PHYSICAL REVIEW B VOLUME 34, NUMBER 10 15 NOVEMBER 1986

Effective dielectric and photoelastic tensors of superlattices in the long-wavelength regime

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(Received 20 May 1986)

The effective photoelastic constants of a superlattice made of thin alternating layers of orthorhombic symmetry (with principal axes along the superlattice axis) are derived as a function of dielectric, elastic, and photoelastic constants of the constituents. As a first step in this calculation we also obtain the effective dielectric constants of the superlattice for any symmetry of the constituents.

I. INTRODUCTION

A superlattice is composed of alternating layers of two (or more) different materials of thickness d and d'; a new period $D = d + d'$ is thus created in the direction perpendicular to the layers. Light and acoustic waves can propagate and interact in superlattices, like in any other medium.[1] This interaction can be schematized in the following manner. The acoustic propagation excites periodic variations of strain which induce modifications of the dielectric tensor, which in turn influence the propagation of light waves. The dielectric tensor is related to the strain through the photoelastic tensor. The photoelastic constants are needed in order to calculate the intensity either of the light diffused by phonons in a Brillouin scattering experiment, or of the deflected and modulated laser beam by ultrasound in an acousto-optical device. The purpose of this study is to obtain the expressions of the photoelastic constants in a superlattice, in the long-wavelength regime, as a function of the dielectric, elastic, and photoelastic properties of the individual layers. The general method of writing the equations of propagation in the different media and using the boundary conditions at the interfaces is rather complicated. However, in the case where the light and acoustic wavelengths are large compared to the thicknesses d and d' (long-wavelength regime), the superlattice behaves like a homogeneous effective medium whose physical properties are characterized by effective parameters obtained by taking some particular averages over the parameters of the constituents. The effective elastic and dielectric constants have been of interest for several years;[2] the effective elastic constants calculated many years ago by Rytov[3] in the case of isotropic layers have been recently generalized to cubic,[4,5] hexagonal,[5] and orthorhombic[6] symmetries. Now we are dealing with the effective photoelastic constants (Sec. III) but before it is necessary to determine the effective dielectric constants (Sec. II).

In the following, all the properties are referred to orthonormal axes of reference, x_3 being normal to the layers. The photoelastic constants are calculated for layers of orthorhombic symmetry with the principal axes parallel to x_1, x_2, x_3 and the notation $x = d/D$, $1-x = d'/D$ will be used.

II. THE EFFECTIVE DIELECTRIC CONSTANTS

Let us call $\mathbf{E},\mathbf{E}'$, and $\mathbf{D},\mathbf{D}'$ the electric and displacement fields in the two constituents of the superlattice and $\mathbf{E}^e$ and $\mathbf{D}^e$ the corresponding fields in the effective medium. We consider the limit of small d and d', where the variations of the fields remain small over each layer (static fields or propagating fields with wavelengths large compared to d and d'); then the boundary conditions on the continuity of the tangential components of $\mathbf{E}$ and of the normal component of $\mathbf{D}$ imply

$$E_1^e = E_1 = E_1' , \tag{1}$$

$$E_2^e = E_2 = E_2' , \tag{2}$$

$$D_3^e = D_3 = D_3' . \tag{3}$$

On the other hand, the voltage variation across one period of the superlattice results from the addition of the corresponding variations across two adjacent layers. This simply gives

$$E_3^e = xE_3 + (1-x)E_3' . \tag{4}$$

Finally by using the additivity of the electric moment, one obtains for the polarization vector (electric moment per unit volume) the relation

$$\mathbf{P}^e = x\mathbf{P} + (1-x)\mathbf{P}' .$$

Combining this last equation with Eqs. (1) and (2), one obtains

$$D_1^e = xD_1 + (1-x)D_1' , \tag{5}$$

$$D_2^e = xD_2 + (1-x)D_2' . \tag{6}$$

Equations (1)–(6) are the basic equations in the superlattice considered as an effective medium. The components of the effective electric and displacement fields are thus either identical to the corresponding components in the different adjacent layers, or equal to their averages. We express Eqs. (4)–(6) as a function only of E_1, E_2, and D_3, using the other Eqs. (1)–(3) as well as the relations between the displacement fields and the electric fields through the dielectric tensors

$$D_i=\sum_j \epsilon_{ij}E_j \;, \tag{7}$$

$$D_i'=\sum_j \epsilon_{ij}'E_j' \;, \tag{8}$$

$$D_i^e=\sum_j \epsilon_{ij}^e E_j^e \;. \tag{9}$$

Then, Eq. (4), for example, becomes

$$E_1\left[\frac{\epsilon_{13}^e}{\epsilon_{33}^e}-\left[x\frac{\epsilon_{13}}{\epsilon_{33}}+(1-x)\frac{\epsilon_{13}'}{\epsilon_{33}'}\right]\right]+E_2\left[\frac{\epsilon_{23}^e}{\epsilon_{33}^e}-\left[x\frac{\epsilon_{23}}{\epsilon_{33}}+(1-x)\frac{\epsilon_{23}'}{\epsilon_{33}'}\right]\right]-D_3\left[\frac{1}{\epsilon_{33}^e}-\left[\frac{x}{\epsilon_{33}}+\frac{1-x}{\epsilon_{33}'}\right]\right]=0 \;. \tag{10}$$

In order to satisfy Eq. (10) for all possible values of E_1, E_2, and D_3 one should have

$$\frac{1}{\epsilon_{33}^e}=\frac{x}{\epsilon_{33}}+\frac{1-x}{\epsilon_{33}'} \;, \tag{11}$$

$$\frac{\epsilon_{i3}^e}{\epsilon_{33}^e}=x\frac{\epsilon_{i3}}{\epsilon_{33}}+(1-x)\frac{\epsilon_{i3}'}{\epsilon_{33}'}, \quad i=1 \text{ or } 2 \;. \tag{12}$$

It is worthwhile to point out that the effective constants ϵ_{33}^e, ϵ_{13}^e, and ϵ_{23}^e are obtained by building some particular averages over the parameters of the two media, that is averages over $1/\epsilon_{33}$, $\epsilon_{13}/\epsilon_{33}$, and $\epsilon_{23}/\epsilon_{33}$, each layer having a weight equal to its relative thickness.

A similar procedure applied to Eqs. (5) and (6) leads to three new relations giving ϵ_{11}^e, ϵ_{22}^e, and ϵ_{12}^e. These relations can be summarized as

$$\epsilon_{ij}^e-\frac{\epsilon_{i3}^e\epsilon_{j3}^e}{\epsilon_{33}^e}=x\left[\epsilon_{ij}-\frac{\epsilon_{i3}\epsilon_{j3}}{\epsilon_{33}}\right]+(1-x)\left[\epsilon_{ij}'-\frac{\epsilon_{i3}'\epsilon_{j3}'}{\epsilon_{33}'}\right] \tag{13}$$

for $ij=11$, 22, or 12; they express that we have taken the averages of the following three combinations of the dielectric constants:

$$\epsilon_{11}-\frac{\epsilon_{13}^2}{\epsilon_{33}},\quad \epsilon_{22}-\frac{\epsilon_{23}^2}{\epsilon_{33}},\quad \text{and } \epsilon_{12}-\frac{\epsilon_{13}\epsilon_{23}}{\epsilon_{33}} \;.$$

Table I summarizes the six combinations of the elements of the effective dielectric tensor which are the averages of the corresponding combinations in the two constituents. These relations enable us to obtain the six independent components ϵ_{ij}^e for all symmetries of the layers. Now if the layers are orthorhombic with their principal axes parallel to x_1, x_2, x_3, the effective medium is also orthorhombic, the nondiagonal elements of the dielectric tensors vanish, and the diagonal elements ϵ_{ii}^e of the effective tensor are obtained by writing that ϵ_{11}^e, ϵ_{22}^e, and $1/\epsilon_{33}^e$ are respectively equal to the averages of the corresponding quantities.

III. THE PHOTOELASTIC TENSOR

The components P_{ijkl} of the photoelastic tensor are defined as[7]

$$\delta\epsilon_{ij}=-\epsilon_{ii}\epsilon_{jj}\sum_{k,l}P_{ijkl}\frac{\partial u_k}{\partial x_l} \;, \tag{14}$$

where the $\delta\epsilon_{ij}$ give the variations of the dielectric tensor in presence of gradients of the mechanical displacement **u**. One can notice that the P_{ijkl} are symmetrical with respect to the two indices i and j ($P_{ijkl}=P_{jikl}$), but not with respect to k and l, contrary to the generally admitted definition,[8] since Pockel, where the elements S_{kl} of the deformation tensor were used in Eq. (14) instead of the displacement gradients. Thus for orthorombic layers there are 15 different components P_{1111}, P_{1122}, P_{1133}, P_{2211}, P_{2222}, P_{2233}, P_{3311}, P_{3322}, P_{3333}, P_{2323}, P_{2332}, P_{3131}, P_{3113}, P_{1212}, and P_{1221}. Actually, the six last components (also called transverse photoelastic components because they are involved in the interaction of light with transverse acoustic waves propagating along the principal axes) are not independent, since

$$P_{ijkl}-P_{ijlk}=\left[\frac{1}{\epsilon_{jj}}-\frac{1}{\epsilon_{ii}}\right](\delta_{ik}\delta_{jl}-\delta_{il}\delta_{jk}) \;, \tag{15}$$

where δ_{ij} is the Kroenecker symbol.

The displacement gradients $\partial u_i/\partial x_j$ in the effective medium and in the layers of the superlattice satisfy the following equations ($i=1$, 2, or 3)

$$\left[\frac{\partial u_i}{\partial x_j}\right]^e=\frac{\partial u_i}{\partial x_j}=\left[\frac{\partial u_i}{\partial x_j}\right]' \quad \text{for } j=1,2 \;, \tag{16}$$

$$\left[\frac{\partial u_i}{\partial x_3}\right]^e=x\frac{\partial u_i}{\partial x_3}+(1-x)\left[\frac{\partial u_i}{\partial x_3}\right]' \;. \tag{17}$$

In particular, the components S_{ij},

$$S_{ij}=\frac{1}{2}\left[\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right] ,$$

of the deformation tensors are related by

$$S_{ij}^e=S_{ij}=S_{ij}' \quad \text{for } ij=11,\ 22, \text{ or } 12 \;, \tag{18}$$

$$S_{ij}^e=xS_{ij}+(1-x)S_{ij}' \quad \text{for } ij=13,\ 23, \text{ or } 33 \;. \tag{19}$$

Combining the last equations with those relating the elements T_{ij} of the stress tensors

$$T_{ij}^e=T_{ij}=T_{ij}' \quad \text{for } ij=13,\ 23, \text{ or } 33 \;, \tag{20}$$

$$T_{ij}^e=xT_{ij}+(1-x)T_{ij}' \quad \text{for } ij=11,\ 22, \text{ or } 12 \;, \tag{21}$$

and using the Hooke's law, Grimsditch[6] was able to find the nine effective elastic constants of the superlattice.[9] Table I indicates the nine combinations of the effective elastic constants which are averages of the corresponding quantities in the two layers.

Let us come back to the variations of the dielectric constants $\delta\epsilon_{ij}$ in presence of a general deformation [Eq. (4)], and consider first the diagonal elements $\delta\epsilon_{ii}$. It is worthwhile to express them as a function of S_{11}, S_{22}, and T_{33}, rather than S_{11}, S_{22}, and S_{33} which appear in Eq. (14), because the first quantities remain invariant over a period of the superlattice according to (18) and (20). Thus we obtain

$$-\frac{\delta\epsilon_{ii}}{\epsilon_{ii}^2}=\left[P_{ii11}-P_{ii33}\frac{C_{13}}{C_{33}}\right]S_{11}+\left[P_{ii22}-P_{ii33}\frac{C_{23}}{C_{33}}\right]S_{22}+P_{ii33}\frac{T_{33}}{C_{33}}\quad (i=1,2,3)\ . \tag{22}$$

The nondiagonal elements $\delta\epsilon_{ij}$ with $ij=12$, 13, 23, can be obtained from (14) as a function of $\partial u_i/\partial x_j$ and $\partial u_j/\partial x_i$ which are not all invariant over the superlattice period. Using Hooke's law and Eq. (15) we obtain

$$-\frac{\delta\epsilon_{12}}{\epsilon_{11}\epsilon_{22}}=P_{1212}\frac{\partial u_1}{\partial x_2}+P_{1221}\frac{\partial u_2}{\partial x_1}\ , \tag{23}$$

$$-\frac{\delta\epsilon_{13}}{\epsilon_{11}\epsilon_{33}}=P_{1313}\frac{T_{13}}{C_{55}}+\left[\frac{1}{\epsilon_{11}}-\frac{1}{\epsilon_{33}}\right]\frac{\partial u_3}{\partial x_1}\ , \tag{24}$$

$$-\frac{\delta\epsilon_{23}}{\epsilon_{22}\epsilon_{33}}=P_{2323}\frac{T_{23}}{C_{44}}+\left[\frac{1}{\epsilon_{22}}-\frac{1}{\epsilon_{33}}\right]\frac{\partial u_3}{\partial x_2}\ . \tag{25}$$

Equations similar to (22)–(25) hold for the second constituent of the superlattice as well as for the effective medium. We now consider particular elastic deformations compatible with the orthorhombic symmetry and combine these last equations with (11)–(13) in order to obtain the effective photoelastic constants.

The propagation along x_3 of an acoustic wave polarized along x_2 (which means $\partial u_3/\partial x_2=0$; $\partial u_2/\partial x_3=2S_{23}=T_{23}/C_{44}$) induces [Eq. (25)] a component $\delta\epsilon_{23}$ of the dielectric tensor in an orthorhomic medium; in the superlattice (12) gives

$$\frac{\delta\epsilon_{23}^e}{\epsilon_{33}^e}=x\frac{\delta\epsilon_{23}}{\epsilon_{33}}+(1-x)\frac{\delta\epsilon_{23}'}{\epsilon_{33}'}\ . \tag{26}$$

Combination of (26) and (25) together with the invariance of T_{23} over the superlattice period leads to

$$\frac{\epsilon_{22}^eP_{2323}^e}{C_{44}^e}=x\frac{\epsilon_{22}P_{2323}}{C_{44}}+(1-x)\frac{\epsilon_{22}'P_{2323}'}{C_{44}'}\ . \tag{27}$$

Likewise combining (24) and (12) we obtain that $\epsilon_{11}^eP_{1313}^e/C_{55}^e$ is the average of the corresponding quantities in the two constituents. Once the expressions of P_{ijij}^e ($ij=13,23$) are known, those of P_{ijji}^e result from the analog of Eq. (15) for the effective medium.

The propagation along x_2 of an acoustic wave polarized along x_1 gives rise to $\delta\epsilon_{12}$. According to (13)

$$\delta\epsilon_{12}^e=x\delta\epsilon_{12}+(1-x)\delta\epsilon_{12}' \tag{28}$$

which combined with (23) gives

$$\epsilon_{11}^e\epsilon_{22}^eP_{1212}^e=x\epsilon_{11}\epsilon_{22}P_{1212}+(1-x)\epsilon_{11}'\epsilon_{22}'P_{1212}'\ . \tag{29}$$

The interchange of the indices 1 and 2 also gives

$$\epsilon_{11}^e\epsilon_{22}^eP_{1221}^e=x\epsilon_{11}\epsilon_{22}P_{1221}+(1-x)\epsilon_{11}'\epsilon_{22}'P_{1221}'\ . \tag{30}$$

In order to calculate the components P_{iijj} of the photoelastic tensor, let us first consider a longitudinal wave along x_3 which induces variations $\delta\epsilon_{ii}$ ($i=1,2,3$) through (22), where $S_{11}=S_{22}=0$ but $T_{33}\neq 0$. Writing these $\delta\epsilon_{ii}$

TABLE I. Effective constants of superlattices in the long-wavelength regime. The effective elastic, dielectric, and photoelastic constants can be obtained by equating for each of the quantity A, its value A^e in the effective medium with its average over the two constituents of the superlattice, i.e., $A^e=xA+(1-x)A'$, where $x=d/D$.

Dielectric tensor (all symmetries)	Elastic constants	Photoelastic tensor components
	(orthorhombic layers	with principal axes parallel to x_1,x_2,x_3)
$1/\epsilon_{33}$	$1/C_{33}$	P_{3333}/C_{33}
$\epsilon_{13}/\epsilon_{33}$	C_{13}/C_{33}	$\epsilon_{11}^2P_{1133}/C_{33}$
$\epsilon_{23}/\epsilon_{33}$	C_{23}/C_{33}	$\epsilon_{22}^2P_{2233}/C_{33}$
$\epsilon_{11}-\epsilon_{13}^2/\epsilon_{33}$	$C_{11}-C_{13}^2/C_{33}$	$P_{3311}-P_{3333}C_{13}/C_{33}$
$\epsilon_{22}-\epsilon_{23}^2/\epsilon_{33}$	$C_{22}-C_{23}^2/C_{33}$	$\epsilon_{11}^2(P_{1111}-P_{1133}C_{13}/C_{33})$
$\epsilon_{12}-\epsilon_{13}\epsilon_{23}/\epsilon_{33}$	$C_{12}-C_{13}C_{23}/C_{33}$	$\epsilon_{22}^2(P_{2211}-P_{2233}C_{13}/C_{33})$
	$1/C_{44}$	$P_{3322}-P_{3333}C_{23}/C_{33}$
		$\epsilon_{11}^2(P_{1122}-P_{1133}C_{23}/C_{33})$
	$1/C_{55}$	$\epsilon_{22}^2(P_{2222}-P_{2233}C_{23}/C_{33})$
	C_{66}	$\epsilon_{11}\epsilon_{22}P_{1212}$
		$\epsilon_{11}\epsilon_{22}P_{1221}$
		$\epsilon_{11}P_{1313}/C_{55}$
		$\epsilon_{11}P_{1331}/C_{55}+\epsilon_{11}/(\epsilon_{33}C_{55})$
		$\epsilon_{22}P_{2323}/C_{44}$
		$\epsilon_{22}P_{2332}/C_{44}+\epsilon_{22}/(\epsilon_{33}C_{44})$

from Eqs. (11) and (13) we obtain

$$\frac{\epsilon_{ii}^{e^2} P_{ii33}^e}{C_{33}^e} = x\frac{\epsilon_{ii}^2 P_{ii33}}{C_{33}} + (1-x)\frac{(\epsilon'_{ii})^2 P'_{ii33}}{C'_{33}} \quad (i=1,2) \;,$$

$$\frac{P_{3333}^e}{C_{33}^e} = x\frac{P_{3333}}{C_{33}} + (1-x)\frac{P'_{3333}}{C'_{33}} \;. \tag{31}$$

These equations give the constants P_{ii33}. We now consider the more general case of a sagittal wave polarized in the x_1x_3 plane (S_{11} and $T_{33} \neq 0$). It results that the following quantities

$$\epsilon_{ii}^{e^2}\left[P_{ii11}^e - P_{ii33}^e \frac{C_{13}^e}{C_{33}^e}\right] \quad \text{for } i=1 \text{ or } 2$$

and

$$P_{3311}^e - P_{3333}^e \frac{C_{13}^e}{C_{33}^e}$$

are averages of the corresponding quantities in the two layers. In the same way the consideration of a saggital wave polarized in the x_2x_3 plane leads to a similar result for the quantities

$$\epsilon_{ii}^2\left[P_{ii22} - P_{ii33}\frac{C_{23}}{C_{33}}\right] \quad \text{for } i=1 \text{ or } 2$$

and

$$P_{3322} - P_{3333}\frac{C_{23}}{C_{33}} \;.$$

Table I summarizes all the combinations of the elastic, dielectric, and photoelastic constants which have to be averaged in order to obtain the effective photoelastic constants of the superlattice.

IV. CONCLUSIONS

In this paper it is shown that the components of the dielectric, elastic and photoelastic tensors of a superlattice are involved into expressions which have to be averaged over the constitutive layers. To each layer corresponds a weight in the summation equal to its relative thickness. Though one generally deals with superlattices composed of two different media, this summation is obviously valid irrespective of the number of layers contained in a period.

Besides, the results reported in Table I apply also to superlattices with layers of higher symmetry. Hexagonal 622 (D_6), $6mm$ (C_{6v}), $\bar{6}m2$ (D_{3h}), and $6/mmm$ (D_{6h}), tetragonal 422 (D_4), $4mm$ (C_{4v}), $\bar{4}2m$ (D_{2d}), $4/mmm$ (D_{4h}), cubic and isotropic layers give the same expressions as is Table I provided that minor changes in the tensors components are carried out.[8]

The intensity of the light scattered in a Brillouin line[10] is proportional to the product n^8p^2/C; here C is the elastic constant, n the refractive index ($n=\sqrt{\epsilon}$), and p the photoelastic constant corresponding to the geometry of the scattering process where a photon and a phonon are involved. Besides, the intensity of a laser beam which is deflected at Bragg incidence in an acousto-optical cell,[1] is proportional to the so-called "figure of merit" $M_2 = n^6p^2/\rho v^3$ (ρ is the density and v the acoustic velocity). In order to calculate M_2 in a superlattice, one has to use the effective values reported in Table I, in addition to the obvious equation $\rho^e = x\rho + x'\rho'$.

The procedure shown in this paper to obtain the expressions of the effective elastic, dielectric, and photoelastic constants is quite general and can be extended to other physical properties (piezoelectricity, ferroelectricity, conductivity, etc.) in the limit where they undergo small variations in the scale of one superlattice period (the superperiods range between 10 and 1000 Å in usual microstructures).

Note added. After the submission of this study, another paper [M. Grimsditch and F. Nizzoli, Phys. Rev. B 33, 5891 (1986)] has appeared which gives a formal generalization of the Grimsditch theory and enables the calculation of the effective elastic constants for any symmetry of the layers in the superlattice. This result, together with the fact that the dielectric tensor calculated in the present paper, is valid for any symmetry of the layers, may make it possible to also calculate (at least numerically) the P_{ijkl} for any symmetry.

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