$e_{jk} = \tfrac{1}{2}(u_{j,k} + u_{k,j}), \quad E_j = -\phi_{,j}, \tag{4}$$

where $u_j(\mathbf{x}) \exp[\pm i\omega t]$ and $\phi(\mathbf{x}) \exp[\pm i\omega t]$ are the displacement and electric scalar potential fields, and the electric field is assumed to be quasi-static.

QUASI-PERIODICITY AND CONTINUITY

A three-dimensional composite with periodic structure is regarded as a collection of identical unit cells which extend in all directions, and each consists of heterogeneous materials. For the sake of simplicity, we assume that the unit cell is a rectangular parallelepiped, whose edges are defined by three vectors $\mathbf{a}_1$, $\mathbf{a}_2$ and $\mathbf{a}_3$, which are parallel to the three coordinate axes, respectively. a_1, a_2 and a_3 are the lengths of vectors $\mathbf{a}_1$, $\mathbf{a}_2$ and $\mathbf{a}_3$, respectively.

The mass-density and the material tensors satisfy the following periodicity condition:

$$\rho(\mathbf{x}) = \rho(\mathbf{x} + m\mathbf{a}_\beta), \quad g_{jk}(\mathbf{x}) = g_{jk}(\mathbf{x} + m\mathbf{a}_\beta),$$

$$g_{jkp}(\mathbf{x}) = g_{jkp}(\mathbf{x} + m\mathbf{a}_\beta), \quad g_{jkpq}(\mathbf{x}) = g_{jkpq}(\mathbf{x} + m\mathbf{a}_\beta), \tag{5}$$

where $\beta = 1, 2, 3$ and m is an integer.

Harmonic waves with wave vector $\mathbf{q}$ satisfy the quasi-periodicity conditions:

$$u_j(\mathbf{x} + \mathbf{a}_\beta) = u_j(\mathbf{x}) \exp[i\mathbf{q} \cdot \mathbf{a}_\beta], \quad \sigma_{jk}(\mathbf{x} + \mathbf{a}) = \sigma_{jk}(\mathbf{x}) \exp[i\mathbf{q} \cdot \mathbf{a}_\beta],$$

$$D_j(\mathbf{x} + \mathbf{a}_\beta) = D_j(\mathbf{x}) \exp[i\mathbf{q} \cdot \mathbf{a}_\beta], \quad \phi(\mathbf{x} + \mathbf{a}_\beta) = \phi(\mathbf{x}) \exp[i\mathbf{q} \cdot \mathbf{a}_\beta], \tag{6}$$

across the boundary of a cell, where $\beta = 1, 2, 3$. For complete bonding at the interface between adjacent materials,

$$u_j(\mathbf{x}^+) = u_j(\mathbf{x}^-), \quad [\sigma_{jk}(\mathbf{x}^+) - \sigma_{jk}(\mathbf{x}^-)]\tau_k = 0, \tag{7}$$

where $\mathbf{x}^+$ and $\mathbf{x}^-$ are points on the opposite sides of the interface, and τ is the unit vector pointing from the minus to the plus side of the interface.

DIMENSIONLESS FIELD VARIABLES AND EQUATIONS

We use a_1 as the unit length, and ρ_0, g_2, g_3 and g_4 as those of the mass-density and the material tensors, i.e. g_{ij}, g_{ijk} and g_{ijpq}, respectively. We take a_1^{-1}, $a_1\sqrt{\rho_0 g_4}$, $1/g_4$, $1/\sqrt{g_2 g_4}$, $\sqrt{g_2/g_4}$ and $a_1\sqrt{g_2/g_4}$ as the units of the wave vector, time, stress, electric

displacement, electric field and electric scalar potential, respectively, to get the corresponding dimensionless field variables. In what follows, we use the same symbols to denote the dimensional and dimensionless field variables.

Equations (1), (3) and (4)–(7) can be regarded as those of dimensionless field variables, as long as $a_1^{-2}(\rho_0 g_4)^{-1}$ is used as the unit with which to measure λ, while eqns (2) are changed to

$$e_{jk} = g_{jkpq}\sigma_{pq} + \sqrt{\varepsilon_P} g_{pjk} D_p, \quad E_j = -\sqrt{\varepsilon_P} g_{jpq}\sigma_{pq} + g_{jk} D_k, \tag{8}$$

where

$$\varepsilon_P = (g_3)^2/(g_2 g_4) \tag{9}$$

is the electromechanical coupling coefficient.

VARIATIONAL PRINCIPLE

It is easily verified that the solution of the set of equations in (1), (4) and (8) render the functional

$$\lambda_N = \{\langle\sigma_{jk}, u_{j,k}\rangle + \langle u_{j,k}, \sigma_{jk}\rangle - \langle g_{jkpq}\sigma_{jk}, \sigma_{pq}\rangle - \sqrt{\varepsilon_P}(\langle g_{pjk} D_p, \sigma_{jk}\rangle + \langle g_{pjk}\sigma_{jk}, D_p\rangle)$$
$$+ \langle D_p, \phi_{,p}\rangle + \langle\phi_{,p}, D_p\rangle + \langle g_{pk} D_k, D_p\rangle\}/\langle\rho u_j, u_j\rangle \tag{10}$$

stationary, and the stationary value implies λ, where

$$\langle gu, v\rangle = V^{-1}\int guv^* \, \mathrm{d}V, \tag{11}$$

g is a real-valued weighting function, u and v are complex-valued functions of space coordinates, v^* is the complex conjugate of v, V is the dimensionless volume of the cell, and the integration extends over the entire cell.

The actual field variables are determined from among those satisfying conditions (6) and (7), through the condition that they make the functional (10) stationary.

MATRIX EIGENVALUE PROBLEM

We use

$$f'(\mathbf{x}) = \exp\left[i\{\mathbf{q}\cdot\mathbf{x} + 2\pi(\alpha x_1 + \beta n_0 x_2 + \gamma m_0 x_3)\}\right], \tag{12}$$

to approximate the field variables as follows:

$$\sigma_{ij}(\mathbf{x}) = \sum_{I=1}^{N} S_{ij}^I f'(\mathbf{x}), \quad u_j(\mathbf{x}) = \sum_{I=1}^{N} U_j^I f'(\mathbf{x}),$$

$$D_j(\mathbf{x}) = \sum_{I=1}^{N} D_j^I f'(\mathbf{x}), \quad \phi(\mathbf{x}) = \sum_{I=1}^{N} W^I f'(\mathbf{x}), \tag{13}$$

where α, β, γ are integers such that $-M \leqslant \alpha, \beta, \gamma \leqslant M$, S_{ij}^I, U_j^I, D_j^I and W^I are the complex coefficients, $I = \alpha + 1 + M + (\beta + M)(2M+1) + (\gamma + M)(2M+1)^2$, $n_0 = a_1/a_2$, $m_0 = a_1/a_3$ and $N = (2M+1)^3$.

Substitute from eqn (12) into eqn (10), and upon differentiation with respect to the unknown coefficients, obtain a set of linear equations for these coefficients as follows:

$$HS + \lambda_N AU = 0, \tag{14}$$

$$KD = 0, \tag{15}$$

$$H^\dagger U + BS + \sqrt{\varepsilon_P} C^\dagger D = 0, \tag{16}$$

$$K^\dagger W + \sqrt{\varepsilon_P} CS - FD = 0, \tag{17}$$

where $\dagger$ means transposed conjugate.

The bold letters stand for vectors and matrices as defined below: S, U and D are the vectors such that

$$S = [S_{11}, S_{12}, S_{13}, S_{22}, S_{23}, S_{33}]^T, \quad U = [U_1, U_2, U_3]^T, \quad D = [D_1, D_2, D_3]^T. \tag{18}$$

where S_{ij}, U_i and D_i are the N-vectors having S_{ij}^I, U_i^I and D_i^I as their Ith components, respectively, similarly, the Ith component of W is W^I; T means transposed. On the other hand,

$$K = [H_1, H_2, H_3], \tag{19}$$

where H_1, H_2 and H_3 are the $N \times N$ diagonal matrices having $i\{q_1 + 2\pi\alpha\}$, $i\{q_2 + 2\pi\beta n_0\}$ and $i\{q_3 + 2\pi\gamma m_0\}$ as their (I, I)-components, respectively.

Matrices H, A, B, C, F are given as follows:

$$H = \begin{bmatrix} H_1 & H_2 & H_3 & 0 & 0 & 0 \\ 0 & H_1 & 0 & H_2 & H_3 & 0 \\ 0 & 0 & H_1 & 0 & H_2 & H_3 \end{bmatrix}, \tag{20}$$

$$B = \begin{bmatrix} G_{1111} & 2G_{1112} & 2G_{1113} & G_{1122} & 2G_{1123} & G_{1133} \\ 2G_{1211} & 4G_{1212} & 4G_{1213} & 2G_{1222} & 4G_{1223} & 2G_{1233} \\ 2G_{1311} & 4G_{1312} & 4G_{1313} & 2G_{1322} & 4G_{1323} & 2G_{1333} \\ G_{2211} & 2G_{2212} & 2G_{2213} & G_{2222} & 2G_{2223} & G_{2233} \\ 2G_{2311} & 4G_{2312} & 4G_{2313} & 2G_{2322} & 4G_{2323} & 2G_{2333} \\ G_{3311} & 2G_{3312} & 2G_{3313} & G_{3322} & 2G_{3323} & G_{3333} \end{bmatrix}, \tag{21}$$

$$C = \begin{bmatrix} G_{111} & 2G_{112} & 2G_{113} & G_{122} & 2G_{123} & G_{133} \\ G_{211} & 2G_{212} & 2G_{213} & G_{222} & 2G_{223} & G_{233} \\ G_{311} & 2G_{312} & 2G_{313} & G_{322} & 2G_{323} & G_{333} \end{bmatrix}, \tag{22}$$

$$F = \begin{bmatrix} G_{11} & G_{12} & G_{13} \\ G_{21} & G_{22} & G_{23} \\ G_{31} & G_{32} & G_{33} \end{bmatrix}, \quad A = \begin{bmatrix} R & 0 & 0 \\ 0 & R & 0 \\ 0 & 0 & R \end{bmatrix}, \tag{23}$$

where R is an $N \times N$ matrix whose (I, J)-components are given by

$$R(I, J) = \langle \rho(x) f^I, f^J \rangle; \tag{24}$$

a similar definition is used for G_{jk}, G_{jkp} and G_{jkpq} whose components are given by the substitution of $g_{jk}(x)$, $g_{jkp}(x)$ and $g_{jkpq}(x)$ for $\rho(x)$ on the right-hand side of eqn (24), 0 is the zero-matrix, $J = (\delta + 1 + M) + (\mu + M)(2M + 1) + (\tau + M)(2M + 1)^2$, and I has been defined before.

Eliminate S, D and W from eqns (14)–(17) to obtain

$$HL^{-1} H^\dagger U - \lambda_N AU = 0, \tag{25}$$

where

$$L = B + \varepsilon_p C^{\dagger} M C, \quad M = F^{-1} - F^{-1} K^{\dagger} N^{-1} K F^{-1}, \quad N = K F^{-1} K^{\dagger}. \tag{26}\ddagger$$

The values of λ_N are given as eigenvalues of eqn (25), and U as their corresponding eigenvectors. D, S and W are given through

$$D = \sqrt{\varepsilon_p} M C S, \quad W = -\sqrt{\varepsilon_p} N^{-1} K F^{-1} C S, \quad S = -L^{-1} H^{\dagger} U. \tag{27}$$

The corresponding field variables are given by the substitution of these solutions into eqn (13).

NUMERICAL EXAMPLE

We calculate the eigenfrequencies of harmonic waves in a three-dimensional composite with ellipsoidal inclusions. The ellipsoidal inclusion is centered with respect to the cell in such a manner that its three axes are placed parallel to each side of the cell, the corresponding diameters being b_1, b_2 and b_3, respectively. Let g_{jk}^f, g_{jkp}^f, g_{jkpq}^f, ρ^f be the material constants of the inclusions, and g_{jk}^m, g_{jkp}^m, g_{jkpq}^m, ρ^m those of the matrix. We put

$$g_2 = \text{Max} \left(n_m |g_{jk}^m| + n_f |g_{jk}^f| \right), \quad g_3 = \text{Max} \left(n_m |g_{jkp}^m| + n_f |g_{jkp}^m| \right),$$

$$g_4 = \text{Max} \left(n_m |g_{jkpq}^m| + n_f |g_{jkpq}^f| \right), \quad \rho_0 = n_m \rho^m + n_f \rho^f, \tag{28}$$

where

$$n_m = 1 - n_f, \quad n_f = (\pi/6) b_1 b_2 b_3 / a_1 a_2 a_3. \tag{29}$$

The unit of frequency of the harmonic waves is given by $1/(a_1 \sqrt{\rho_0 g_4})$ and that of their phase velocity by $1/\sqrt{\rho_0 g_4}$.

The (I, J)-components of R, G_{jk}, G_{jkp} and G_{jkpq} are given by the substitution of those dimensionless parameters for g^f and g^m in the right-hand side of

$$G(I, J) = n_m g^m + n_f g^f \qquad \text{if} \quad I = J,$$

$$= 3 n_f (g^f - g^m) R^{-2} \{ R^{-1} \sin(R) - \cos(R) \} \quad \text{if} \quad I \neq J, \tag{30}$$

where

$$R = \pi \{ (b_1/a_1)^2 (\delta - \alpha)^2 + (b_2/a_2)^2 (\mu - \beta)^2 + (b_3/a_3)^2 (\tau - \gamma)^2 \}^{1/2}, \tag{31}$$

and we have used $J_{3/2}(R) = \{ 2/(\pi R) \}^{1/2} \{ R^{-1} \sin(R) - \cos(R) \}$ (see Minagawa and Nemat-Nasser, 1976).

We calculate the case where the composite is composed of gallium arsenide (matrix) and lithium niobate (inclusions). These crystals—the former is cubic and the latter trigonal—are placed in such a manner that their standard reference frames are identical to

‡ Note that N is an $N \times N$-matrix and $K^{\dagger} N^{-1} K$ is an $3N \times 3N$-matrix such that

$$\begin{bmatrix} H_1^{\dagger} N^{-1} H_1 & H_1^{\dagger} N^{-1} H_2 & H_1^{\dagger} N^{-1} H_3 \\ H_2^{\dagger} N^{-1} H_1 & H_2^{\dagger} N^{-1} H_2 & H_2^{\dagger} N^{-1} H_3 \\ H_3^{\dagger} N^{-1} H_1 & H_3^{\dagger} N^{-1} H_2 & H_3^{\dagger} N^{-1} H_3 \end{bmatrix}.$$

Table 1. Material constants

		GaAs	LiNbO₃
Elastic constants (× 10¹⁰ Nm⁻²)	c_{11}	11.81	20.3
	c_{33}		24.5
	c_{12}	5.32	5.3
	c_{13}		7.5
	c_{14}		0.9
	c_{44}	5.94	6.0
	c_{66}		7.4
Piezoelectric constant (cm⁻²)	e_{14}	−0.16	
	e_{15}		3.76
	e_{22}		2.43
	e_{31}		0.23
	e_{33}		1.33
Dielectric constant (× 10⁻¹⁰ Fm⁻¹)	ε_{11}	1.108	3.922
	ε_{33}		2.470
Mass density (× 10³ kgm⁻³)	ρ	5.317	4.64

Table 2. Phase velocities of harmonic waves in a three-dimensional composite with ellipsoidal inclusions (GaAs/LiNbO₃)

ε_p	0.0		0.4989E − 2	
q	0.001	0.5	0.001	0.5
Acoustical	0.2980E + 4	0.2974E + 4	0.3083E + 4	0.3070E + 4
	0.3023E + 4	0.3013E + 4	0.3110E + 4	0.3101E + 4
	0.5684E + 4	0.5678E + 4	0.5732E + 4	0.5728E + 4
Optical	0.4108E + 7	0.6292E + 7	0.4264E + 4	0.6526E + 4
	0.4108E + 7	0.6709E + 7	0.4288E + 4	0.6886E + 4
	0.4112E + 7	1.0103E + 7	0.4320E + 4	1.0409E + 4

$(a_1 : a_2 : a_3 = 1 : 2 : 3, \quad b_1/a_1 = 0.9, \quad b_2/a_2 = 0.8, \quad b_3/a_3 = 0.7,$
$q_1 = q_2 = q_3 = q).$

the coordinate frame so that the material constants are given as in Table 1. The g_{jk}, g_{jkp} and g_{jkpq} are estimated from these parameters by the method of matrix-inversion, and the values of g_2, g_3, g_4 and ε_p are given through eqns (9) and (28). The lowest six phase velocities are given for the two values of q in Table 2, with those of an unrealistic limiting case where the piezoelectric stress constants of both the matrix and inclusions are zero, while the other parameters are unchanged. The computations were carried out by the crudest approximation such as $M = 1$ and $N = 27$, and the other parameters used in computations are given in Table 2.

REFERENCES

American National Standard Institute (1978). IEEE standard on piezoelectricity. IEEE, Inc.
Cady, W. G. (1946). *Piezoelectricity*. McGraw-Hill. (Also Dover, 1964.)
Minagawa, S. and Nemat-Nasser, S. (1976). Harmonic waves in three-dimensional elastic composites. *Int. J. Solids Structures* **12**, 769-777.
Minagawa, S. and Nemat-Nasser, S. (1977). On harmonic waves in layered composites. *J. Appl. Mech.* **99**, 689-695.
Minagawa, S., Nemat-Nasser, S. and Yamada, M. (1981). Finite element analysis of harmonic waves in layered and fiber-reinforced composites. *Int. J. Numer. Meth. Engng* **17**, 1335-1353.
Nemat-Nasser, S. (1972). General variational methods for waves in elastic composites. *J. Elasticity* **2**, 73-90.
Nemat-Nasser, S., Fu, F. C. L. and Minagawa, S. (1975). Harmonic waves in one-, two- and three-dimensional composites: bounds for eigenfrequencies. *Int. J. Solids Structures* **11**, 617-642.