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Nonlinear surface waves on cubic materials

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ABSTRACT

The effect of nonlinearity on the propagation of surface Rayleigh waves on an elastic medium of cubic symmetry is examined by applying the results of an earlier analysis for general anisotropic materials. Explicit calculations are given of the parameters relating to the generation of higher harmonics in an initially sinusoidal wave for a series of thirty-five materials for which experimental measurements of the third-order moduli are available.

1. Introduction

In an earlier paper Lardner [1]* has examined the effect of nonlinearities on the propagation of Rayleigh waves in a homogeneous, general anisotropic elastic medium. The technique used was an extension of the method of multiple scales used earlier for similar investigations in isotropic materials by Kalyanasundaram [2,3] and Lardner [4-6]. The end result of this analysis is a coupled system of differential equations for quantities directly related to the Fourier components of the surface displacements (eqn. (I.54) or (I.58)).

The purpose of the present paper is to apply the general analysis in I to the particular case of cubic materials. In Sections 2 and 3 we shall give algebraic simplications of the various expressions given in I appropriate for the cubic case when the free surface is a plane of symmetry and the direction of propagation is one of the cubic axes. In Section 2 we simplify those quantities that depend only on the second-order elastic moduli of the material. Several of the results in this section will be familiar from linear Rayleigh wave theory and may be compared, for example, with the investigations of Chadwick and Smith [7] or Farnell [8] which also contain extensive references to previous studies. In Section 3, explicit expressions are derived for the quantities that involve the third-order elastic moduli and finally for the kernel $H(k,k')$ occurring in the system of differential equations (I.58).

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* Subsequently, this paper will be referred to as I and equations in it will be designated by (I.1) etc.

In Section 4 the numerical calculations are described and related to observable quantities. The parameters occurring in the generation of higher harmonics in an initially sinusoidal wave are calculated for a series of thirty-five cubic materials for which data on the second and third-order moduli are available. Finally, in that section, the implications of these are discussed and representative numerical results are presented in tabular and graphical form.

2. Linear Rayleigh waves in cubic† materials

We consider a half-space of homogeneous, elastic material which is cubically symmetric† in its elastic response and, in its reference configuration, occupies the region $x_2 < 0$. A slowly modulated wave is supposed to be propagating subsonically in the positive x_1-direction over the free surface $x_2 = 0$. The coordinate axes are situated so that $x_2 = 0$ is a plane of symmetry and the x_1-axis is a cubic axis of the material.

We use the standard abbreviated two-index notation c_{pq} for the elastic moduli $c_{ijk\ell}$ by means of which index pairs (ij) are represented by a single index according to the following scheme : (11) → 1, (22) → 2, (33) → 3, (23) or (32) → 4, (13) or (31) → 5, (12) or (21) → 6. Then in a cubic material there are three independent second-order moduli and the nine non-zero moduli are

$$c_{11} = c_{22} = c_{33}$$

$$c_{12} = c_{23} = c_{13} \text{ (} = c_{21}\text{, etc. by symmetry)}$$

$$c_{44} = c_{55} = c_{66}.$$

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† Crystal class 432, $\overline{4}3m$, m3m

We introduce the dimensionless ratios

$$r = c_{11}/c_{44}\,, \qquad \delta = (c_{12} + c_{44})/c_{44}$$

and use r, δ and c_{44} as the three linear elastic constants. For elastic stability they must satisfy the restrictions

$$c_{44} > 0, \quad r > 0, \quad -\tfrac{1}{2}r < \delta - 1 < r.$$

It is also useful to note that in the isotropic limit

$$c_{44} \to \mu, \quad r \to (\lambda + 2\mu)/\mu \quad \delta \to r - 1 \qquad (1)$$

where λ and μ are the usual Lamé elastic constants. Thus in particular, r has the same significance in the isotropic limit as in the earlier papers [4-6] on nonlinear surface waves in isotropic materials.

The matrix, whose elements $L_{ij}(s)$ are defined by (I.16), is found in this cubic case to be

$$\left(L_{ij}(s)\right) = c_{44}\begin{pmatrix} s^2 + r - 1 + p^2 & \delta s & 0 \\ \delta s & rs^2 + p^2 & 0 \\ 0 & 0 & s^2 + p^2 \end{pmatrix}$$

where

$$p^2 = 1 - \rho c^2/c_{44},$$

ρ being the uniform rest density and c the Rayleigh wave speed. Setting $\det[L_{ij}(s)] = 0$ we obtain that $s^{(3)} = -ip$ while $s^{(1)}$ and $s^{(2)}$ are the two roots with negative imaginary parts of the equation

$$rs^4 + \left(p^2 + rp^2 + r^2 - r - \delta^2\right)s^2 + p^2\left(r - 1 + p^2\right) = 0. \qquad (2)$$

It can be proved that two cases may arise

Case (i) : The bi-quadratic equation (2), when solved for s^2 has real and negative roots. In this case $s^{(1)}$ and $s^{(2)}$ will be pure imaginary with negative imaginary parts, and so will have complex conjugates given by $\overline{s^{(1)}} = - s^{(1)}$, $\overline{s^{(2)}} = - s^{(2)}$. The isotropic limit falls into this case.

Case (ii): Equation (2) has two conjugate complex roots for s^2. In this case $s^{(1)}$ and $s^{(2)}$ have non-zero real parts, and $\overline{s^{(2)}} = - s^{(1)}$.

Note that in both the above cases the product $s^{(1)} s^{(2)}$ is real and negative while the sum $s^{(1)} + s^{(2)}$ is imaginary with negative imaginary part.

Corresponding to each $s^{(\ell)}$ we take the following solutions of (I.17)

$$\left(a_j^{(\ell)}\right) = \begin{pmatrix} rs^{(\ell)2} + p^2 \\ - \delta s^{(\ell)} \\ 0 \end{pmatrix} \quad (\ell = 1,\ 2)\ , \qquad \left(a_j^{(3)}\right) = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} .$$

From (I.20) the matrix $\left(M_{i\ell}\right)$ can be constructed and written in the form

$$\left(M_{i\ell}\right) = c_{44} \begin{pmatrix} s^{(1)}\left(rs^{(1)2} + p^2 - \delta\right) & s^{(2)}\left(rs^{(1)2} + p^2 - \delta\right) & 0 \\ - rs^{(1)2} + p^2(\delta - 1) & - rs^{(2)2} + p^2(\delta - 1) & 0 \\ 0 & 0 & - ip \end{pmatrix}.$$

The condition $\det\left(M_{i\ell}\right) = 0$ can be simplified, using the fact that $s^{(1)}$ and $s^{(2)}$ are roots of (2), to the equation

$$p\{(\delta - 1)^2 + r(1 - r - p^2)\} = (1 - p^2)\ \{r(r - 1 + p^2)\}^{\frac{1}{2}}, \qquad (3)$$

which determines p and hence c. It can be shown that this is equivalent to the usual equation for the Rayleigh wave speed.

The quantities $\left(\beta_\ell\right)$ and $\left(\beta_i'\right)$ are solutions of $M_{i\ell}\beta_\ell = 0$ and $\beta_i' M_{i\ell} = 0$ respectively. They are taken to be

$$\beta_1 = s^{(2)}\left(rs^{(2)2} + p^2 - \delta\right), \qquad \beta_2 = - s^{(1)}\left(rs^{(1)2} + p^2 - \delta\right), \quad \beta_3 = 0$$

$$\beta_1' = rs^{(1)2} + p^2(\delta - 1) \quad , \qquad \beta_2' = \quad s^{(1)}\left(rs^{(1)2} + p^2 - \delta\right), \quad \beta_3' = 0.$$

$\Gamma^{(\ell)}$, $\Delta^{(\ell)}$ and $\theta^{(\ell)}$ defined by (I.41) can be evaluated, and they turn out to be, for $\ell = 1, 2$,

$$\Gamma^{(\ell)} = 2c_{44}\ \{r\left(rs^{(\ell)2} + p^2\right)^2 - \delta^2 s^{(\ell)2}\left(rs^{(\ell)2} + p^2 - 1\right)\}$$

$$\Delta^{(\ell)} = 2c_{44}\ s^{(\ell)}\{\left(rs^{(\ell)2} + p^2\right)^2 - \delta^2 p^2\}$$

$$\theta^{(\ell)} = 2\rho c\ \{\left(rs^{(\ell)2} + p^2\right)^2 + \delta^2 s^{(\ell)2}\}\ .$$

The identity (I.42) is readily checked using the fact that $s^{(\ell)}$ (ℓ=1,2) is a root of (2). For $\ell = 3$, we find

$$\Gamma^{(3)} = 2c_{44}, \quad \Delta^{(3)} = -\ 2i\rho c_{44}, \quad \theta^{(3)} = 2\rho c$$

and again (I.42) is clearly satisfied.

The inverse matrix $\left(U_{ij}^{(\ell)}\right)$ can be constructed from (I.45). For $\ell = 1, 2$ it turns out to be

$$\left(U_{ij}^{(\ell)}\right) = \frac{1}{c_{44}D}\begin{pmatrix} \delta^2 s^{(\ell)2} & \delta s^{(\ell)}\left(rs^{(\ell)2} + p^2\right) & 0 \\ \delta s^{(\ell)}\left(rs^{(\ell)2} + p^2\right) & \left(rs^{(\ell)2} + p^2\right)^2 & 0 \\ 0 & 0 & D/\left(s^{(\ell)2} + p^2\right) \end{pmatrix} \quad (4)$$

where

$$D = \{\left(rs^{(\ell)2} + p^2\right)^2 + \delta^2 s^{(\ell)2}\}^2/\left(rs^{(\ell)2} + p^2\right)\ .$$

The matrix $\left(U_{ij}^{(3)}\right)$ does not enter later expressions and so is not given here.

Finally we can calculate $F_j^{(\ell)}$ and $G_j^{(\ell)}$ from equations (I.47). These quantities are non-zero only when j and ℓ are 1 or 2, and in such a case are given, for ℓ = 1, 2, by

$$F_1^{(\ell)} = -\delta s^{(\ell)} F_0^{(\ell)}, \qquad F_2^{(\ell)} = -\left(rs^{(\ell)2} + p^2\right)F_0^{(\ell)}$$

$$G_1^{(\ell)} = \delta s^{(\ell)2} F_0^{(\ell)}, \qquad G_2^{(\ell)} = s^{(\ell)}\left(rs^{(\ell)2} + p^2\right)F_0^{(\ell)} \qquad (\ell = 1, 2)$$

where

$$F_0^{(\ell)} = \delta(r-1)\left(s^{(\ell)2}+1\right)\left(rs^{(\ell)2}+p^2\right) / D.$$

Note that condition (I.48) is met.

Later we shall also need the inverse matrix $\left(L_{ij}^{-1}(s)\right)$. Its elements with i, j = 1 or 2 are given by

$$L_{11}^{-1}(s) = \left(rs^2 + p^2\right) / B(s), \qquad L_{22}^{-1}(s) = \left(s^2 + r^2 - 1 + p^2\right) / B(s)$$

$$L_{12}^{-1}(s) = L_{21}^{-1}(s) = -\delta s/B(s), \qquad B(s) = c_{44} r\left(s^2 - s^{(1)2}\right)\left(s^2 - s^{(2)2}\right). \qquad (6)$$

3. Calculation of quantities involving third-order moduli

Theoretical and experimental calculations of the third-order elastic moduli of many materials have been undertaken quite extensively. The numerical data available is discussed and presented, together with comprehensive references to this work and its applications, in an excellent review article by Hearmon [9] which claims to give general literature coverage through to late 1977.

Using the same abbreviated notation for index pairs as for the linear moduli in Section 2, the third-order moduli $c^{(3)}_{ijk\ell mn}$ can be denoted by c_{pqr} with the three indices running from 1 to 6. By virtue of the symmetry, we need only list these moduli for $p \leq q \leq r$. For a cubic material, there are six independent third-order moduli and the twenty non-zero moduli are

$$c_{111} = c_{222} = c_{333}$$

$$c_{112} = c_{113} = c_{122} = c_{133} = c_{223} = c_{233}$$

$$c_{123}$$

$$c_{144} = c_{255} = c_{366}$$

$$c_{155} = c_{166} = c_{244} = c_{266} = c_{344} = c_{355}$$

$$c_{456} \; .$$

In the isotropic limit, these moduli take the form

$$\begin{aligned} c_{111} &= 6(\alpha + \beta + \gamma), \quad & c_{112} &= 6\alpha + 2\beta, \quad & c_{123} &= 6\alpha, \\ c_{144} &= \beta \quad , & c_{155} &= \beta + \frac{3}{2}\gamma, & c_{456} &= \frac{3}{4}\gamma \end{aligned} \tag{7}$$

where α, β, γ are the isotropic third-order moduli used in earlier work on nonlinear Rayleigh waves by Kalyanasundaram [2,3] and Lardner [5,6].

In the analysis in I it is found to be more convenient to write the stress-displacement equations in terms of $c_{ijk\ell}$ and $d_{ijk\ell mn}$ rather than the second and third-order moduli directly.

The quantities $d_{ijk\ell mn}$ are defined by (I.5). While symmetrical among the three pairs (ij), $(k\ell)$ and (mn) they are not symmetrical between i and j or between k and ℓ or m and n. Consequently the abbreviated notation must be modified for these quantities, and we adopt the following convention: (11) → 1, (22) → 2, (33) → 3, (23) → 4, (13) → 5, (12) → 6, (32) → 7, (31) → 8, (21) → 9 in denoting $d_{ijk\ell mn}$ by d_{pqr} ($p \leq q \leq r$) with the indices taking the values 1 to 9. From the one hundred and sixty five such constants which must be considered, there are only ten distinct d_{pqr} for our cubic material which are given by

$$d_{111} = \frac{1}{2}(c_{111} + 3c_{11}) \qquad d_{112} = \frac{1}{2}(c_{112} + c_{12})$$

$$d_{123} = \frac{1}{2} c_{123} \qquad d_{144} = \frac{1}{2}(c_{144} + c_{12})$$

$$d_{147} = \frac{1}{2} c_{144} \qquad d_{155} = \frac{1}{2}(c_{155} + c_{12} + 2c_{44})$$

$$d_{158} = \frac{1}{2}(c_{155} + c_{44}) \qquad d_{188} = \frac{1}{2}(c_{155} + c_{11})$$

$$d_{456} = \frac{1}{2}(c_{456} + c_{44}) \qquad d_{468} = \frac{1}{2} c_{456}$$

and the forty-five non-zero d_{pqr} (with $p \leq q \leq r$) are

$$d_{111} = d_{222} = d_{333}$$

$$d_{112} = d_{113} = d_{122} = d_{133} = d_{223} = d_{233}$$

$$d_{123}$$

$$d_{144} = d_{177} = d_{255} = d_{288} = d_{366} = d_{399}$$

$$d_{147} = d_{258} = d_{369}$$

$$d_{155} = d_{166} = d_{244} = d_{299} = d_{377} = d_{388}$$

$$d_{158} = d_{169} = d_{247} = d_{265} = d_{347} = d_{358}$$

$$d_{188} = d_{199} = d_{266} = d_{277} = d_{344} = d_{355}$$

$$d_{456} = d_{459} = d_{489} = d_{567} = d_{678} = d_{789}$$

$$d_{468} = d_{579}.$$

Having listed the non-zero elastic moduli, we must now derive representations for the various quantities needed to ultimately reach our objective of evaluating the kernel $H(k,k')$, given by (I.55) and (I.56), for cubic materials.

The non-zero elements among the $D_{ijm\ell}$, $D'_{ijm\ell}$ and $D''_{ijm\ell}$, computed from (I.23), are given in Table 1. These are then used in

Insert Table 1 about here

(I.24) - (I.26) to compute $N^{(p)}_{i\ell n}$ for p = 1, 2, 3. Only the elements with i, ℓ, and n equal to 1 or 2 enter the later expressions and these are given by the following expressions:

$$
\begin{aligned}
N^{(1)}_{1\ell n} = {} & \left(rs^{(\ell)2} + p^2\right)\left(rs^{(n)2} + p^2\right)\left[d_{111} + 2s^{(\ell)}s^{(n)}d_{155} + s^{(n)2}d_{155}\right] \\
& - \delta s^{(n)}\left(rs^{(\ell)2} + p^2\right)\left[s^{(\ell)}d_{158} + s^{(n)}\left(d_{112} + d_{158}\right) + s^{(\ell)}s^{(n)2}d_{188}\right] \\
& - \delta s^{(\ell)}\left(rs^{(n)2} + p^2\right)\left[s^{(\ell)}d_{112} + 2s^{(n)}d_{158} + s^{(\ell)}s^{(n)2}d_{188}\right] \\
& + \delta^2 s^{(\ell)}s^{(n)}\left[d_{188} + s^{(\ell)}s^{(n)}\left(d_{112} + d_{158}\right) + s^{(n)2}d_{158}\right]
\end{aligned}
$$

$$
\begin{aligned}
N^{(1)}_{2\ell n} = {} & \left(rs^{(\ell)2} + p^2\right)\left(rs^{(n)2} + p^2\right)\left[s^{(\ell)}d_{158} + s^{(n)}\left(d_{112} + d_{158}\right) + s^{(\ell)}s^{(n)2}d_{188}\right] \\
& - \delta s^{(n)}\left(rs^{(\ell)2} + p^2\right)\left[d_{188} + 2s^{(\ell)}s^{(n)}d_{158} + s^{(n)2}d_{112}\right] \\
& - \delta s^{(\ell)}\left(rs^{(n)2} + p^2\right)\left[d_{188} + s^{(\ell)}s^{(n)}\left(d_{112} + d_{158}\right) + s^{(n)2}d_{158}\right] \\
& + \delta^2 s^{(\ell)}s^{(n)}\left[s^{(\ell)}d_{155} + 2s^{(n)}d_{155} + s^{(\ell)}s^{(n)2}d_{111}\right] .
\end{aligned}
$$

$N^{(2)}_{i\ell n}$ is obtained from $N^{(1)}_{i\ell n}$ by complex conjugating every $s^{(\ell)}$ while $N^{(3)}_{i\ell n}$ is obtained from $N^{(1)}_{i\ell n}$ by conjugating every $s^{(n)}$.

From equations (I.31) - (I.33) we find the following expressions for $C^{(p)}_i$:

$$C^{(1)}_1 = c_{44}\delta^2 rs^{(1)}s^{(2)}\left(s^{(1)}+s^{(2)}\right)\left(s^{(1)}-s^{(2)}\right)^2\{s^{(1)}s^{(2)}\left(\delta+r-p^2\right) + p^2\left(\delta-2+r+p^2\right)\}$$

$$C^{(1)}_2 = \delta^2\left(s^{(1)}-s^{(2)}\right)^2\ \{U+V\left(s^{(1)}+s^{(2)}\right)^2\}$$

$$C^{(2)}_2 = \delta^2\left|s^{(1)}-s^{(2)}\right|^2\{U+V\left|s^{(1)}+s^{(2)}\right|^2\}$$

$$C^{(2)}_1 = 0, \quad C^{(p)}_3 = 0 \qquad (p = 1, 2)$$

where

$$U = d_{112}\left[\bar{p}^2(\delta-1) + rs^{(1)}\bar{s}^{(2)}\right]\left[\bar{p}^2(\delta-1) + rs^{(1)}\bar{s}^{(2)} - 2s^{(1)}s^{(2)}(\delta-p^2+rs^{(1)}s^{(2)})\right] + d_{111}\ s^{(1)2}s^{(2)2}\left(\delta-p^2+rs^{(1)}s^{(2)}\right)^2 .$$

$$V = \frac{1}{2}c_{44}(r+\delta-1)\ r^2 s^{(1)2}s^{(2)2} .$$

From (I.41) we can now compute $\Lambda^{(\ell)}$ to obtain

$$\Lambda^{(\ell)} = \left(rs^{(\ell)2}+p^2\right)N^{(1)}_{1\ell\ell} - \delta s^{(\ell)}N^{(1)}_{2\ell\ell}$$

while from the last of (I.47) we find using (4) that

$$H^{(\ell)}_1 = \delta s^{(\ell)}H^{(\ell)}_0 , \qquad H^{(\ell)}_2 = \left(rs^{(\ell)2}+p^2\right)H^{(\ell)}_0 \qquad (\ell = 1, 2)$$

where

$$H^{(\ell)}_0 = \frac{1}{c_{44}D}\{\delta s^{(\ell)}N^{(1)}_{1\ell\ell} + \left(rs^{(\ell)2}+p^2\right)N^{(1)}_{2\ell\ell}\}$$

and D is given by (5). $H^{(\ell)}_3 = 0$, while $H^{(3)}_j$ do not enter subsequent expressions.

From (I.51) - (I.53) we obtain the following expressions for Q, P´ and Q´:

$$Q = c_{44} \sum_{\ell=1,2} \beta_\ell \left\{ - \beta_1' \left[\delta s^{(\ell)} + \left(rs^{(\ell)2} + p^2\right) \frac{\Gamma^{(\ell)}}{\Delta^{(\ell)}} \right.\right.$$
$$\left. + \left(rs^{(\ell)2} + p^2 + \delta s^{(\ell)2}\right) F_0^{(\ell)} \left(s^{(\ell)} + \frac{\Gamma^{(\ell)}}{\Delta^{(\ell)}}\right) \right]$$
$$+ \beta_2' \left[(\delta - 1)\left(rs^{(\ell)2} + p^2\right) + r\delta s^{(\ell)} \frac{\Gamma^{(\ell)}}{\Delta^{(\ell)}} \right.$$
$$\left.\left. - s^{(\ell)} \{r\left(rs^{(\ell)2} + p^2\right) + \delta(\delta - 1)\} F_0^{(\ell)} \left(s^{(\ell)} + \frac{\Gamma^{(\ell)}}{\Delta^{(\ell)}}\right) \right] \right\}$$

$$P' = - \beta_1' C_1^{(1)} + c_{44} \sum_{\ell=1,2} \beta_\ell^2 \left\{ \beta_1' \left[\left(rs^{(\ell)2} + p^2\right) \frac{\Lambda^{(\ell)}}{\Delta^{(\ell)}} \right.\right.$$
$$\left. + \left(rs^{(\ell)2} + p^2 + \delta s^{(\ell)2}\right) \left(H_0^{(\ell)} + F_0^{(\ell)} \frac{\Lambda^{(\ell)}}{\Delta^{(\ell)}}\right) \right]$$
$$+ \beta_2' \left[- r\delta s^{(\ell)} \frac{\Lambda^{(\ell)}}{\Delta^{(\ell)}} + s^{(\ell)} \{r\left(rs^{(\ell)2} + p^2\right) + \delta(\delta-1)\} \times \right.$$
$$\left.\left. \times \left(H_0^{(\ell)} + F_0^{(\ell)} \frac{\Lambda^{(\ell)}}{\Delta^{(\ell)}}\right) \right] \right\}$$

$$Q' = - 2\beta_2' C_2^{(2)} .$$

Finally from (I.55) and (I.56) we obtain the following expressions for H(k,k´). For $k' < k$,

$$H(k,k') = \frac{P'}{Q} + \frac{2c_{44}(k-k')}{Qk} \sum_{\substack{m,\ell,n=1,2 \\ (\ell \neq n)}} \beta_\ell \beta_n N_{m\ell n}^{(1)} \Omega_m(z_{\ell n})$$

while for $k' > k$,

$$H(k,k') = \frac{Q'}{Q} + \frac{2c_{44}}{Qk} \sum_{m,\ell,n=1,2} \beta_\ell \bar{\beta}_n \left[k' N^{(2)}_{mn\ell} + (k - k')N^{(3)}_{m\ell n}\right] \Omega_m\left(w_{\ell n}\right)$$

where

$$z_{\ell n} = [s^{(\ell)} k' + s^{(n)} (k-k')]/k, \quad w_{\ell n} = [s^{(\ell)} k' + \overline{s^{(n)}} (k-k')]/k$$

and

$$\Omega_m(s) = [\beta_1' s + (\delta - 1)\beta_2'] L^{-1}_{1m}(s) + [\beta_1' + r\beta_2' s] L^{-1}_{2m}(s)$$

where the elements of the inverse matrix $\left(L^{-1}_{ij}(s)\right)$ are given in (6).

4. Computational Aspects

A computer program has been written to calculate the above $H(k,k')$ for any given values of the second and third-order elastic moduli, c_{pq} and c_{pqr}. Equation (3) is first solved numerically for p, then (2) is solved for $s^{(1)}$ and $s^{(2)}$, and after that the successive formulas given in Sections 2 and 3 are evaluated. As a check on the computation, it has been confirmed that in the isotropic limit defined by (1) and (7), the values of $H(k,k')$ are consistent with those obtained from the isotropic formulas given by Lardner in [4,5]*.

In the integral equation (I.54), $H(k,k')$ in the region $0 < k' < k$ can be replaced by the symmetrized kernel

$$H_s(k,k') = \frac{1}{2}[H(k,k') + H(k,k - k')]$$

---

* Equation (A.21) in [4] contains a misprint. On the second line the first square bracket should contain $[d_1 + d_3 p_2^2 + c_2^2 (1 - p_2^2)^2]$. A corresponding error occurs in the second line of equation (A.17) in [5] where $2d_1$ should be replaced by $d_1(1 + p_2^2)$.

without changing the equation. In comparing with the isotropic results, this symmetrized kernel must be used. The symmetrized form will also be used in the results to be presented below.

Let us define

$$\gamma(k,\xi,\tau) = \begin{cases} \sigma\,\tilde{\gamma}(k,\xi,\tau) & (k > 0) \\ \bar{\sigma}\,\tilde{\gamma}(k,\xi,\tau) & (k < 0) \end{cases}$$

where σ is the constant scaling factor defined by

$$\sigma^{-1} = \sum_{\ell} \beta_\ell\, a_1^{(\ell)} = \delta\{rs^{(1)} s^{(2)} + p^2(\delta - 1)\}\left(s^{(2)} - s^{(1)}\right) .$$

Then with this re-scaling, we see from (I.22) that $\tilde{\gamma}$ becomes exactly equal to the Fourier transform of the longitudinal surface displacement:

$$u_1(x,0,t) = \int_{-\infty}^{\infty} \tilde{\gamma}(k,\xi,\tau)e^{ik(x-ct)}\, dk \qquad (8)$$

with $\tilde{\gamma}(-k,\xi,\tau) = \overline{\tilde{\gamma}(k,\xi,\tau)}$. The normal surface displacement is then

$$u_2(x,0,t) = iK\int_{0}^{\infty} \tilde{\gamma}\,(k,\xi,\tau)e^{ik(x-ct)}\, dk + CC \qquad (9)$$

where K is the (real) constant defined by

$$K = -\,i\sigma \sum_{\ell} \beta_\ell a_2^{(\ell)} = irs^{(1)} s^{(2)}\left(s^{(1)}+s^{(2)}\right) / \{rs^{(1)} s^{(2)} + p^2(\delta-1)\}$$

and CC denotes complex conjugate.

The integral equation (I.54) can then be written as

$$\tilde{\gamma}_\xi(k,\xi,\tau) + c^{-1}\tilde{\gamma}_\tau\,(k,\xi,\tau) + \int_0^\infty \tilde{H}(k,k')k'(k-k')\tilde{\gamma}(k',\xi,\tau)\tilde{\gamma}(k-k',\xi,\tau)dk' = 0 \quad (10)$$

where

$$\tilde{H}(k,k') = \begin{cases} \sigma H_s(k,k') & (0 < k' < k) \\ \bar{\sigma} H(k,k') & (k' > k). \end{cases}$$

For the basic problem of harmonic generation by a sinusoidal source at $\xi = 0$, we take the fundamental to have wave-number $k = 1$ and replace (8) by

$$u_1(x,0,t) = \sum_{k=-\infty}^{\infty} \tilde{\gamma}_k(\xi)e^{ik(x-ct)}, \quad \tilde{\gamma}_{-k}(\xi) = \overline{\tilde{\gamma}_k(\xi)} \ .$$

Then, with an obvious extension of our notation, (10) becomes

$$\frac{d\tilde{\gamma}_k}{d\xi} + \sum_{k'=1}^{\infty} \tilde{H}_{kk'}\, k'(k - k')\tilde{\gamma}_{k'}\, \tilde{\gamma}_{k-k'} = 0$$

and the initial conditions at $\xi = 0$ are $\gamma_1 = a$, $\gamma_k = 0$ for $k > 1$ where a is the given amplitude of the fundamental. Seeking the solution for each $\tilde{\gamma}_k$ as a power series in ξ, the first few expressions are easily seen to be

$$\tilde{\gamma}_1/a = 1 - w_1\xi_1^2 + \dots$$

$$\tilde{\gamma}_2/a = w_2\xi_1\left(1 - w_4\xi_1^2 + \dots\right)$$

$$\tilde{\gamma}_3/a = w_3\xi_1^2 + \dots$$

where we have taken a to be real, which can always be achieved by choosing a suitable time origin, $\xi_1 = a\xi$ and the w_k are given by

$$w_1 = \tilde{H}_{12}\,\tilde{H}_{21}\,, \qquad w_2 = -\tilde{H}_{21}$$

$$w_3 = \left(\tilde{H}_{31} + \tilde{H}_{32}\right)\tilde{H}_{21}$$

$$w_4 = \frac{2}{3}\tilde{H}_{21}\,\tilde{H}_{12} + \tilde{H}_{23}\left(\tilde{H}_{31} + \tilde{H}_{32}\right) .$$

When the fundamental has wave number k_0, the only change necessary in these formulas is to re-define $\xi_1 = k_0^2\, a\xi$. We note also that $\xi = \epsilon x$ and the physical displacement components are ϵu_i so that the product $a\xi$ is equal to $(\epsilon a)x$, and ϵa is the amplitude of the physical longitudinal displacement at the source. Typical graphs of $\tilde{\gamma}_1/a$, $\tilde{\gamma}_2/a$ and $\tilde{\gamma}_3/a$ as a function of ξ_1 are shown in Figure 1. This figure is drawn for the material MgO.

Insert Figure 1 about here

Values of w_1, w_2, w_3 and w_4 as well as the constant K appearing in (9) have been calculated for thirty-five different cubic materials. Experimentally measured values of the second and third-order elastic moduli have been taken from Hearmon [9] and Teodosiu [10, p.72]. They are tabulated for ease of reference in Table 2. The variations in the measurements of the second-order

Insert Table 2 about here

moduli are relatively small and so Hearmon presents only an average value with the coefficient of variation for each material for which there are three or more sets of data. If more than ten sets are available he uses only the ten most recent and acceptable sets for his calculations. However, the third-order moduli should be accepted with more caution. It will be observed that for a number of the materials, several sets of values of the third-order moduli are given, corresponding to different experimental determinations. The discrepancies between these sets of values indicate the lack of reliability which can be placed in these moduli values. The computed values of w_1, ..., w_4 and K are summarized in Table 3.

Insert Table 3 about here

It can be seen that the discrepancies in the experimental third-order moduli produce rather large differences between the computed values of the w_k . The exception here is NaCℓ where the five sets of values are fairly close together. However in most cases, one can do little better than estimate the order of magnitude of the w_k without more reliable information on the moduli.

Among the materials examined, the nonlinear effects are largest for MgO and LiF and among the metals they are largest for Aℓ. Figure 1 has been constructed using the computed values of the w_k for MgO.

As a measure of the magnitude of the nonlinear effects we may consider the generation of second harmonics via the term $w_2 \xi$. Let x_{10} denote the distance from the source at which the amplitude $\tilde{\gamma}_2$ of the second harmonic reaches 10% of the initial value a of the fundamental amplitude. Then if $\lambda_0 = 2\pi/k_0$ is the wavelength of the fundamental, it can be seen that

$$\frac{x_{10}}{\lambda_0} = \frac{0.1}{\pi w_2 e_m}$$

where $e_m = [\partial(\varepsilon u_1)/\partial x_1]_{max} = 2\varepsilon a k_0$ is the maximum longitudinal strain on the surface for the initial sinusoidal wave. For example, if $e_m = 0.001$, x_{10} is 37.5 wavelengths for MgO and varies between 263 and 491 wavelengths for Si depending on which of the four sets of third-order moduli are used. At these values of x, the ratio $\left(w_4 \xi_1^2\right) = 0.01 w_4/w_2^2$ of the nonlinear to the linear term in $\tilde{\gamma}_2$ is equal to 0.023 for MgO and varies between 0.015 and 0.019 for the four sets of Si moduli.

It can be seen by inspection of the quantities involved in evaluating the $\tilde{H}_{kk}$, that, for our cubic materials, c_{111}, c_{112} and c_{155} are the only third-order moduli on which the w_k depend. In fact, w_2 varies linearly while w_1, w_3 and w_4 vary quadratically with c_{111}, c_{112} and c_{155}. It is of interest to enquire how susceptible our computed values of the w_k are to the experimental variations in the third-order moduli. A series of numerical calculations was therefore undertaken for Ge in which each of c_{111}, c_{112} and c_{155} was varied in turn over the range of the data given in Table 2 while the other moduli are kept fixed at their average values. The w_k are found to be extremely sensitive to these changes. Curves for Ge showing the above variations of $10^4 w_1$ and $-10^3 w_2$ with (a) c_{111} (b) c_{112} (c) c_{155}, are presented in Figures 2 and 3, respectively.

Insert Figures 2 and 3 about here

Acknowledgements

The authors would like to take this opportunity to thank Dr. S. B. Palmer and Professor G. A. Saunders for their correspondence concerning the third-order moduli.

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Table 1

(ijm)	$D_{ijm\ell}$	$D'_{ijm\ell}$	$D''_{ijm\ell}$
111	d_{111}	$2s^{(\ell)}d_{155}$	d_{155}
112	$s^{(\ell)}d_{158}$	$d_{112} + d_{158}$	$s^{(\ell)}d_{188}$
121	$s^{(\ell)}d_{112}$	$2d_{158}$	$s^{(\ell)}d_{188}$
122	d_{188}	$s^{(\ell)}(d_{112} + d_{158})$	d_{158}
133	d_{188}	$s^{(\ell)}(d_{144} + d_{456})$	d_{456}
211	$s^{(\ell)}d_{158}$	$d_{112} + d_{158}$	$s^{(\ell)}d_{188}$
212	d_{188}	$2s^{(\ell)}d_{158}$	d_{112}
221	d_{188}	$s^{(\ell)}(d_{112} + d_{158})$	d_{158}
222	$s^{(\ell)}d_{155}$	$2d_{155}$	$s^{(\ell)}d_{111}$
233	$s^{(\ell)}d_{456}$	$d_{456} + d_{144}$	$s^{(\ell)}d_{188}$
313	d_{188}	$2s^{(\ell)}d_{456}$	d_{144}
323	$s^{(\ell)}d_{144}$	$2d_{456}$	$s^{(\ell)}d_{188}$
331	d_{188}	$s^{(\ell)}(d_{144} + d_{456})$	d_{456}
332	$s^{(\ell)}d_{456}$	$d_{144} + d_{456}$	$s^{(\ell)}d_{188}$

TABLE 2

MATERIAL	C11	C12	C44	C111	C112	C123	C144	C155	C456
AG	123.0	92.0	45.3	-843.0	-529.0	189.0	56.0	-637.0	83.0
AL	108.0	62.0	28.3	-1060.0	-315.0	36.0	-23.0	-340.0	-30.0
AU	190.0	161.0	42.3	-1730.0	-922.0	-233.0	-13.0	-648.0	-12.0
CU (1)	169.0	122.0	75.3	-1271.0	-814.0	-50.0	-3.0	-780.0	-95.0
(2)	169.0	122.0	75.3	-1500.0	-850.0	-250.0	-135.0	-645.0	-16.0
(3)	169.0	122.0	75.3	-1950.0	-1150.0	-420.0	-125.0	-725.0	12.0
(4)	169.0	122.0	75.3	-2000.0	-1220.0	-500.0	-132.0	-705.0	25.0
(5)	169.0	122.0	75.3	-1427.0	-778.0	-265.0	-6.0	-771.0	117.0
(6)	169.0	122.0	75.3	-1427.0	-687.0	-177.0	-63.0	-744.0	66.0
(7)	169.0	122.0	75.3	-1240.0	-620.0	-110.0	-100.0	-700.0	70.0
(8)	169.0	122.0	75.3	-1270.0	-820.0	-72.0	-69.0	-67.0	40.0
(9)	169.0	122.0	75.3	-1350.0	-800.0	-120.0	-66.0	-720.0	-32.0
NB	245.0	132.0	28.4	-2560.0	-1140.0	-467.0	-343.0	-168.0	137.0
NI	247.0	153.0	122.0	-2030.0	-1040.0	-220.0	-138.0	-910.0	-70.0
CO-32 AT% NI	238.7	155.3	131.5	-2550.0	-1210.0	-10.0	-160.0	-1020.0	-120.0
CU-3.1 AT% AL	167.5	121.6	76.2	-1360.0	-797.0	-80.0	-42.0	-706.0	-32.0
CU-7.4 AT% AL	165.0	120.7	77.3	-1330.0	-793.0	-75.0	-20.0	-700.0	-43.0
CU-10.8 AT% AL	162.0	120.4	78.1	-1320.0	-781.0	-98.0	-66.0	-666.0	-36.0
CU-9 AT% NI	178.0	124.0	79.9	-1450.0	-838.0	-169.0	-131.0	-660.0	-90.0
CU-23 AT% NI	188.0	133.0	87.4	-1480.0	-880.0	-175.0	-180.0	-720.0	-80.0
CU-44.3 AT% ZN	125.0	108.0	81.0	-1220.0	-511.0	-440.0	-460.0	-509.0	-269.0
CU-48.3 AT% ZN	124.1	104.2	80.9	-1250.0	-475.0	-467.0	-385.0	-396.0	-399.0
GE (1)	129.0	48.0	67.1	-732.0	-290.0	216.0	-8.0	-304.0	-41.0
(2)	129.0	46.0	67.1	-710.0	-389.0	-18.0	-23.0	-292.0	-53.0
(3)	129.0	48.0	67.1	-716.0	-403.0	-18.0	-53.0	-315.0	-47.0
(4)	129.0	48.0	67.1	-720.0	-380.0	-30.0	-10.0	-305.0	-45.0
(5)	129.0	48.0	67.1	-760.0	-410.0	-70.0	0.0	-310.0	-46.0
(6)	129.0	46.0	67.1	-780.0	-420.0	-70.0	-10.0	-310.0	33.0
(7)	129.0	48.0	67.1	-820.0	-400.0	-50.0	-70.0	-350.0	319.0
(8)	129.0	48.0	67.1	-743.0	-374.0	-51.0	-1.0	-303.0	-82.0
(9)	129.0	48.0	67.1	-743.0	-391.0	-59.0	9.0	-296.0	-114.0
(10)	129.0	48.0	67.1	-681.0	-363.0	-9.0	9.0	-306.0	-43.0
SI (1)	165.0	64.0	79.2	-744.0	-418.0	2.0	29.0	-315.0	-70.0
(2)	165.0	64.0	79.2	-825.0	-451.0	-64.0	12.0	-310.0	-64.0
(3)	165.0	64.0	79.2	-795.0	-445.0	-75.0	15.0	-310.0	-86.0
(4)	165.0	64.0	79.2	-658.0	-511.0	60.0	65.0	-336.0	-86.0
BA.F2	90.7	41.0	25.3	-584.0	-299.0	-206.0	-121.0	-89.0	-27.0
CA.F2	165.0	46.0	33.9	-1246.0	-400.0	-254.0	-124.0	-214.0	-75.1
CD.S	76.0	55.0	23.0	-250.0	-260.0	-190.0	30.0	-60.0	40.0
GA.AS (1)	118.0	53.5	59.4	-675.0	-402.0	-4.0	-70.0	-320.0	-69.0
(2)	118.0	53.5	59.4	-622.0	-387.0	-57.0	2.0	-269.0	-39.0
GA.SB	68.4	40.3	43.4	-475.0	-308.0	-44.0	50.0	-216.0	-25.0
IN.SB	66.0	35.8	30.1	-314.0	-210.0	-48.0	9.0	-118.0	0.2
K.CL (1)	40.5	6.9	6.3	-701.0	-22.0	13.0	13.0	-24.5	12.0
(2)	40.5	6.9	6.3	-726.0	-24.0	11.0	23.0	-26.0	16.0
LI.F (1)	112.0	46.0	63.5	-1420.0	-264.0	156.0	85.0	-273.0	94.0
(2)	112.0	46.0	63.5	-1920.0	-330.0	-40.0	100.0	-325.0	43.0
MG.O	294.0	93.0	155.0	-4900.0	-95.0	-69.0	113.0	-659.0	147.0
NA.CL (1)	49.1	12.8	12.8	-880.0	-57.0	26.0	26.0	-61.0	27.0
(2)	49.1	12.8	12.8	-843.0	-50.0	46.0	29.0	-60.0	26.0
(3)	49.1	12.8	12.8	-823.0	2.0	53.0	23.0	-61.0	20.0
(4)	49.1	12.8	12.8	-864.0	-50.0	9.0	7.0	-59.0	13.0
(5)	49.1	12.8	12.8	-950.0	-79.0	90.0	19.0	-83.0	19.0
NA.F	97.0	24.2	28.1	-1460.0	-270.0	280.0	46.0	-114.0	0.0
RB.BR	31.5	4.8	3.8	-560.0	-30.0	28.0	30.0	-27.0	-31.0
RB.CL	36.4	6.3	4.7	-617.0	-67.0	87.0	25.0	-26.0	-38.0
RB.F	55.1	14.5	9.2	-671.0	-18.0	5.0	11.0	-17.0	14.0
RB.I	25.6	3.6	2.8	-463.0	-20.0	20.0	24.0	-22.0	-26.0
RB.MN.F3	116.0	42.0	32.0	-1640.0	-240.0	40.0	-60.0	-180.0	-50.0
SR.F2	124.0	45.0	31.7	-821.0	-309.0	-181.0	-95.0	-175.0	-42.0
SR.TI.O3	316.0	102.0	123.6	-4960.0	-770.0	20.0	-810.0	-300.0	90.0
Y.FE GARNET	269.0	110.0	76.6	-2330.0	-717.0	-33.0	-148.0	-306.0	-97.0

TABLE 3

MATERIAL	W1	W2	W3	W4	KCAP
AG	0.0536177	-0.2315550	0.0967009	0.0805232	1.1394349
AL	0.1496577	-0.3066562	0.3272664	0.3773898	1.4516596
AU	0.0709897	-0.2664389	0.1397617	0.1361117	1.1723123
CU (1)	0.0371406	-0.1927191	0.0666753	0.0550370	1.1095045
(2)	0.0506145	-0.2249766	0.0982464	0.0933928	1.1095045
(3)	0.0923466	-0.3036892	0.1860031	0.1981916	1.1095045
(4)	0.0860627	-0.2933645	0.1726299	0.1740078	1.1095045
(5)	0.0653666	-0.2556726	0.1266649	0.1200470	1.1095045
(6)	0.0456094	-0.2135637	0.0851387	0.0755456	1.1095045
(7)	0.0254105	-0.1594068	0.0440516	0.0339714	1.1095045
(8)	0.0000343	-0.0058545	-0.0000888	0.0001306	1.1095045
(9)	0.0436321	-0.2088830	0.0816225	0.0727060	1.1095045
NB	0.0074008	0.0860281	0.0179032	0.0239369	2.3066834
NI	0.0435166	-0.2086064	0.0876046	0.0890992	1.1276225
CU-32 AT% NI	0.1112408	-0.3335278	0.2322031	0.2469719	1.0900619
CU-3.1 AT% AL	0.0453302	-0.2129088	0.0852532	0.0766714	1.1032160
CU-7.4 AT% AL	0.0432341	-0.2079281	0.0805737	0.0712852	1.0949044
CU-10.8 AT% AL	0.0443542	-0.2106043	0.0826845	0.0736578	1.0848696
CU-9 AT% NI	0.0359122	-0.1895052	0.0684193	0.0629593	1.1195519
CU-23 AT% NI	0.0332066	-0.1822274	0.0616729	0.0542227	1.1066586
CU-44.3 AT% ZN	0.2484090	-0.4984065	0.4889947	0.4761201	1.0202453
CU-48.3 AT% ZN	0.2594724	-0.5093644	0.5126288	0.5022046	1.0238157
GE (1)	0.0028321	-0.0532175	0.0067956	0.0089827	1.1940670
(2)	0.0000301	-0.0054865	0.0001330	0.0003717	1.1940670
(3)	0.0006453	-0.0254022	0.0016235	0.0022930	1.1940670
(4)	0.0006009	-0.0245142	0.0015622	0.0023066	1.1940670
(5)	0.0017172	-0.0414393	0.0040752	0.0053026	1.1940670
(6)	0.0023987	-0.0489766	0.0055874	0.0070774	1.1940670
(7)	0.0121437	-0.1101985	0.0265619	0.0306366	1.1940670
(8)	0.0012937	-0.0359677	0.0031830	0.0043586	1.1940670
(9)	0.0006391	-0.0252800	0.0016065	0.0024710	1.1940670
(10)	0.0001011	-0.0100561	0.0003355	0.0006748	1.1940670
SI (1)	0.0072033	0.0848721	0.0133955	0.0116051	1.2256579
(2)	0.0041957	0.0647746	0.0074677	0.0061112	1.2256579
(3)	0.0056154	0.0749360	0.0102656	0.0067676	1.2256579
(4)	0.0146511	0.1210418	0.0287659	0.0278851	1.2256579
BA.F2	0.0260140	0.1612886	0.0511094	0.0496000	1.5235384
CA.F2	0.0012933	-0.0359626	0.0026215	0.0026802	1.9391717
CD.S	0.0664068	0.2576951	0.1503859	0.1827732	1.2185339
GA.AS (1)	0.0012677	-0.0356047	0.0026461	0.0028370	1.1825390
(2)	0.0010185	0.0319138	0.0020531	0.0020801	1.1825390
GA.SB	0.0002632	0.0162246	0.0005279	0.0005304	1.1916527
IN.SB	0.0106489	0.1041580	0.0233194	0.0261836	1.1861470
K.CL (1)	0.0003576	-0.0189090	0.0000318	-0.0002365	2.3358291
(2)	0.0011531	-0.0339566	0.0011455	-0.0000101	2.3358291
LI.F (1)	0.2625443	-0.5123908	0.5785255	0.6748379	1.1490751
(2)	0.6868638	-0.8287725	1.5014158	1.7300540	1.1490751
MG.O	0.7097777	-0.8424851	1.5031674	1.6490672	1.2026043
NA.CL (1)	0.0969196	-0.3113191	0.1921395	0.1893265	1.7102810
(2)	0.0823124	-0.2869014	0.1628593	0.1599418	1.7102810
(3)	0.0852086	-0.2919051	0.1687367	0.1659579	1.7102810
(4)	0.0864964	-0.2941026	0.1708108	0.1672109	1.7102810
(5)	0.2046263	-0.4523564	0.4166894	0.4292642	1.7102810
NA.F	0.0588965	-0.2426851	0.1168363	0.1152522	1.6207434
RB.BR	0.0078510	-0.0886061	0.0141081	0.0116873	2.6821730
RB.CL	0.0014830	-0.0385093	0.0019457	0.0007133	2.5813624
RB.F	0.0120728	0.1098762	0.0302329	0.0424246	2.1824832
RB.I	0.0084010	-0.0916572	0.0153475	0.0130911	2.8491514
RB.MN.F3	0.1165133	-0.3413405	0.2383931	0.2475021	1.6001104
SR.F2	0.0001977	0.0140615	0.0002260	0.0000403	1.6655631
SR.TI.O3	0.1456646	-0.3816603	0.2997689	0.3142158	1.3632658
Y.FE GARNET	0.0002918	0.0170830	0.0004481	0.0002641	1.5411635

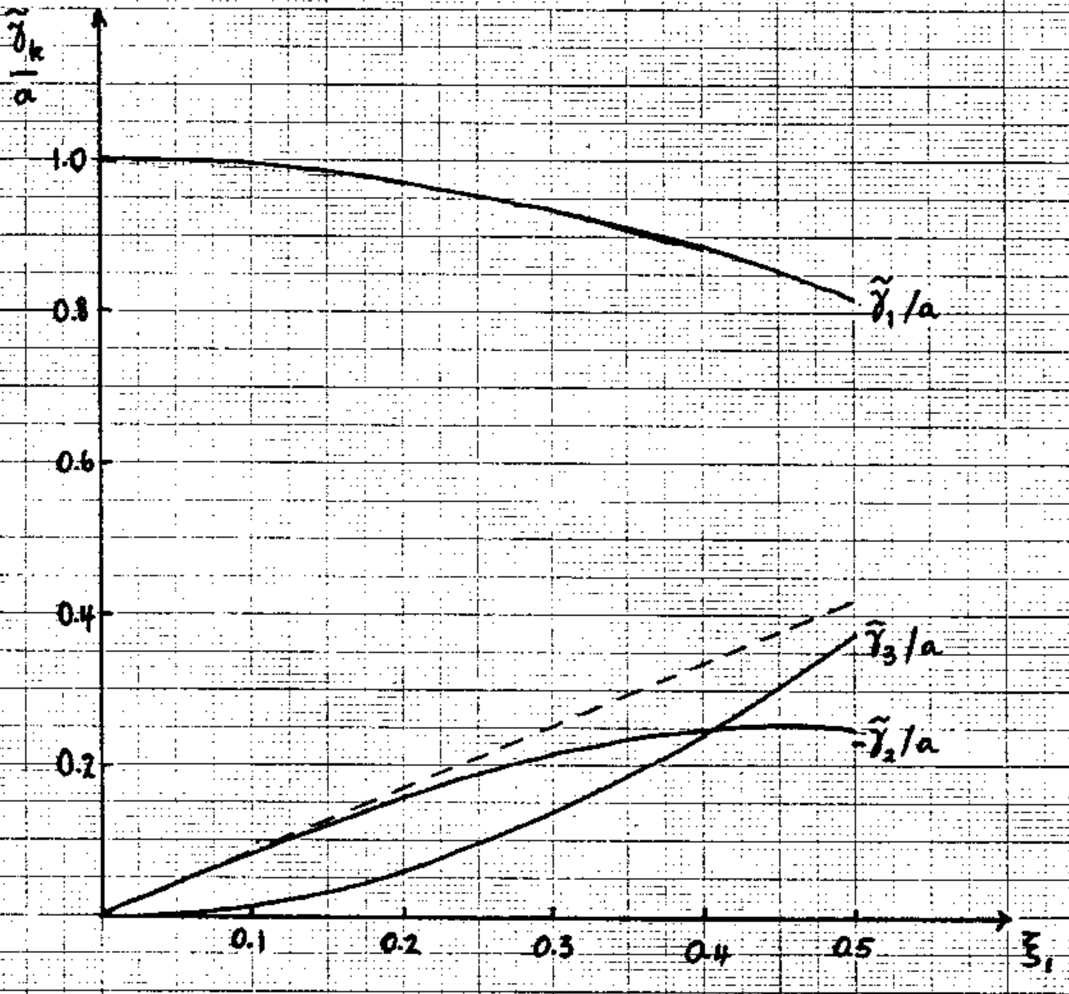
$\tilde{\gamma}_k / a$
1.0
0.8
0.6
0.4
0.2
0.1
0.2
0.3
0.4
0.5
ξ_1
$\tilde{\gamma}_1 / a$
$\tilde{\gamma}_3 / a$
$\tilde{\gamma}_2 / a$

Figure 1

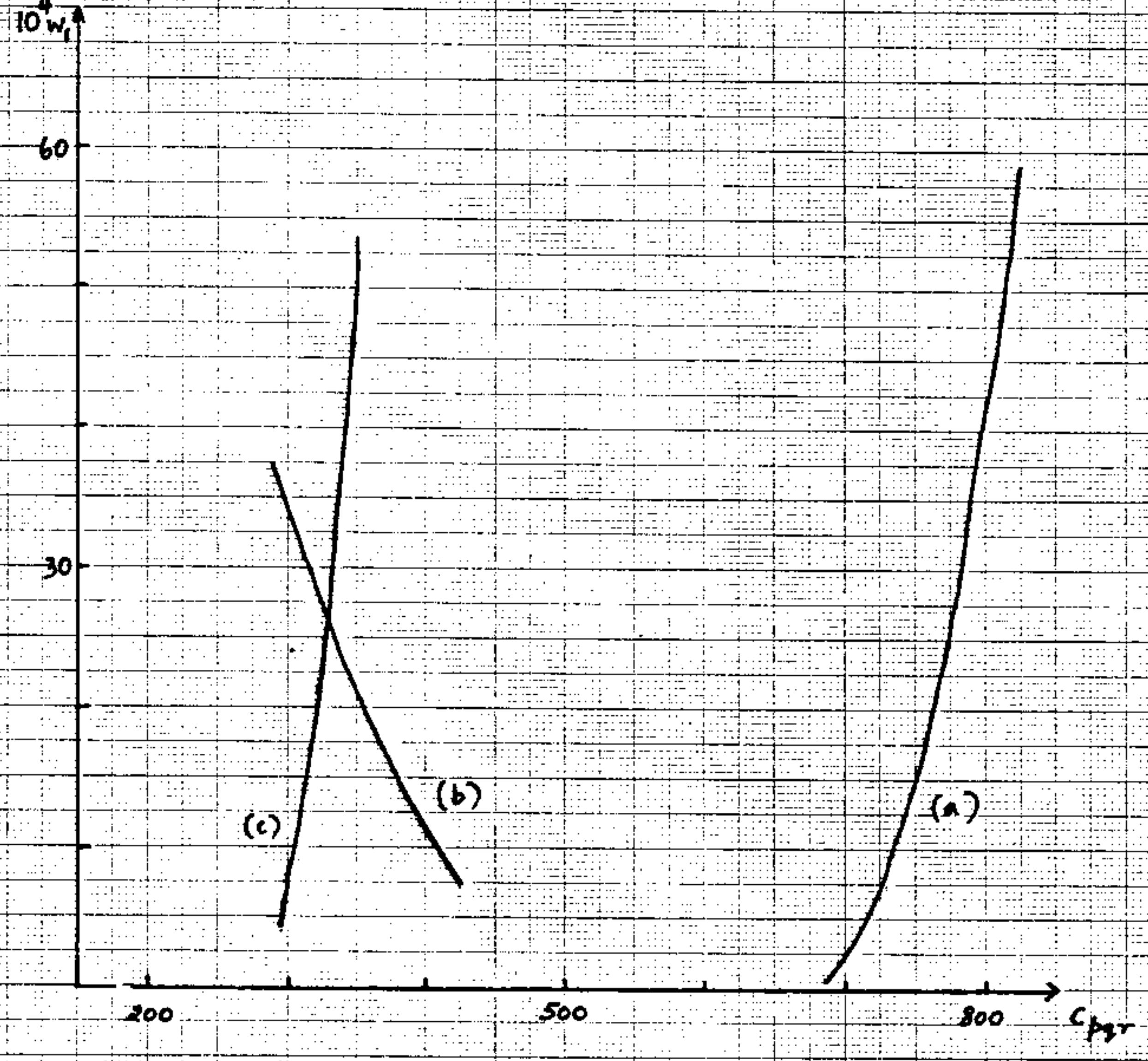

Figure 2

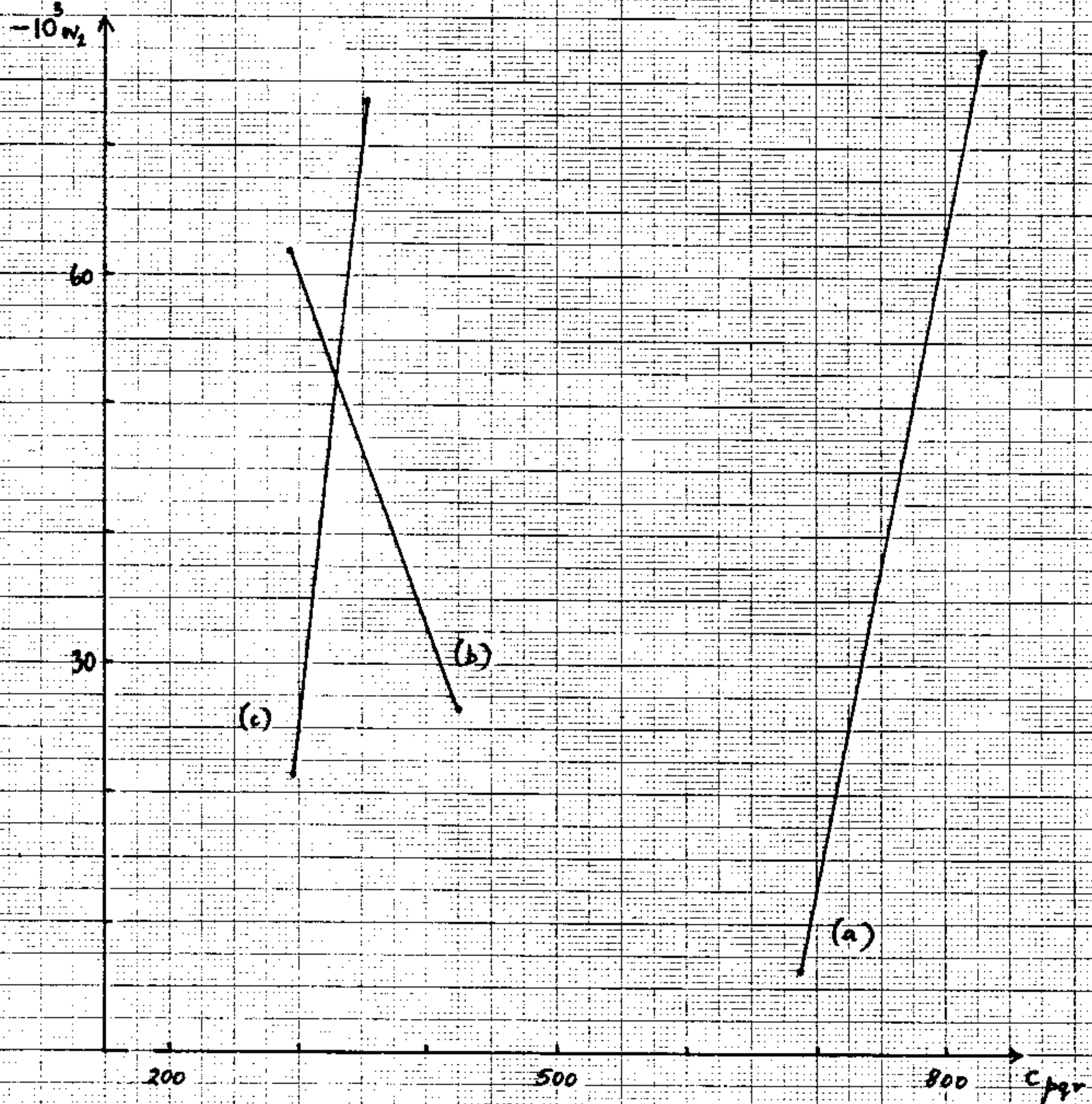

Figure 3

LEGEND OF TABLES

Table 1. The non-zero elements $D_{ijm\ell}$, $D'_{ijm\ell}$ and $D''_{ijm\ell}$

Table 2. Elastic moduli of cubic materials (units 10^9 NM^{-2})

Table 3. Parameters for harmonic generation: w_1 is the coefficient of the quadratic decay of the fundamental amplitude; w_2 is the coefficient of linear growth of the second harmonic; w_3 is the coefficient of quadratic growth of the third harmonic; w_4 is the coefficient of the nonlinear term in the second harmonic.

LEGEND OF FIGURES

Figure 1. Variations of amplitudes of fundamental and second and third harmonics with distance x from the source. Here $\xi_1 =$ $k_0^2(\varepsilon a)x$ where k_0 is the wave number of the fundamental and εa is the amplitude of the longitudinal surface displacement at the source. The graphs are computed for Mg 0.

Figure 2. Variations of $10^4 w_1$ with (a) c_{111}, (b) c_{112} and (c) c_{155}, computed for germanium.

Figure 3. Variations of $-10^3 w_2$ with (a) c_{111}, (b) c_{112} and (c) c_{155}, computed for germanium.