PHYSICAL REVIEW B VOLUME 46, NUMBER 20 15 NOVEMBER 1992-II

Pressure tuning of strains and piezoelectric fields in cubic superlattices and heterostructures: Linear effects

E. Anastassakis
Physics Department, National Technical University, Zografou Campus, Athens 157 80, Greece

(Received 6 April 1992; revised manuscript received 4 August 1992)

Strained superlattices and heterostructures under hydrostatic pressure exhibit changes in the elastic strain and stress components which, in the lowest order, are linear in the applied pressure. An arbitrary direction of growth is assumed. Criteria are established for predicting the form of such changes in any combination of material constituents. The pressure dependence of the tetragonal distortion is shown to affect the built-in piezoelectric fields, wherever present. Expressions are derived for the effective linear compressibilities parallel and perpendicular to the direction of growth, and for the effective bulk compressibilities and bulk moduli of the system.

I. INTRODUCTION

Strained superlattices (SL) and heterostructures (HS) have been studied extensively in recent years under hydrostatic pressure P. Interesting changes have been observed in the phonon spectra through Raman spectroscopy,[1–3] in the electronic band structure through photoluminescence[4] or other optical spectroscopic techniques,[5] and in the type conversions and phase transitions of the constituents.[6] A constantly increasing variety of constituents is involved in these studies. It will be useful, therefore, to have some general criteria for predicting the behavior under P of a particular combination of constituents. In a very recent publication,[7] Tuchman and Herman presented a theoretical discussion of the effect of P on the in-plane strain of HS based, mainly, on physical arguments; the direction of growth presumably is along [001] and the analysis includes nonlinear terms in P, which turn out to be of importance for pressures beyond the linear range.

Here, the problem is treated theoretically in its most general form, and concerns the pressure dependence of the complete strain and stress tensors in strained SL and HS grown along a general direction. Only linear terms in P are considered; thus, all conclusions are subject to a linearity criterion, which is quantified by setting an upper limit to P. In order to determine the latter, we assume that the pressure-induced linear change $\delta B = B'P$ of the bulk modulus B of either constituent is negligible compared to B (we assume the same is true for all elastic constants). The upper limit $P_{\max}$ of that constituent then satisfies $P_{\max} \ll B/B'$; for practical purposes we can set $P_{\max} \simeq B/B'^2$. [For the III-V and II-VI materials, the slope $B' = dB/dP$ is around 4.5 (Ref. 7); a rule of thumb then is to take $P_{\max} \simeq B/20$.] In general, we can define $P_{\max}$ for the system as the lower of the $P_{\max}$ pressures of the two constituents. In short, the present work concerns pressures $P \leq P_{\max}$.

It is assumed that these structures are coherently grown, with no interfacial disorder, and that the elastic-continuum theory can be applied. For simplicity, the SL are regarded as being in a free-standing state. The results are easily extended to include buffer effects [see discussion following Eq. (4)].

Of central importance is the P dependence of the in-plane and normal-to-the-plane strain components $\varepsilon^{\parallel}(P)$ and $\varepsilon^{\perp}(P)$, respectively, and also the P dependence of the tetragonal distortion

$$\Delta\varepsilon(P) = \varepsilon^{\parallel}(P) - \varepsilon^{\perp}(P) .$$

For all combinations of constituents, these functions are linear in P, in the lowest order. Furthermore, in some combinations of constituents, $\varepsilon^{\parallel}(P)$, $\varepsilon^{\perp}(P)$, and $\Delta\varepsilon(P)$ can be tuned by P to positive, zero, or negative values, depending on the bulk values of the lattice constants and bulk moduli. The piezoelectric fields that may exist in piezoelectric constituents are shown to depend on P in a similar manner. The effective values of the linear compressibilities parallel and normal to the direction of growth are derived explicitly in terms of the corresponding constituent's properties, and likewise for the effective bulk compressibilities and bulk moduli of the system.

Section II includes the necessary background information and notation, followed by the derivation of the P-dependent strain and stress components, independently for SL and HS in Secs. III and IV. Compressibilities and piezoelectric fields are treated in Secs. V and VI, respectively. The results are summarized and discussed in Sec. VII.

II. BACKGROUND INFORMATION AND NOTATION FOR THE $P = 0$ STATE

A detailed treatment of the elastic strains and stresses for cubic constituents at $P = 0$ (more precisely, at 1 bar) can be found in Refs. 8–10. Only the necessary results are repeated here. This and the following section concern SL. Similar results for HS are presented in Sec. IV.

By a_ν and h_ν (ν denotes layer 1 or layer 2) we designate the bulk lattice constants and the layer thicknesses of the two constituents. The SL consists of equal numbers of layers 1 and 2, say, m. Thus, the total thickness is

$$h_{\text{tot}} = m(h_1 + h_2) < h_c \ ,$$

where h_c is the critical thickness for which misfit dislocations start to appear (subcritical). Since we have assumed coherent growth, the direction cosines and all their functions are common to both layers. All other layer parameters should carry the layer index ν. Wherever obvious, ν will be omitted for simplicity. The lattice misfit is defined here as $f = (a_2/a_1) - 1$.

We designate the cubic axes by $x_1 \| [100]$, $x_2 \| [010]$, $x_3 \| [001]$, and the SL axes by $x'_1 \| [l_1 m_1 n_1]$, $x'_2 \| [l_2 m_2 n_2]$ (in-plane axes), and $x'_3 \| [l_3 m_3 n_3] \equiv \mathbf{N}$ (direction of growth), $l_\lambda, m_\lambda, n_\lambda$ being the direction cosines of x'_λ relative to x_λ ($\lambda = 1-3$). Hereafter, all primed (unprimed) components refer to the primed (unprimed) system, and all latin (greek) indices run from 1 (1) to 6 (3). Latin indices refer to suppressed indices, i.e., $11 \to 1$, $22 \to 2$, $33 \to 3$, $23 = 32 \to 4$, $31 \to 5$, $12 \to 6$.

Within each layer, the in-plane strain is isotropic. The tetragonal distortion of either layer is defined as the difference of the in-plane strain $\varepsilon^{\|}$ and the normal-to-the-plane strain $\varepsilon^{\perp}$. It is given by[8]

$$\Delta\varepsilon = \varepsilon^{\|} - \varepsilon^{\perp} = \frac{3B\varepsilon^{\|}}{\Delta}[C_{44}^2 + CC_{44}(1 - T_{33}) + 3C^2(l_3 m_3 n_3)^2] \ , \tag{1}$$

i.e., it is expressed in terms of $l_3 m_3 n_3$, the corresponding elastic stiffnesses C_{ij}, and the in-plane strain. The bulk modulus of the layer is $B = (C_{11} + 2C_{12})/3$, and

$$C = C_{11} - C_{12} - 2C_{44} \ , \tag{2a}$$

$$T_{33} = l_3^4 + m_3^4 + n_3^4 \ , \tag{2b}$$

$$\Delta = C_{11}C_{44}^2 + (CC_{44}/2)(C_{11} + C_{12})(1 - T_{33}) + C^2(C_{11} + 2C_{12} + C_{44})(l_3 m_3 n_3)^2 \ . \tag{2c}$$

The reduced tetragonal distortion, defined from Eq. (1) as

$$\Delta\tilde{\varepsilon} = \Delta\varepsilon/\varepsilon^{\|} \ , \tag{1'}$$

is readily computed from l_3, m_3, n_3 and C_{ij}. It is an important parameter and will be used extensively in the following analysis. Having determined the value of $\Delta\tilde{\varepsilon}$ for each layer, the relevant elastic properties are obtained as follows.

A positive-definite property, usually defined as the shear modulus of the layer, is given by[9]

$$G_\nu = 3B_\nu(3 - \Delta\tilde{\varepsilon}_\nu) \ . \tag{3}$$

Within an $\mathbf{N}$-dependent multiplication factor,[9] the in-plane lattice constant at $P = 0$ for both layers is

$$a^{\|} = \frac{h_1 G_1 a_1 + h_2 G_2 a_2}{h_1 G_1 + h_2 G_2} \ . \tag{4}$$

To be precise, Eq. (4) corresponds to the free-standing state only and is derived from the requirement of minimal elastic free-energy density.[9] If the SL is grown on a buffer (h_b, G_b, a_b) the following three possibilities exist: (i) The SL is grown on the buffer incoherently; the buffer then remains practically unstrained; the SL remains in its own free-standing state and Eq. (4) continues to hold; (ii) the SL is grown on the buffer coherently; if $h_b \geq h_\nu$, the buffer is also strained, as if it were a third constituent of the SL; Eq. (4) is valid with the terms $h_b G_b a_b$ and $h_b G_b$ added to the numerator and denominator, respectively; (iii) as in (ii), but with $h_b \gg h_\nu$; the buffer is practically unstrained and $a^{\|} = a_b$. Analogous definitions apply to HS. For simplicity we consider from now on only case (i).

The in-plane strains of the two layers ($\nu = 1,2$) are, by definition,

$$\varepsilon_1^{\|} = (a^{\|}/a_1) - 1 = \left[\frac{h_2 G_2}{h_1 G_1 + h_2 G_2} \right] f \ , \tag{5a}$$

$$\varepsilon_2^{\|} = (a^{\|}/a_2) - 1 = \left[\frac{-h_1 G_1}{h_1 G_1 + h_2 G_2} \right] f \ , \tag{5b}$$

and the normal-to-the-plane strains of the two layers are

$$\varepsilon_1^{\perp} = \varepsilon_1^{\|} - \Delta\varepsilon_1 \ , \tag{6a}$$

$$\varepsilon_2^{\perp} = \varepsilon_2^{\|} - \Delta\varepsilon_2 \ . \tag{6b}$$

The shear strains and the stresses of either layer (ν) are

$$\varepsilon'_{\nu,4} = \frac{3B_\nu \varepsilon_\nu^{\|} C_\nu}{\Delta_\nu}[C_{44}T_{34} + C(T_{31}T_{34} - T_{35}T_{36})]_\nu = 2\varepsilon'_{\nu,23} \ , \tag{7a}$$

$$\varepsilon'_{\nu,5} = \frac{3B_\nu \varepsilon_\nu^{\|} C_\nu}{\Delta_\nu}[C_{44}T_{35} + C(T_{32}T_{35} - T_{36}T_{34})]_\nu = 2\varepsilon'_{\nu,31} \ , \tag{7b}$$

and

$$\sigma'_{\nu,1} = 3B_\nu \varepsilon_\nu^{\|} - (C_{12} + CT_{31})_\nu \Delta\varepsilon_\nu + C_\nu(T_{14}\varepsilon'_4 + T_{15}\varepsilon'_5)_\nu = \sigma'_{\nu,11} \ , \tag{8a}$$

$$\sigma'_{\nu,2} = 3B_\nu \varepsilon_\nu^{\|} - (C_{12} + CT_{32})_\nu \Delta\varepsilon_\nu + C_\nu(T_{24}\varepsilon'_4 + T_{25}\varepsilon'_5)_\nu = \sigma'_{\nu,22} \ , \tag{8b}$$

$$\sigma'_{\nu,6} = -C_\nu T_{36}\Delta\varepsilon_\nu + C_\nu(T_{25}\varepsilon'_4 + T_{14}\varepsilon'_5)_\nu = \sigma'_{\nu,12} \ , \tag{8c}$$

where

$$T_{ij} = T_{ji} = T_{\lambda\mu\kappa\rho} = l_\lambda l_\mu l_\kappa l_\rho + m_\lambda m_\mu m_\kappa m_\rho + n_\lambda n_\mu n_\kappa n_\rho \tag{9}$$

is a fully symmetric third-rank tensor, and i and j are the suppressed indices for $\lambda\mu$ and $\kappa\rho$, respectively. To avoid confusion between tensor indices 1–6 and layer indices $\nu = 1,2$ we add the latter explicitly in Eqs. (7) and (8), and in some of the following equations, wherever omitting ν may cause confusion.

In summary, at $P = 0$ the generalized Hook's law for crystals combined with the strain and stress boundary conditions yield the following strain and stress component arrays for each layer ν

$$\varepsilon'_v=(\varepsilon^{\parallel},\varepsilon^{\parallel},\varepsilon^{\perp},\varepsilon'_4,\varepsilon'_5,0)_v\ , \tag{10a}$$

$$\sigma'_v=(\sigma'_1,\sigma'_2,0,0,0,\sigma'_6)_v\ . \tag{10b}$$

Of these components, only $\varepsilon_v^{\parallel}$ is readily computed from Eqs. (5); all others are expressed in terms of $\varepsilon_v^{\parallel}$. Notice that $\varepsilon_v^{\parallel}\varepsilon_v^{\perp}<0$, i.e., a contractive (negative) in-plane strain is accompanied by a tensile (positive) normal-to-the-plane strain, and vice versa. On the other hand, Eq. (5) suggests that $\varepsilon_1^{\parallel}\varepsilon_2^{\parallel}<0$. We therefore conclude that the strains $\varepsilon_1^{\parallel}$, $\varepsilon_2^{\perp}$ have the same sign as f, and the strains $\varepsilon_1^{\perp},\varepsilon_2^{\parallel}$ have the opposite sign of f.

Finally, for later use we introduce the following positive parameters:

$$\alpha_1^{\parallel}\equiv\varepsilon_1^{\parallel}/f=\left[\frac{h_2G_2}{h_1G_1+h_2G_2}\right]<1\ ,$$

$$\alpha_1^{\perp}\equiv-\varepsilon_1^{\perp}/f=\alpha_1^{\parallel}(\Delta\tilde{\varepsilon}_1-1)\ , \tag{11a}$$

$$\alpha_2^{\parallel}\equiv-\varepsilon_2^{\parallel}/f=\left[\frac{h_1G_1}{h_1G_1+h_2G_2}\right]<1\ ,$$

$$\alpha_2^{\perp}\equiv\varepsilon_2^{\perp}/f=\alpha_2^{\parallel}(\Delta\tilde{\varepsilon}_2-1)\ . \tag{11b}$$

They are independent of f and can be computed straightforwardly.

III. PRESSURE-DEPENDENT STRAINS AND STRESSES IN SUPERLATTICES

As usual, the hydrostatic pressure is defined as negative and set equal to $-P$, so that $P>0$. Because of the isotropic nature of P, no new components are induced by P in the arrays of Eqs. (10), provided no phase transition is caused by P. Instead, each component becomes a linear function of P, in the lowest order ($P\le P_{\max}$, see the Introduction). To determine these functions, we write the generalized Hook's law for each layer as follows:

$$C'_{ij}\varepsilon'_j(P)=\begin{cases}\sigma'_i(P)-P\ , & i=1-3 & \text{(12a)}\\ \sigma'_i(P)\ , & i=4-6\ . & \text{(12b)}\end{cases}$$

Upon combining Eqs. (12) with the P-dependent counterpart of (10), we find that the expressions for $\Delta\varepsilon$, ε'_4, ε'_5, σ'_1, σ'_2, and σ'_6 can be transcribed to the corresponding P-dependent components by imposing the substitution

$$3B\varepsilon^{\parallel}\rightarrow3B\varepsilon^{\parallel}(P)+P\ . \tag{13}$$

Again, all P-dependent strain and stress components turn out to be proportional to $\varepsilon^{\parallel}(P)$. In order to determine $\varepsilon^{\parallel}(P)$ itself, the P-dependent free-energy density must be minimized. Following the same procedure[9] that has led to Eq. (4), we find

$$a^{\parallel}(P)=\frac{h_1G_1a_1(1-P/3B_1)+h_2G_2a_2(1-P/3B_2)}{h_1G_1+h_2G_2} \tag{14a}$$

$$=a^{\parallel}-\frac{P}{3B_1B_2}\left[\frac{h_1G_1a_1B_2+h_2G_2a_2B_1}{h_1G_1+h_2G_2}\right]\ , \tag{14b}$$

where the linearity condition has been taken into account. Within the same approximation, the P-dependent in-plane strains relative to the $P=0$ state (net strains) for the two layers become, to first order in f,

$$\varepsilon_1^{\parallel}(P)=\frac{a^{\parallel}(P)}{a_1}-1=\left[\frac{h_2G_2}{h_1G_1+h_2G_2}\right]f(P)-\frac{P}{3B_1}$$

$$\equiv\varepsilon_{1P}^{\parallel}-\frac{P}{3B_1} \tag{15a}$$

$$=\varepsilon_1^{\parallel}-\frac{P}{3B_1B_2}\left[\frac{h_1G_1B_2+h_2G_2B_1}{h_1G_1+h_2G_2}\right] \tag{15b}$$

$$=\varepsilon_1^{\parallel}-\frac{P}{3B_1B_2}(B_2-\varepsilon_1^{\parallel}\Delta B/f) \tag{15c}$$

$$=\varepsilon_1^{\parallel}-\frac{P}{3B_1B_2}(B_2-\alpha_1^{\parallel}\Delta B)\ , \tag{15d}$$

$$\varepsilon_2^{\parallel}(P)=\frac{a^{\parallel}(P)}{a_2}-1=\left[\frac{-h_1G_1}{h_1G_1+h_2G_2}\right]f(P)-\frac{P}{3B_2}$$

$$\equiv\varepsilon_{2P}^{\parallel}-\frac{P}{3B_2} \tag{16a}$$

$$=\varepsilon_2^{\parallel}-\frac{P}{3B_1B_2}\left[\frac{h_1G_1B_2+h_2G_2B_1}{h_1G_1+h_2G_2}\right] \tag{16b}$$

$$=\varepsilon_2^{\parallel}-\frac{P}{3B_1B_2}(B_1-\varepsilon_2^{\parallel}\Delta B/f) \tag{16c}$$

$$=\varepsilon_2^{\parallel}-\frac{P}{3B_1B_2}(B_1+\alpha_2^{\parallel}\Delta B)\ , \tag{16d}$$

where always $\Delta B=B_2-B_1$, $f=a_2/a_1-1$, and

$$f(P)=a_2(P)/a_1(P)-1=f+\frac{P\Delta B}{3B_1B_2}\ , \tag{17}$$

$$\varepsilon_{1P}^{\parallel}\equiv\left[\frac{h_2G_2}{h_1G_1+h_2G_2}\right]f(P)=\varepsilon_1^{\parallel}\left[1+\frac{P\Delta B}{3B_1B_2f}\right]\ , \tag{18a}$$

$$\varepsilon_{2P}^{\parallel}\equiv\left[\frac{-h_1G_1}{h_1G_1+h_2G_2}\right]f(P)=\varepsilon_2^{\parallel}\left[1+\frac{P\Delta B}{3B_1B_2f}\right]\ . \tag{18b}$$

$f(P)$ is the lattice misfit at $P\neq0$. In view of Eqs. (15a), (16a), and (18), the substitution (13) becomes

$$\varepsilon_v^{\parallel}\rightarrow\varepsilon_v^{\parallel}\left[1+\frac{P\Delta B}{3B_1B_2f}\right]\ . \tag{13'}$$

Thus, in order to have, in lowest order, the P-dependent counterparts of $\Delta\varepsilon$, ε'_4, ε'_5, σ'_1, σ'_2, and σ'_6 for both layers, it suffices to multiply the latter by the factor $(1+P\Delta B/3B_1B_2f)$. The tetragonal distortion of Eq. (1), in particular, takes the form

$$\Delta\varepsilon_v(P)=\Delta\varepsilon_v\left[1+\frac{P\Delta B}{3B_1B_2f}\right]\ , \tag{19a}$$

and, for nearly matched constituents ($\Delta\varepsilon_v\simeq0$),

$$\Delta\varepsilon_\nu(P)=\frac{P\Delta B}{3B_1B_2}(\Delta\varepsilon_\nu/f)=\pm\frac{P\Delta B}{3B_1B_2}\alpha_\nu^{\parallel}\Delta\tilde{\varepsilon}_\nu\ , \tag{19b}$$

where the upper (lower) sign holds for $\nu=1$ (2). A P-dependent tetragonal distortion begins to develop even in lattice-matched systems, provided $B_1\neq B_2$.

In a similar manner we find for the P-dependent normal-to-the-plane strains

$$\varepsilon_1^{\perp}(P)=\varepsilon_1^{\parallel}(P)-\Delta\varepsilon_1(P)=\varepsilon_1^{\perp}-\frac{P}{3B_1B_2}(B_2-\varepsilon_1^{\perp}\Delta B/f) \tag{20a}$$

$$=\varepsilon_1^{\perp}-P\left[\frac{1}{3B_1}+\frac{\varepsilon_1^{\perp}}{P_m}\right] \tag{20b}$$

$$=\varepsilon_1^{\perp}-\frac{P}{3B_1B_2}(B_2+\alpha_1^{\perp}\Delta B)\ , \tag{20c}$$

$$\varepsilon_2^{\perp}(P)=\varepsilon_2^{\parallel}(P)-\Delta\varepsilon_2(P)=\varepsilon_2^{\perp}-\frac{P}{3B_1B_2}(B_1-\varepsilon_2^{\perp}\Delta B/f) \tag{21a}$$

$$=\varepsilon_2^{\perp}-P\left[\frac{1}{3B_2}+\frac{\varepsilon_2^{\perp}}{P_m}\right] \tag{21b}$$

$$=\varepsilon_2^{\perp}-\frac{P}{3B_1B_2}(B_1-\alpha_2^{\perp}\Delta B)\ , \tag{21c}$$

where, for $\Delta B\neq 0$ only,

$$P_m\equiv-\frac{3B_1B_2f}{\Delta B}=\frac{3B_1B_2}{a_1}\left[\frac{a_2-a_1}{B_1-B_2}\right]\ . \tag{22}$$

According to Eqs. (15b) and (16b), the in-plane strains $\varepsilon_1^{\parallel}(P)$ and $\varepsilon_2^{\parallel}(P)$ have the same (negative) slope. On the contrary, Eqs. (20a), and (21a) suggest that the slopes of the normal-to-the-plane strains $\varepsilon_1^{\perp}(P)$ and $\varepsilon_2^{\perp}(P)$ are not equal, in general, except when $\Delta B=0$, in which case they are also equal to the slopes of $\varepsilon_\nu^{\parallel}(P)$. It is emphasized that all strains here are defined relative to the $P=0$ state; therefore, Eqs. (15), (16), (20), and (21) include the anisotropic as well as the isotropic part $-P/3B_\nu$. The latter cancels out in the expression for the tetragonal distortion.

The normal-to-the-plane lattice constant at $P\neq 0$ follows immediately from the definition of $\varepsilon_\nu^{\perp}(P)$ since, within the same proportionality factor applied to Eq. (4), we can write

$$a_\nu^{\perp}(P)=a_\nu[1+\varepsilon_\nu^{\perp}(P)]\ . \tag{23}$$

The critical pressure P_m appearing in Eqs. (20b) and (21b) has a particular physical meaning, provided $P_m\leq P_{\max}$. According to Eqs. (17) and (19), the P-dependent lattice misfit and tetragonal distortion of both layers become zero at P_m, i.e.,

$$f(P_m)=\Delta\varepsilon_\nu(P_m)=0\ . \tag{24}$$

The condition $P_m>0$ requires that $a_2>a_1$ and $B_1>B_2$, or $a_2<a_1$ and $B_1<B_2$, in short, $f\Delta B<0$. Satisfying either of these two requirements is, as we shall see shortly, a necessary but not sufficient condition for the tetragonal distortion to be zero at P_m. The unit cells of both layers recover their cubic shape at P_m, and the net (hydrostatic) strains become

$$\varepsilon_{1m}^{\parallel,\perp}=fB_2/\Delta B<0\ , \tag{25a}$$

$$\varepsilon_{2m}^{\parallel,\perp}=fB_1/\Delta B<0\ . \tag{25b}$$

In view of (14a), (23), and (25), the lattice constant of both layers in the linear approximation becomes at P_m

$$a_m^{\parallel,\perp}=a_1(1+fB_2/\Delta B)=a_2(1+fB_1/\Delta B)\ . \tag{26}$$

It is also clear that $f(P)$, $\Delta\varepsilon_1(P)$, and $\Delta\varepsilon_2(P)$ reverse their signs at $P=P_m$. Like $a^{\parallel}(P)$, the critical pressure P_m is a parameter characterizing the system as a whole and not the layers individually, to first order in f. Contrary to $a^{\parallel}(P)$, the critical pressure P_m is isotropic in that it does not depend on **N**. Furthermore, it is independent of the thicknesses h_ν. For most combinations of constituents, P_m turns out to be between 1 and 70 GPa according to Eq. (22).

It is important to emphasize that the critical pressure P_m reached from Eq. (22) is physically meaningful and practically useful only as long as its value falls in the region of linearity, i.e., $P_m\leq P_{\max}$. Otherwise, the linear approach expressed by the result of Eq. (22) is not sufficient and one should include nonlinear terms in determining P_m (Ref. 7). We consider three examples: For ZnSe/GaAs and GaSb/ZnTe superlattices or heterostructures, the above condition is satisfied, i.e., $P_m=2.2<P_{\max}\simeq B/B'^2=2.6$ GPa (see Introduction) and $1.2<2.2$, respectively. At least for a ZnSe/GaAs heterostructure the value of P_m has been confirmed experimentally.[3] On the other hand, in InAs/ZnTe HS or SL, the above condition is not satisfied ($6.3>2.2$). The nonlinear approach of Ref. 7 places P_m around 13 GPa, much higher than the value of 6.3 GPa reached from Eq. (22). For all these numerical applications, and the ones that follow, we have used the values of a, B, and B' from Table I of Ref. 7. It is noted at this point that the definition of strain used here (net strain) is different than that used in Ref. 7 (nonhydrostatic strain) and this should be remembered when comparing any conclusions about strains in the present work and in Ref. 7.

An additional restriction concerning P_m, in either linear or nonlinear approach, is that its value should be lower than the lower of the critical pressures P_g where phase transitions for the layers may take place. Most of the well-known combinations of constituents do not satisfy this restriction and, therefore, P_m carries no physical meaning.[3,7] Examples of combinations where this is not true, i.e., $P_m<P_g$, are ZnSe/GaAs, and GaSb/ZnTe, with $P_g=1.4$ and 6.2 GPa, respectively.[7] On the other hand, in InAs/ZnTe the value of $P_g\simeq 8.4$ GPa falls between the linear (6.3) and nonlinear (13 GPa) value of P_m, and this shows the importance of knowing in advance the extent of validity of the linear approach.

A geometrical presentation of the functions $\varepsilon_1^{\parallel}(P)$ and $\varepsilon_1^{\perp}(P)$ in the form of Eqs. (15d) and (20c) is quite helpful in following the behavior under P of any combination of constituents. Regardless of the sign of $\varepsilon_1^{\parallel}$ (i.e., of f), the

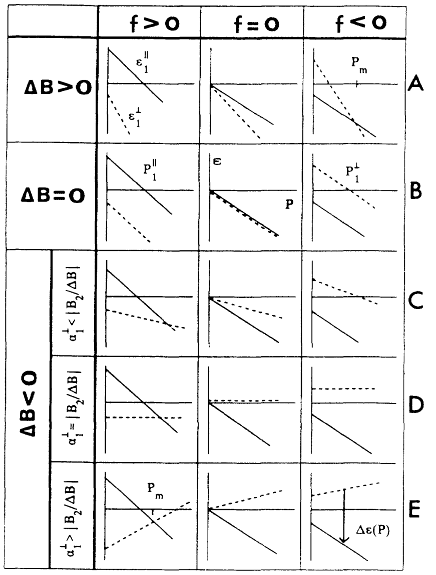

FIG. 1. Geometrical presentation of the in-plane strain $\varepsilon_1^{\parallel}(P)$ (solid lines) and normal-to-the-plane strain $\varepsilon_1^{\perp}(P)$ (dashed lines) vs pressure $P(>0)$ for constituent 1 in a superlattice grown along an arbitrary direction **N**. The bulk moduli differ by $\Delta B = B_2 - B_1$; lattice misfit $f=(a_2/a_1)-1$. In rows C, D, and E, the conditions imposed by $\alpha_1^{\perp}$ refer to superlattices. The same conditions become $2C_{12} \lesseqgtr 3B_s$ when referred to a [001]-grown heterostructure with 1→layer (no index) and 2→substrate (index s). The tetragonal distortion $\Delta\varepsilon(P)$ is shown by an arrow. The critical pressures P_m, $P_1^{\parallel,\perp}$ are discussed in the text. To demonstrate the P dependence of the lattice constants in a similar way, use Eqs. (38). The configurations describing constituent 2 in superlattices correspond to $-\Delta B$ and $-f$, while for the $\alpha_1^{\perp}$ conditions indices 1 and 2 should be switched. Only the range of pressures satisfying the linearity criterion $P \le P_{\max}$ (see the Introduction) is applicable for each combination of materials.

slope of $\varepsilon_1^{\parallel}(P)$ is always negative. On the contrary, the slope of $\varepsilon_1^{\perp}(P)$ can be positive, zero, or negative, depending on the sign of $B_2+\alpha_1^{\perp}\Delta B$, where $\alpha_1^{\perp}>0$ and $B_2>0$ (remember that $\varepsilon_1^{\parallel}\varepsilon_1^{\perp}<0$). Using these facts, we find a total of 15 configurations for the slopes of $\varepsilon_1^{\parallel}(P)$ and $\varepsilon_1^{\perp}(P)$, in pairs. They are shown schematically in Fig. 1 for the various signs of f and ΔB. It is understood that in Fig. 1, only the range $P \le P_{\max}$ is applicable for each combination of materials; moreover, it is assumed that P_g does not occur in that range. The configurations that correspond to $f=0$ and $\Delta B=0$ are included for completeness and for consistency checks. It is emphasized that these configurations are intended to show the functions $\varepsilon_1^{\parallel}(P)$ (solid lines) and $\varepsilon_1^{\perp}(P)$ (dashed lines) only qualitatively. Each configuration is designated by a row index (A to E) and a column index $>, =, <$, according to the sign of f. Configuration B= corresponds to the trivial case of a single bulk material under P (isotropic contraction). Notice that the two top rows are independent of **N** and h_1, h_2. On the contrary, the three lowest rows (C, D, and E) depend on **N** and h_1, h_2 through $\alpha_1^{\perp}$ of Eq. (11a).

There are four configurations where the two lines intercept each other. These are the cases where f and ΔB have opposite signs, thus rendering P_m positive. The crossing points correspond to the negative strain at P_m according to Eqs. (25), and a zero value for $\Delta\varepsilon(P_m)$, provided that $P_m \le P_{\max}$. The P-dependent tetragonal distortion

$$\Delta\varepsilon(P)=\varepsilon^{\parallel}(P)-\varepsilon^{\perp}(P)$$

is represented in each configuration by the difference between the two lines. Clearly, the effect of P in these four configurations is to reduce $\Delta\varepsilon(P)$, thus increasing the elastic stability of the system.

There are critical pressures $P_1^{\parallel}$ and $P_1^{\perp}$ in Fig. 1, for which $\varepsilon_1^{\parallel}(P_1^{\parallel})=0$ and $\varepsilon_1^{\perp}(P_1^{\perp})=0$, independently. The pressure $P_1^{\parallel}$ requires $f>0$ and is given by

$$P_1^{\parallel}=\frac{3B_1B_2f\alpha_1^{\parallel}}{B_2-\alpha_1^{\parallel}\Delta B}>0 . \tag{27a}$$

The pressure $P_1^{\perp}$ occurs with either $f>0$ or $f<0$ and is given by

$$P_1^{\perp}=-\frac{3B_1B_2f\alpha_1^{\perp}}{B_2+\alpha_1^{\perp}\Delta B}>0 . \tag{27b}$$

Since the net strain parallel (normal) to the plane is zero at $P_1^{\parallel}$ ($P_1^{\perp}$), the corresponding in-plane (normal-to-the-plane) lattice constant at this pressure acquires its unperturbed bulk value.

Figure 1 can also be used to follow the behavior under P of constituent 2. Once the configuration of constituent 1 with specific signs for f and ΔB is identified, the configuration of constituent 2 corresponds to $-f$, $-\Delta B$, and the conditions $\alpha_1^{\perp} \lesseqgtr |B_2/\Delta B|$ (defined as the $\alpha^{\perp}$ criterion from now on) become $\alpha_2^{\perp} \lesseqgtr |B_1/\Delta B|$. Suppose, for instance, that constituent 1 is represented by one of the configurations C>, D>, E>. Then, the corresponding constituent 2 is represented by configuration A<. Inversely, constituent 2 at A< has its constituent 1 in one of C>, D>, E>, to be specified by the $\alpha^{\perp}$ criterion. The critical pressures $P_2^{\parallel}$ and $P_2^{\perp}$ are

$$P_2^{\parallel}=-\frac{3B_1B_2f\alpha_2^{\parallel}}{B_1+\alpha_2^{\parallel}\Delta B}>0 , \tag{28a}$$

$$P_2^{\perp}=\frac{3B_1B_2f\alpha_2^{\perp}}{B_1-\alpha_2^{\perp}\Delta B}>0 . \tag{28b}$$

The vast majority of known SL belong to the upper three of Fig. 1. Thus, from these criteria one easily finds that A< is the configuration appropriate to describe, in the linear region of P, constituent 1 in the following superlattices:

$$\frac{1}{2}=\mathrm{InP/GaAs},\quad \mathrm{InAs/GaAs},\quad \mathrm{GaAs/GaP},\quad \mathrm{InAs/InP},\quad \mathrm{GaSb/InAs},$$

$$\mathrm{ZnTe/ZnSe},\quad \mathrm{CdTe/ZnTe}, \mathrm{ZnSe/ZnS}\ ,$$

$$\mathrm{Ge/Si}\ ,$$

$$\mathrm{GaAs/Si},\quad \mathrm{GaP/Si},\quad \mathrm{InAs/Si},\quad \mathrm{ZnTe/GaSb},\quad \mathrm{ZnTe/InAs},\quad \mathrm{ZnSe/GaAs}\ .$$

Likewise, constituent 2 of these SL follows, in the linear region of P, one of the C>, D>, E> configurations, to be specified by the $\alpha^{\perp}$ criterion, most likely C>. In AlAs/GaAs we have $f \lesssim 0$ and $\Delta B < 0$ at 300 K; the configuration for constituent 1 is between C= and C<, and the configuration for constituent 2 is between $A=$ and A>, depending on the exact value of f. The situation is expected to change at different temperatures. Similarly, in AlSb/InAs we have $f<0$, $\Delta B \lesssim 0$; the configuration for constituent 1 is between C< and B<, and the configuration for constituent 2 is between A> and B>, depending on the exact value of ΔB. In HgTe/CdTe we have $f>0$ and $\Delta B \gtrsim 0$; the configuration for constituent 1 is between A> and B>, and the configuration for constituent 2 is between C> and B<, depending on the exact value of ΔB. In AlSb/GaSb, constituent 1 follows one of the C<, D<, E< configurations, to be specified by the $\alpha^{\perp}$ criterion, and constituent 2 follows A>. Notice the ambiguity in some assignments, due to the fact that the values of f and/or ΔB are not accurately specified.

The lowest two rows are rather unlikely to occur, because of the stringent conditions imposed by the $\alpha^{\perp}$ criterion. Good candidates for the lowest two rows would be SL involving thin diamond layers alternating with thicker layers of III-V or II-VI compounds, provided the growth of such SL is technically possible.

As shown in Ref. 7, many combinations of constituents from among the same series of II-VI, III-V, or group-IV semiconductors happen to satisfy the condition $f\Delta B<0$; therefore, with increasing pressure these structures become elastically more stable than at $P=0$. There are situations, however, in which these trends are not followed, e.g., AlAs/GaAs, AlSb/GaSb, and HgTe/CdTe. Moreover, this stability condition is satisfied by constituents from different series as well, e.g., ZnSe/GaAs and GaSb/ZnTe. The safest way, therefore, to decide on the trends of $\Delta\varepsilon(P)$ and the concomitant elastic stability in the linear region, is to consult Fig. 1, regardless of the series of the individual constituents. The effects of nonlinearities on P_m and the relation of the latter to P_g constitute independent problems for which physical trends can be established only through microscopic models, as was done in Ref. 7.

IV. PRESSURE-DEPENDENT STRAINS IN HETEROSTRUCTURES

The results of the preceding section are easily adapted to HS, i.e., thin films (constituent 1, no index) grown coherently along an arbitrary direction **N** on much thicker substrates (constituent 2, index s). For $P=0$, Eq. (1) is still valid and $f=(a_s/a)-1$, $\Delta B=B_s-B$. With $h_s \gg h$, Eqs. (5), (6), (11), and (4) give

$$\varepsilon^{\parallel}=f,\quad \varepsilon^{\perp}=f-\Delta\varepsilon,\quad \varepsilon_s^{\parallel}=\varepsilon_s^{\perp}=\Delta\varepsilon_s=0\ , \tag{29a}$$

$$\alpha^{\parallel}=1,\quad \alpha^{\perp}=\Delta\tilde{\varepsilon}-1,\quad \alpha_s^{\parallel}=\alpha_s^{\perp}=0\ , \tag{29b}$$

$$a^{\parallel}=a_s\ . \tag{30a}$$

Furthermore,[9]

$$\begin{aligned} a^{\perp}&=a(1+\varepsilon^{\perp})=a_s(1-\Delta\tilde{\varepsilon})+a\Delta\tilde{\varepsilon}\\ &=a_s-a\Delta\varepsilon=a_s-\Delta a\Delta\tilde{\varepsilon}\ , \end{aligned} \tag{30b}$$

where $\Delta a=a_s-a$ is the absolute lattice misfit.

For $0<P\leq P_{\max}$, Eqs. (14a), (15), (20c), (19a), and (21c) give

$$a^{\parallel}(P)=a_s(P)=a_s\left[1-\frac{P}{3B_s}\right]\ , \tag{31}$$

$$\varepsilon^{\parallel}(P)=f(P)-\frac{P}{3B}=f-\frac{P}{3B_s}\ , \tag{32a}$$

$$\varepsilon^{\perp}(P)=\varepsilon^{\perp}-\frac{P}{3BB_s}(B+\Delta\tilde{\varepsilon}\Delta B)\ , \tag{32b}$$

$$\Delta\varepsilon(P)=\Delta\varepsilon\left[1+\frac{P\Delta B}{3BB_sf}\right]\ , \tag{33}$$

$$\varepsilon_s^{\parallel}(P)=\varepsilon_s^{\perp}(P)=-\frac{P}{3B_s},\quad \Delta\varepsilon_s(P)=0\ . \tag{34}$$

Equations (22)–(26) continue to hold, and

$$P^{\parallel}=3B_sf>0,\quad P^{\perp}=-\frac{3BB_sf(\Delta\tilde{\varepsilon}-1)}{B+\Delta\tilde{\varepsilon}\Delta B}>0\ , \tag{35a}$$

$$P_s^{\parallel}=P_s^{\perp}=0\ . \tag{35b}$$

Figure 1 is valid under the same conditions as for SL, especially in regard to the linearity condition $P\leq P_{\max}$. For growth along [001] we have $\Delta\tilde{\varepsilon}=3B/C_{11}$ and $\alpha^{\perp}=2C_{12}/C_{11}$. The conditions $\alpha_1^{\perp}\lesseqgtr B_2/|\Delta B|$ become $2C_{12}\lesseqgtr 3B_s$. It is emphasized that constituent 2 (substrate) contracts isotropically, always following configuration B=, while constituent 1 (layer) may follow any of the configurations in Fig. 1. Thus, a ZnSe film grown on a GaAs substrate follows configuration A<. A diamond film on a Si substrate follows C>. On the contrary, a diamond film on a GaAs substrate would follow configuration E>. In fact, if the ratio h/h_s, which, for HS is practically zero, starts increasing, the configuration of the corresponding SL passes quickly through D> and terminates in C>. This is an example where the geometric parameters alone dictate the behavior of the system under pressure.

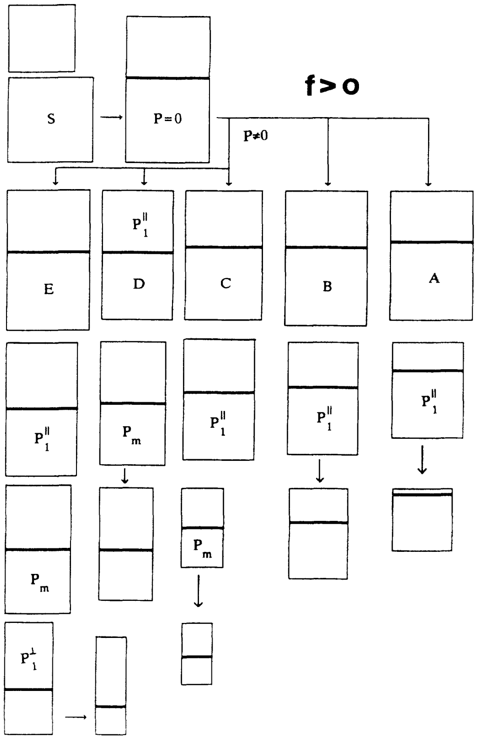

FIG. 2. Schematic presentation of the change, with pressure increasing downwards, of the cubic unit cells in a [001]-grown heterostructure with $f>0$. The row indices A–E are the same as those used for the corresponding strains in Fig. 1, i.e., each column of blocks here corresponds to the configuration in the first column of Fig. 1 which bears the same letter index. The critical pressures are marked explicitly. The dimensions of the cells change with P at arbitrary (and rather exaggerated) rates, but in a consistent way within each column. Only the range of pressures satisfying the linearity criterion $P \le P_{\max}$ (see the Introduction) is applicable for each combination of materials.

An alternative presentation emphasizing the evolution in the shape of the unit cells, in the linear range, for a [001]-grown HS, is shown in Fig. 2 for $f>0$. Here the cubic unit cells of the layer (upper square) and substrate (lower square) are depicted in various stages, i.e., before growth (top left) and after growth, at $P=0$ and $P\neq 0$ (P increases downwards). Each column of blocks is consistent with the configuration in the first column of Fig. 1 bearing the same letter index. Notice that the substrate's cell maintains its cubic shape at all pressures P, while the layer's cell becomes cubic again only at P_m.

V. COMPRESSIBILITIES AND BULK MODULI OF SUPERLATTICES AND HETEROSTRUCTURES

It is possible now to deduce the linear compressibilities of the layers, for directions parallel and perpendicular to the direction of growth. Such information may be particularly useful in analyzing experimental data of x-ray diffraction under P.

The linear compressibility κ of cubic materials is related to their bulk modulus by[11]

$$\kappa = 1/3B = (C_{11}+2C_{12})^{-1} . \tag{36}$$

$C_{11}+2C_{12}$ is invariant under rotation and so is κ. Therefore, in cubic materials κ is isotropic. The same is not true in SL and HS, as shown next.

The lowest-order dependence on P of the in-plane and normal-to-the-plane lattice constants of a SL can be expressed by

$$a^{\parallel}(P) = a^{\parallel}(1-\kappa^{\parallel}_{\mathrm{SL}}P) , \tag{37a}$$

$$a^{\perp}_{\nu}(P) = a^{\perp}_{\nu}(1-\kappa^{\perp}_{\nu}P) , \tag{37b}$$

where $\kappa^{\parallel}_{\mathrm{SL}}$ ($\kappa^{\perp}_{\nu}$) is the linear compressibility governing the in-plane (normal-to-the-plane) linear lattice contraction under P of the entire SL (constituent ν). The linear compressibilities $\kappa^{\parallel}_{\mathrm{SL}}$ and $\kappa^{\perp}_{\nu}$ are expected to be functions of the bulk values of the constituent's linear compressibilities κ_{ν} and to exhibit a weak dependence on P through the P dependence of κ_{ν}. The expressions of $a^{\parallel}$ and $a^{\parallel}(P)$ are given by Eqs. (4) and (14). Furthermore, the definitions of the P-dependent strains, relative to the $P=0$ state, i.e., Eqs. (15), (16), and (23) yield

$$\varepsilon^{\parallel}_{\nu}(P) = \frac{a^{\parallel}(P)}{a_{\nu}} - 1, \quad \varepsilon^{\perp}_{\nu}(P) = \frac{a^{\perp}_{\nu}(P)}{a_{\nu}} - 1 , \tag{38}$$

from which we obtain by subtraction,

$$a^{\perp}_{\nu}(P) = a^{\parallel}(P) - a_{\nu}\Delta\varepsilon_{\nu}(P) , \tag{39a}$$

$$a^{\perp}_{\nu} = a^{\parallel} - a_{\nu}\Delta\varepsilon_{\nu} . \tag{39b}$$

Upon combining Eqs. (37a), (4), and (14b) we obtain,

$$\kappa^{\parallel}_{\mathrm{SL}} = -\frac{da^{\parallel}(P)}{dP}\Big/ a^{\parallel} = \frac{h_1G_1a_1\kappa_1 + h_2G_2a_2\kappa_2}{h_1G_1a_1 + h_2G_2a_2} \equiv \frac{1}{3B^{\parallel}_{\mathrm{SL}}} , \tag{40a}$$

with

$$B^{\parallel}_{\mathrm{SL}} = \frac{1}{3\kappa^{\parallel}_{\mathrm{SL}}} = \frac{h_1G_1a_1 + h_2G_2a_2}{h_1G_1a_1/B_1 + h_2G_2a_2/B_2} . \tag{40b}$$

Equation (40a) describes the in-plane linear compressibility of the SL as a whole. It is isotropic within the plane and depends on **N** through the shear moduli G_{ν}.

Likewise, from Eqs. (37b), (39b), and (14b) we obtain, in the lowest order,

$$\kappa^{\perp}_{\nu} = -\frac{da^{\perp}_{\nu}(P)}{dP} / a^{\perp}_{\nu} = \kappa^{\parallel}_{\mathrm{SL}} - \Delta\kappa\Delta\varepsilon_{\nu}/f . \tag{41a}$$

The normal-to-the-plane compressibility of the entire SL is easily shown to be

$$\kappa^{\perp}_{\mathrm{SL}} = \frac{h_1\kappa^{\perp}_1 + h_2\kappa^{\perp}_2}{h_1+h_2} \equiv \frac{1}{3B^{\perp}_{\mathrm{SL}}} , \tag{41b}$$

with

$$\frac{1}{B^{\perp}_{\mathrm{SL}}} = \frac{1}{B^{\parallel}_{\mathrm{SL}}} + \frac{\Delta B}{B_1B_2f} \left[\frac{h_1\Delta\varepsilon_1 + h_2\Delta\varepsilon_2}{h_1+h_2} \right] , \tag{41c}$$

where $\Delta\kappa = \kappa_2 - \kappa_1$, $\Delta B = B_2 - B_1$, and $\Delta\varepsilon_{\nu}/f = \pm\alpha^{\parallel}_{\nu}\Delta\tilde{\varepsilon}_{\nu}$, the + (−) sign corresponding to $v=1$ (2). Equations (41a) and (41b) describe the normal-to-the-plane linear compressibilities of the individual layers and of the SL as a whole, respectively. They depend on **N** through $\Delta\varepsilon_v$ and G_v.

We can now define the effective bulk compressibility K_{SL} and bulk modulus B_{SL} of the entire SL as

$$K_{\mathrm{SL}}=2\kappa_{\mathrm{SL}}^{\parallel}+\kappa_{\mathrm{SL}}^{\perp}=\frac{2}{3B_{\mathrm{SL}}^{\parallel}}+\frac{1}{3B_{\mathrm{SL}}^{\perp}} \tag{42a}$$

$$=\frac{1}{B_{\mathrm{SL}}^{\parallel}}+\frac{\Delta B}{3B_1B_2f}\left[\frac{h_1\Delta\varepsilon_1+h_2\Delta\varepsilon_2}{h_1+h_2}\right]=\frac{1}{B_{\mathrm{SL}}} . \tag{42b}$$

For HS, the corresponding results are obtained from Eqs. (37)–(42). To avoid confusion, we use explicit indices s (e) for the substrate (epilayer),

$$a^{\parallel}(P)\equiv a_e^{\parallel}(P)=a_s^{\parallel}(P)=a_s^{\perp}(P)=a_s(P)$$

$$=a_s\left[1-\frac{P}{3B_s}\right]=a^{\parallel}(1-\kappa_{\mathrm{HS}}^{\parallel}P) , \tag{43}$$

$$a_e^{\perp}(P)=a_e^{\perp}(1-\kappa_e^{\perp}P)=a_s(P)-a_e\Delta\varepsilon_e(P) , \tag{44}$$

$$\kappa_{\mathrm{HS}}^{\parallel}=\kappa_s^{\parallel}=\kappa_s^{\perp}=\kappa_e^{\parallel}=\kappa_s , \tag{45a}$$

$$\kappa_e^{\perp}=\kappa_s-[\kappa_s-\kappa_e]\Delta\varepsilon_e/f , \tag{45b}$$

$$\kappa_{\mathrm{HS}}^{\perp}=\kappa_s , \tag{45c}$$

$$K_e=2\kappa_e^{\parallel}+\kappa_e^{\perp}=3\kappa_s-\Delta\kappa\Delta\varepsilon_e/f\equiv 1/B_e , \tag{45d}$$

$$K_{\mathrm{HS}}=2\kappa_{\mathrm{HS}}^{\parallel}+\kappa_{\mathrm{HS}}^{\perp}=3\kappa_s=1/B_s\equiv 1/B_{\mathrm{HS}} , \tag{45e}$$

where

$$h_s \gg h_e,\ \Delta B=B_s-B_e ,\ \text{and}\ \Delta\kappa=\kappa_s-\kappa_e . \tag{46}$$

VI. PRESSURE DEPENDENCE OF PIEZOELECTRIC FIELDS

Strained piezoelectric (PZ) layers are capable of exhibiting PZ fields.[12,13] A number of theoretical and experimental works have appeared in recent years that deal with this problem. Depending on the magnitude of the strains and the PZ constants, the fields may reach significant values, exceeding 10^5 V/cm, provided the concentration of mobile carriers is low enough to keep the fields unscreened. In the presence of PZ fields the overall behavior of the layered system is modified. Changes in the electronic band structure and the degeneracy and frequency of the long-wavelength optical phonons, by analogy to similar effects induced by strains, are among the most important consequences. The PZ fields, for a general direction of coherent growth, assuming cubic PZ materials, have been examined in detail in Ref. 14.

According to the phenomenological definition of the PZ effect,[11] the strains in each layer may induce an electric polarization **P**. Only the normal-to-the-plane component P_3' is allowed by the boundary conditions of electrostatics to induce a PZ field **E** which is also oriented along **N**. The resulting expression for the PZ field at zero pressure is

$$E_3'=-\frac{P_3'}{\varepsilon_0\kappa_s} ,\quad E_1'=E_2'=0 , \tag{47}$$

where

$$P_3'=-e(T_{333}\Delta\varepsilon-T_{323}\varepsilon_4'-T_{313}\varepsilon_5') \tag{48a}$$

$$=\left[-\frac{3B\varepsilon^{\parallel}e}{\Delta}\right][(C_{11}-C_{12})^2+2C_{44}^2-C^2T_{33}](l_3m_3n_3) . \tag{48b}$$

Here, e is the PZ constant of the bulk material, and

$$T_{\lambda\mu\kappa}=(l_\lambda m_\mu+l_\mu m_\lambda)n_\kappa+\text{c.p.}$$

$$=2(l_\lambda m_\mu n_\kappa+\text{c.p.})-\varepsilon_{\lambda\mu\kappa} \tag{49}$$

is a fully symmetric third-rank tensor analogous to $T_{\lambda\mu\kappa\rho}$ of Eq. (9), $\varepsilon_{\lambda\mu\kappa}$ is the antisymmetric unit tensor, and c.p. means cyclic permutation over l, m, n. The vacuum permittivity is ε_0 and κ_s is the static (relative) dielectric constant of the layer (not to be confused with κ_s of Sec. V). It has been assumed that no external charges are present and the dielectric constant is uniform throughout the layer. Equation (48b) suggests that PZ fields are induced only for those directions of growth for which all three direction cosines l_3, m_3, and n_3 are nonzero. Often in the literature, such directions of growth are stated as polar axes. Thus, PZ fields are expected to exist for **N** along [111], [11$\bar{2}$], [211], [113], etc., but not for [100], [110], [120], etc.

A hydrostatic pressure cannot induce PZ fields in bulk materials, because of the form of the PZ tensor. On the other hand, the pressure modifies the strain and stress components, as we have already seen in the preceding sections. This results in a P-dependent PZ field in those SL or HS which, according to the above general rule, are allowed to exhibit such a field. In view of Eqs. (47), (48a), (19a), and the comments following (13b), the P-dependent PZ field in each layer becomes, to terms linear in P,

$$E_3'(P)=E_3'\left[1+\frac{P\Delta B}{3B_1B_2f}\right]=\frac{E_3'}{\Delta\varepsilon}\Delta\varepsilon(P) . \tag{50}$$

One may also consider the P dependence of C_{ij}, e, and κ_s, which will impose on $E_3'(P)$ an additional slow variation with P. Otherwise, Eq. (50) suggests that $E_3'(P)$ can be tuned by P to any positive or negative value, or even be zeroed at P_m, since $\Delta\varepsilon(P_m)=0$, provided that $P\le P_{\max}$. Figure 1 shows indirectly that evolution of $E_3'(P)$ in a PZ constituent through the difference between the solid and dashed lines. Thus, in a [111]-grown ZnSe/GaAs superlattice, the ZnSe layer exhibits a PZ field that is proportional to $\Delta\varepsilon_1(P)$; according to configuration A<, the latter decreases with P, becomes zero and reverses sign at P_m, and then continues to increase. On the other hand, the GaAs constituent develops a PZ field that is proportional to $\Delta\varepsilon_2(P)$; the latter has a different magnitude and opposite sign of $\Delta\varepsilon_1(P)$ but, otherwise depends on P in a similar manner, according to Eq. (19a). It should be mentioned at this point that, with no pressure applied, the sign of P_3' (and E_3') for a strained layer (i.e., whether it points along **N** or $-\mathbf{N}$), depends on four factors: (i) the polarity (cation A or anion B) of the layer's face nearest to the free surface, (ii) the sign of the PZ constant, (iii) the sign of the in-plane strain, and (iv) the direction of growth, through the sign of the product $(l_3 m_3 n_3)$, according to Eq. (48b). [It is assumed that the bracket of Eq. (48b) is positive, as is the case for most materials under consideration.] By definition, a positive component P'_3 points from the layer's B face towards its A face. In principle, a fifth parameter, the pressure, may be added to those factors affecting the sign of PZ fields.

VII. DISCUSSION AND CONCLUSION

The first-order effects of hydrostatic pressure on strained SL and HS grown along arbitrary directions have been examined in detail. Only the range of pressures satisfying the linearity criterion $P \le P_{\max}$ is considered. Criteria were established for the direct assessment of the P dependence of all strain and stress components and of the tetragonal distortion for any combination of constituents. The criteria are shown schematically in Fig. 1 and require essentially the lattice misfit f and the bulk moduli B_ν of the two constituents. In SL, the geometrical parameters h_ν and l_3, m_3, n_3, enter through Eqs. (11) and (1)–(6). In HS, Fig. 1 concerns only the epilayer ($\nu = 1$), the substrate being contracted isotropically. Figure 1 can also be used to obtain information on the P-dependent lattice constants, according to Eq. (38). From the analysis it has become possible to deduce the linear compressibilities of the system for directions parallel and perpendicular to the direction of growth, as well as the effective bulk compressibility and bulk modulus of the system as a whole.

Throughout the present work, the strains $\varepsilon^{\parallel}(P)$ and $\varepsilon^{\perp}(P)$ are defined relative to the $P=0$ state of the system, according to Eq. (38). In this way, the results include the net effect of P, i.e., all equations for the P-dependent strain components and all figures include the total hydrostatic part, as well as the shear part. This is to be borne in mind when making a comparison of the present results with analogous results in the literature where, most often, the strain is defined relative to the bulk state of the constituents at pressure P.

The critical pressure P_m at which the tetragonal distortion becomes zero is simply expressed in terms of f, B_1, and B_2 through Eq. (22). The value of P_m was measured recently from Raman experiments under P, in a coherently-grown [001] ZnSe/GaAs heterostructure, and was found equal to the value predicted by Eq. (22), i.e., ~ 2.2 GPa (Ref. 3). It is emphasized that Eq. (22) is valid only in the linear approximation, i.e., under the assumption that $P \le P_{\max}$. For pressures beyond $P_{\max}$ one should consider nonlinear terms.[7]

It has been shown here that the built-in PZ fields, wherever present, can be modified by pressure according to Eq. (50). This fact should be taken into account when analyzing data of electronic transitions across field-modified energy gaps, in the presence of pressure.

Raman-scattering measurements under P on HS grown along [001], [110], and [111], have been shown to lead to values for the phonon deformation potentials, namely, the tensor components that are necessary to convert the observed (through Raman or any other technique) optical-phonon frequency shifts to strains[15] or PZ fields,[14,16] and vice versa. In view of the extensive use of Raman spectroscopy for routine strain characterization of SL and HS, the above technique for obtaining phonon-deformation potentials is particularly suitable in types of materials such as AlAs where other techniques cannot be employed.

The layers have been treated here as homogeneous and dislocation-free (subcritical); we have not considered corrections due to internal displacement (i.e., due to the internal strain parameter ζ). In HS, all present results concern the epilayer, with $\varepsilon^{\parallel} = f$. In SL, a free-standing state has been assumed and the results concern each layer ν independently, with $\varepsilon_\nu^{\parallel}$ given by Eqs. (5). Often, on the other hand, overcritical HS or SL systems are completely relaxed at the growth temperature T_g because of misfit dislocations. In such cases, the in-plane strain $\varepsilon_\nu^{\parallel}$ at room temperature T_0 (and $P=0$) is no longer determined from Eqs. (5), which are valid only for coherently-grown subcritical systems. Instead, it is given by

$$-(\beta^{\parallel} - \beta_\nu)(T_g - T_0) \equiv \delta\beta\Delta T \ ,$$

where β_ν is the linear thermal-expansion coefficient for layer ν and $\beta^{\parallel}$ is a coefficient governing the in-plane linear thermal expansion of the entire system; the value of $\beta^{\parallel}$ is given by an equation similar to Eq. (4), with $a^{\parallel}$ and a_ν replaced by $\beta^{\parallel}$ and β_ν, respectively[17] (more precisely, $\beta^{\parallel}$ and β_ν stand for their mean values in the temperature range $\Delta T = T_g - T_0$). In HS, β_ν and $\beta^{\parallel}$ correspond to the linear thermal-expansion coefficients of the layer and substrate, respectively. Often, in SL and HS the strains at T_g are not fully relaxed; the analysis, then, should take into account contributions from both f and $-\delta\beta\Delta T$ in proportion to the degree of relaxation.

Since much of the experimental work with either subcritical or overcritical SL and HS under P is carried out below room temperature, the entire subject of simultaneous variation of P and T becomes of interest and will be treated independently.[17]

ACKNOWLEDGMENTS

This work has been supported in part by the General Secretariat for Research and Technology, Greece. Thanks are due to B. A. Weinstein for making available the data of Ref. 3 prior to their publication.

---

[1] P. Seguy, J. C. Maan, G. Martinez, and K. Ploog, Phys. Rev. B **40**, 8452 (1989); M. Holtz, K. Syassen, and K. Ploog, *ibid.* **40**, 2988 (1989).

[2] Z. Sui, I. P. Herman, and J. Bevk, Appl. Phys. Lett. **58**, 2351 (1991).

[3] L. J. Cui, U. D. Venkateswaran, B. A. Weinstein, and B. T. Jonker, Phys. Rev. B **44**, 10 949 (1991).

[4] I. L. Spain, M. S. Skolnick, G. W. Smith, M. K. Saker, and C.

R. Whitehouse, Phys. Rev. B **43**, 14 091 (1991), and references therein; K. Takarabe, S. Minomura, M. Nakayama, and H. Kato, J. Phys. Soc. Jpn. **58**, 2242 (1989); Meera Chandrasekhar and H. R. Chandrasekhar, in *Proceedings of the 29th European High Pressure Research Group,* edited by G. A. Kourouklis and S. Ves (Gordon and Breach, Paris, 1992), Vols. 9 and 10, p. 57, and references therein.

[5] L. M. Claessen, J. C. Maan, M. Altarelli, P. Wyder, L. L. Chang, and L. Esaki, Phys. Rev. Lett. **57**, 2556 (1986); B. Rockwell, H. R. Chandrasekhar, M. Chandrasekhar, A. K. Ramdas, M. Kobayashi, and R. L. Gunshor, Phys. Rev. B **44**, 11 307 (1991), and references therein.

[6] Y. Yamada, Y. Masumoto, T. Taguchi, and K. Takemura, Phys. Rev. B **44**, 1801 (1991); M. Gerling, M.-E. Pistol, L. Samuelson, W. Seifert, J.-O. Fornell, and L. Ledebo, Appl. Phys. Lett. **59**, 806 (1991); D. J. Dunstan, A. D. Prins, B. Gil, and J. P. Faurie, Phys. Rev. B **44**, 4017 (1991); U. D. Venkateswaran, L. J. Cui, B. A. Weinstein, and F. A. Chambers, *ibid.* **45**, 9237 (1992).

[7] Judah A. Tuchman and Irving P. Herman, Phys. Rev. B **45**, 11 929 (1992).

[8] E. Anastassakis, J. Appl. Phys. **68**, 4561 (1990).

[9] E. Anastassakis, Solid State Commun. **78**, 347 (1991).

[10] E. Anastassakis, J. Cryst. Growth **114**, 647 (1991).

[11] J. F. Nye, *Physical Properties of Crystals* (Clarendon, Oxford, 1964).

[12] D. L. Smith, Solid State Commun. **57**, 919 (1986).

[13] D. L. Smith and C. Mailhiot, J. Appl. Phys. **63**, 2717 (1988).

[14] E. Anastassakis, in *Proceedings of the 29th European High Pressure Research Group* (Ref. 4), p. 101; Phys. Rev. B **46**, 4744 (1992).

[15] E. M. Anastassakis, in *Dynamical Properties of Solids,* edited by G. K. Horton and A. A. Maradudin (North-Holland, New York, 1980), Vol. 4, p. 157; E. M. Anastassakis, in *Light Scattering from Semiconductor Structures and Superlattices,* edited by D. J. Lockwood and J. F. Young (Plenum, New York, 1991), p. 173.

[16] E. Anastassakis, Solid State Commun. **84**, 47 (1992).

[17] E. Anastassakis (unpublished).