

General trends in changing epilayer strains through the application of hydrostatic pressure

Judah A. Tuchman and Irving P. Herman

Department of Applied Physics, Columbia University, New York, New York 10027

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It is shown that the magnitude of in-plane strains decreases with applied hydrostatic pressure for several general classes of lattice-mismatched heterostructures, thereby making the structures more stable. In particular, the mismatch strain in strained-layer systems composed only of semiconductors from the same series, such as II-VI, III-V, or group-IV semiconductors, will generally decrease with the initial application of hydrostatic pressure, but will never vanish at any pressure. Strain-free conditions under pressure are only possible in heterostructures composed of semiconductors from different series, and then only when a phase transition does not occur first. The importance of using the exact form of Murnaghan's equation, rather than a linear approximation, in analyzing strains is also demonstrated.

I. INTRODUCTION

Semiconductor heterostructures may be grown pseudomorphically to substrates provided that the thickness of the layers is less than the "critical thickness."^{1,2} For these systems, elastic strains accommodate lattice mismatch and affect the mechanical and electronic properties of the system, such as the electronic band offsets at interfaces. The effect of applied hydrostatic pressure on these systems has been shown to alter the degree of mismatch, and subsequently the elastic strains. In particular, it has been shown that lattice mismatch decreases with increasing pressure for several common epilayer-substrate systems, such as in Si/Ge (Ref. 3) and ZnSe/GaAs (Refs. 4–6) heterostructures. This results from differences in the bulk moduli of the substrate and the epilayer. For example, it has been shown^{4–6} that for ZnSe epilayers on GaAs substrates the effect of hydrostatic pressure is to decrease the inherent biaxially compressive strains until a lattice-matching pressure is obtained, whereupon the subsequent addition of pressure results in the generation of biaxially tensile strains. The main intent of this report is to demonstrate that for several general classes of lattice-mismatched systems, the application of hydrostatic pressure initially decreases the magnitude of strains, thereby increasing the stability of these strained-layer heterostructures. However, strain-free conditions will never occur at any pressure for heterostructures involving semiconductors from the same series, such as only II-VI, III-V, or group IV. Rather, pressure-induced lattice matching in strained-layer heterostructures is only possible for semiconductors from different series, and then only when the pressure at which matching occurs is lower than the phase-transition pressure for each of the layered components.

II. STRAIN CONDITIONS

The degree of lattice mismatch in a coherently grown layered structure is reflected in the nonhydrostatic strain components within each layer, which are of the form

$$\epsilon_{xx}^{(b)} = \epsilon_{yy}^{(b)} = \frac{a_{\text{eq}}(p) - a(p)}{a(p)} = \epsilon(p), \quad (1)$$

$$\epsilon_{zz}^{(b)} = -\frac{2C_{12}}{C_{11}}\epsilon_{xx}^{(b)}, \quad (2)$$

where a_{eq} represents the equilibrium, or actual lattice parameter for the strained layer, a is the lattice parameter of the equivalent strain-free layer, C_{11} and C_{12} are elastic constants of the film, and p is the hydrostatic pressure.

The equilibrium lattice constant depends on the particular system of interest. In the case of an epilayer grown pseudomorphically to a substrate, the in-plane lattice constant for the epilayer is that of the substrate ($a_{\text{eq}} = a_{\text{sub}}$). However, for more complicated heterostructures, the equilibrium lattice constant depends on the lattice constants of the component materials, and is weighted by their relative thicknesses.^{2,7} For example, for a free-standing strained-layer superlattice composed of two materials,

$$a_{\text{eq}}(p) = \frac{a_1 t_1 + a_2 t_2}{t_1 + t_2}, \quad (3)$$

where the lattice constants a_1, a_2 , and the total thicknesses t_1, t_2 of the two component materials, which may include buffer films, are all functions of pressure. Accordingly, strain conditions for a thin film on a substrate can be described as a special case of Eq. (3) with t_2 , the thickness of the substrate, $\rightarrow \infty$.

Externally applied hydrostatic pressure modifies the degree of biaxial strain through the inherent pressure dependences of Eqs. (1)–(3). This is demonstrated using Murnaghan's equation⁸

$$a(p) = a(1 \text{ bar}) \left[1 + p \frac{B'}{B} \right]^{-1/3B'} \quad (4a)$$

which reduces to

$$a(p) = a(1 \text{ bar})(1 - p/3B) \quad (4b)$$

in the low-pressure limit. $B = (C_{11} + 2C_{12})/3$ is the bulk modulus and $B' = dB/dp$. The overall layer thicknesses in Eq. (3) vary as does the lattice constant in Eq. (4). Therefore, using Eqs. (1)–(4a) and keeping terms to second order in p , the biaxial strain varies with pressure according to

$$\epsilon(p) = \frac{a_{\text{eq}}}{a} \left\{ 1 + \frac{p}{3} \left[\frac{1}{B} - \frac{1}{B_{\text{eq}}} \right] + \frac{p^2}{18} \left[\frac{3B'_{\text{eq}} + 1}{B_{\text{eq}}^2} - \frac{3B' + 1}{B^2} + \frac{2}{B} \left[\frac{1}{B} - \frac{1}{B_{\text{eq}}} \right] \right] \right\} - 1. \quad (5)$$

The equilibrium bulk modulus also depends on the par-

TABLE I. Lattice constants a , bulk moduli B , and their pressure derivatives $B' = dB/dp$ are given at room temperature, together with the pressures of the first phase transition p_t , for group-IV, III-V, II-VI, and IV-VI semiconductors, each listed by increasing lattice constant. The sources of these values are discussed in Ref. 12, with multiple values representing different values in the literature. Data are for the zinc-blende structure (zb), except where explicitly noted as hexagonal (hex).

		a (Å)	B (kbar)	dB/dp	p_t (kbar)	
Group IV	C	3.566 83	4423	4.07		
	SiC	4.359 6	2280			
	Si	5.430 72	960,979, 988,992	3.20,3.94, 4.24,4.68	125	
	Ge	5.657 906 0	689,744, 750	4.55,4.76	80,105	
	α -Sn	6.489 2	425		0	
III-V	GaP	5.450 6	882,887, 899	4.78	215,220	
	AlP	5.467	860		140,170	
	GaAs	5.653 25	747,755	4.49,4.67	172	
	AlAs	5.660	773,781		123	
	InP	5.868 7	711,725	4.6	100	
	InAs	6.058 3	579	4.79	84	
	GaSb	6.095 93	563,578	4.78	62,80	
	AlSb	6.135 5	582,593		77,83	
	InSb	6.479 37	433,456, 465	4.58,4.88	22.5	
	II-VI	ZnS	5.4102	748,769, 784,800, 841	4.91	150
ZnSe		5.6676, 5.6687	595,607, 624,640, 657,667	4.77	137	
CdS		5.825 (zb) 5.818 (zb)	549 (hex), 615 (hex)		27	
β -HgS		5.851	686,597		0	
CdSe		6.052 (zb)	530 (hex), 550 (hex)		29	
HgSe		6.084	486,497, 516,576	4.88	7	
ZnTe		6.1037, 6.100	480,509, 513	4.7,5.04	95	
HgTe		6.461	408,423	3.78	14	
CdTe		6.481	420,421, 424,429	6.4	33,39	
IV-VI		PbS	5.9362	572		
		PbSe	6.1243	541		
		PbTe	6.454	409,456		

ticular system of interest. For the simple case of a commensurate epilayer on a thick substrate, the bulk modulus is that of the substrate ($B_{\text{eq}} = B_{\text{sub}}$). However, for a free-standing superlattice

$$\frac{1}{B_{\text{eq}}} = \left[2 \frac{a_1}{a_{\text{eq}}} - 1 \right] \frac{t_1}{t_1 + t_2} \frac{1}{B_1} + \left[2 \frac{a_2}{a_{\text{eq}}} - 1 \right] \frac{t_2}{t_1 + t_2} \frac{1}{B_2} \quad (6)$$

in the low-pressure limit, and therefore B_{eq} is intermediate to B_1 and B_2 . Again, the thin film on a substrate case can be viewed as the limiting case of $t_2 \rightarrow \infty$.

Exact theory of course includes terms to higher order. However, as will be seen, Eq. (5) is sufficient to demonstrate the physical trends related to the exact theory. It is also worth mentioning that the more commonly used quasilinear result obtained by combining Eqs. (1) and (4) in the low-pressure limit of Eq. (4b) ($B' \rightarrow 0$) is even less accurate than the linear analysis. Specifically, if $\epsilon(p)$ in the quasilinear model were expanded in powers of p , only the final term in the bracketed p^2 expression in Eq. (5) would be recovered. However, the other terms in the brackets that would remain in the $B' \rightarrow 0$ limit would not be recovered. Of course, the pressure-dependent strains may be calculated for any semiconductor heterostructure using the above equations and the relevant parameters, which are given in Table I,⁹⁻¹² either exactly, or in the linear, quasilinear (low-pressure, $B' \rightarrow 0$), or quadratic approximations. However, certain general trends should be noted.

It is evident from Eq. (1) that at ambient pressure, the strain is tensile $\epsilon > 0$ (compressive $\epsilon < 0$) for $a_{\text{eq}} > a$ ($a_{\text{eq}} < a$), while from Eq. (5) it follows that $d\epsilon/dp > 0$ for $B_{\text{eq}} > B$ and $d\epsilon/dp < 0$ for $B_{\text{eq}} < B$. Therefore, if the heterostructure material with the larger lattice constant also has the smaller bulk modulus, the immediate effect of pressure is to reduce the magnitude of strain in each layer. Indeed, this inverse relationship between lattice constant and bulk modulus exists for many systems, as will now be shown.

III. GENERAL TRENDS IN EPILAYER STRAINS

Keyes¹³ noted several trends among the elastic constants of tetrahedrally bonded semiconductors, including the observation that within the same series the elastic constants are approximately proportional to $1/b^4$, where b is the distance between nearest-neighbor atoms ($b \propto a$). Indeed, a similar trend has been demonstrated between the bulk modulus and lattice constant for the alkali halides,^{14,15} metals,^{16,17} and other solids,^{15,16,18} with the general result that $B = B_0 a^{-n}$, where n is determined by the dependence of the interatomic potential on distance and B_0 is determined by the type of chemical bond. In Table I, this general decrease of B with a is seen for binary II-VI semiconductors, binary III-V semiconductors, and for the group-IV materials. Small variations that exist between the different series are due to differing ionicity and effective valence charge.¹⁹

Recent work has more accurately characterized the relationship between bulk modulus, lattice parameter, and

bond character.^{20,21} Notably, by considering how the bond stretching and bending force constants and the localized effective charge depend on bond distance and ionicity, Neumann²¹ has shown that the bulk modulus for diamond and zinc-blende semiconductors can be related to the lattice constant a and the spectroscopically defined bond ionicity f_i by

$$B = 105.25(1 - 0.25f_i)/a^{3.613}, \quad (7)$$

where B is in kbar and a is in nm. Within each series f_i is fairly constant and the bulk modulus generally depends on lattice constant as $\sim 1/a^{3.6}$. For each semiconductor series, the data in Table I are well fit by this $1/a^{3.6}$ dependence, which is superior to a $1/a^4$ fit.

Ternary II-VI and III-V alloys are thought to fall on these universal curves if their ionicities are similar to those of the corresponding binary compounds. Exceptions to this trend are found among the diluted magnetic semiconductors. For example, the elastic constants and bulk moduli of $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$ and $\text{Hg}_{1-x}\text{Mn}_x\text{Te}$ decrease with increasing Mn concentration, though their lattice parameters decrease.^{22,23} Explanation is offered in terms of reduced bond charges (and consequently increased ionicity) in these compounds with increasing concentrations of Mn.^{23,24} On the other hand, as the Mn fraction increases in $\text{Zn}_{1-x}\text{Mn}_x\text{Se}$ (thereby increasing a and b) the elastic constants and bulk modulus decrease faster than a^4 , again because the added Mn also decreases bond charge.²⁵

It therefore follows that for all strained heterostructures consisting only of binaries or ordinary ternaries selected from among a single series of II-VI, III-V, or group-IV semiconductors, the immediate effect of pressure must generally be to reduce the magnitude of strain at ambient pressure, resulting in increased elastic stability. This results because for $a_{\text{eq}} > a$ then $B_{\text{eq}} < B$, and vice versa, and applies to epilayers grown pseudomorphically to substrates, for which $a_{\text{eq}} = a_{\text{sub}}$ and $B_{\text{eq}} = B_{\text{sub}}$, free-standing and strain-symmetrized strained-layer superlattices, and to more general strained-layer heterostructures. Nonetheless, exceptions to this trend do exist, as for example in the cases of AlSb/GaSb and HgTe/CdTe heterostructures, where biaxial strain increases with pressure. This results from small deviations from the inverse functional dependence between B and a .

For heterostructures composed of semiconductors from different series, the inverse relationship between B and a does not generally apply. Nonetheless, it does happen to apply in many such heterostructures, including ZnSe/GaAs . By using Eq. (7), which is from Ref. 21, a general relation can be established for such different-series heterostructures. For example, for an epilayer on a substrate with $a_1 > a_2$, where a_1 may refer to either the epilayer or the substrate, epilayer strain will decrease with applied pressure if

$$\frac{B_1}{B_2} = \frac{1 - 0.25f_{i1}}{1 - 0.25f_{i2}} \left[\frac{a_2}{a_1} \right]^{3.613} < 1. \quad (8)$$

Figures 1-3 show how the in-plane strain changes with applied hydrostatic pressure in several representative het-

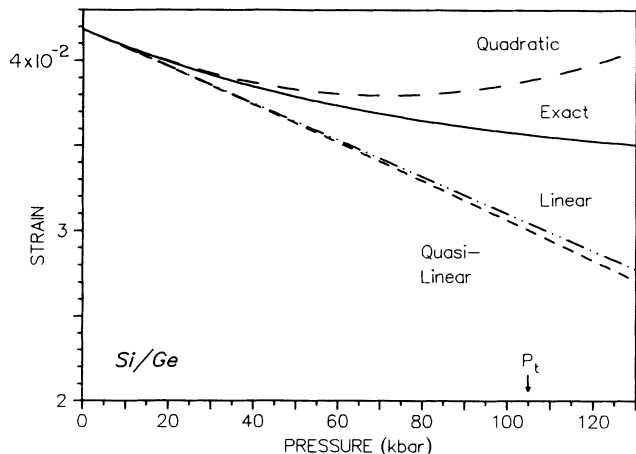


FIG. 1. Linear, quasilinear, quadratic, and exact results for biaxial strain at room temperature are plotted vs applied hydrostatic pressure for a Si epilayer grown on a Ge substrate, which is a same-series semiconductor heterostructure. p_t denotes the lower of the two phase-transition pressures of the heterostructure components, i.e., for Ge.

erostructures at room temperature. Figure 1 demonstrates the general decrease in the magnitude of strain with pressure in same-series heterostructures, while Figs. 2 and 3 demonstrate this same variation for specific different-series heterostructures. These figures compare the exact model of epilayer strains with the linear, quasilinear, and quadratic approximations. It is immediately evident that the commonly used quasilinear theory is not

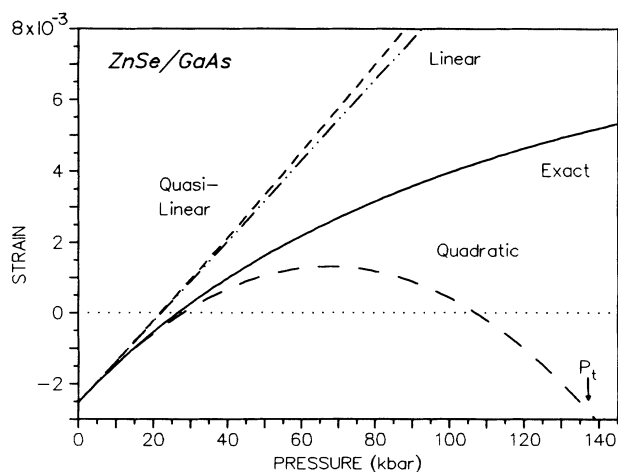


FIG. 2. Linear, quasilinear, quadratic, and exact results for biaxial strain at room temperature are plotted vs applied hydrostatic pressure for a ZnSe epilayer grown on a GaAs substrate. In this different-series semiconductor heterostructure, each model predicts crossover through a strain-free condition at pressures lower than the phase-transition pressure in each layer, which is in contrast to what happens in most other different-series heterostructures. p_t denotes the lower of the two phase-transition pressures of the heterostructure components, i.e., for ZnSe.

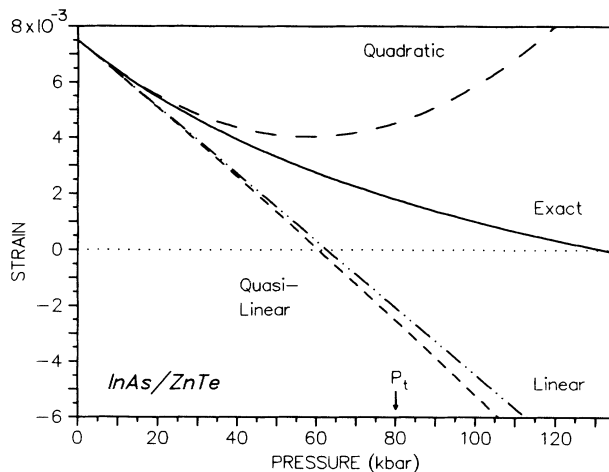


FIG. 3. Linear, quasilinear, quadratic, and exact results for biaxial strain at room temperature are plotted vs applied hydrostatic pressure for an InAs epilayer grown on a ZnTe substrate. In this different-series semiconductor heterostructure, exact theory predicts a crossover at a pressure far exceeding the transition pressure of each semiconductor. p_t denotes the lower of the two phase-transition pressures of the heterostructure components, i.e., for InAs.

adequate in most cases.

It should be noted that because strains involve lattice constant differences, it is even more critical to use the exact form of $a(p)$ in analyzing biaxial strain in heterostructures than in analyzing lattice constants in bulk materials. This is clear in comparing the strain for Si films on Ge at 1 bar and at 50 kbar. Exact theory predicts fractional changes in the Si and Ge lattice constants (from 1 bar to 50 kbar) that are 10% and 14% smaller than the changes predicted by quasilinear theory. However, the fractional change in the biaxial strain for Si/Ge predicted by exact theory is 26% smaller than that predicted by the linear model as seen in Fig. 1. Though this specific example used the values of B' from Table I, this conclusion is not very sensitive to the exact values of B' .

IV. STRAIN-FREE CONDITIONS

Using only terms linear in p in Eq. (5), it is seen that for heterostructures with $a_{eq} > a$ and $B_{eq} < B$ or vice versa, with continued increase in hydrostatic pressure the magnitude of strain in each layer continues to decrease until a strain-free condition is attained. With a further increase in pressure the magnitude of biaxial strain increases, but now layers that were formerly compressive are tensile, and vice versa. However, the potential for such a crossover (through a strain-free condition) depends on two factors. First, if any layer undergoes a phase transition at the applied hydrostatic pressure, the interface will no longer be commensurate. Any crossover must therefore precede a phase transition in any of the layered components. For semiconductors, the first phase transition usually occurs at $p_t \sim 10\text{--}220$ kbar (Table I). Second, the nonlinear dependence of volume on pressure in Eq. (4a) must also be considered. Higher-order terms

may prevent crossover before the phase-transition pressure.

To see the effect of higher-order pressure terms more clearly, Eq. (5) may be rewritten as

$$\epsilon(p) = \frac{1 - \frac{p}{B} \frac{\beta}{3} + \left(\frac{p}{B}\right)^2 \frac{\beta}{18} \alpha}{1 + \Delta} - 1, \quad (9)$$

where $\Delta = a/a_{\text{eq}} - 1 \sim -\epsilon$ (1 bar), $\beta = B/B_{\text{eq}} - 1$, and $\alpha = 6B'_{\text{eq}} + \beta(3B'_{\text{eq}} + 1) + (3/\beta)(B'_{\text{eq}} - B')$. Physically, crossover ($\epsilon=0$) can only occur for $\Delta/\beta < 0$, and then, at a pressure $p = p_c$, for which,

$$\frac{\Delta}{\beta} = -\frac{1}{3} \frac{p_c}{B} + \frac{\alpha}{18} \left(\frac{p_c}{B}\right)^2. \quad (10)$$

For a heterostructure composed of two semiconductors from an identical series (e.g., two II-VI or two III-V semiconductors), $\Delta/\beta \sim -1/3.6$ because $B \propto 1/a^{3.6}$. This assumes that the magnitude of $\Delta \ll 0.1$, which is anyhow generally the case, since biaxial strains in strained layers seldom exceed a few percent.²⁶ If the quadratic term in Eq. (10) were ignored (linear approximation), one would obtain the condition $p_c = (3/3.6)B$, which is typically ~ 500 kbar, and far exceeds the phase-transition pressures of semiconductors. Moreover, when the quadratic term is included in Eq. (10), it is seen that a solution for p_c exists only when $-1/2\alpha \leq \Delta/\beta \leq 0$, where $1/2\alpha \sim 0.017$. The lower limit is an estimate using reasonable values for B' , etc., from Table I. (For most II-VI and III-V semiconductors $B' \sim 4-5$. The first term in α is therefore $\sim 24-30$. Though the magnitude of the second term depends on the materials involved, it is typically $\sim 10-20\%$ of the first term. The third term is usually negligible. Therefore, α is ~ 30 for many II-VI and III-V semiconductor heterostructures and is only weakly dependent on the details of the specific system.)

Consequently, for a heterostructure composed of two semiconductors in the same series there is no solution for p_c . This means that contrary to linear theory, a strain-free condition can never be attained (even when considering $p > p_t$) by applying hydrostatic pressure to these structures. The use of the exact form of Murnaghan's equation (instead of the expansion to the p^2 term) and corrections for the small deviations from the $B \propto 1/a^{3.6}$ dependence do not change this conclusion. This is confirmed for the case of a Si epilayer grown on a thick Ge substrate ($\Delta/\beta = -0.132$; $B_{\text{Si}} = 979$ kbar; $B_{\text{Ge}} = 750$ kbar; $B'_{\text{Si}} = 3.94$; $B'_{\text{Ge}} = 4.76$ from Table I), as is shown in Fig. 1. Linear and quasilinear theory predict a crossover (offscale in the figure), albeit above the (lowest) phase-transition pressure. However, quadratic and exact theory predict that in fact no crossover can ever occur. A similar situation exists for InAs/GaSb heterostructures ($\Delta/\beta = -0.218$). In this latter case Δ/β is relatively near $-1/3.6$, which is typical for III-V and II-VI heterostructures.

However, for heterostructures composed of semiconductors from different series (or those which do not strictly follow a $B \propto 1/a^{3.6}$ dependence), a solution to Eq.

(10) can sometimes be obtained. For example, because the lattice mismatch is very small for ZnSe/GaAs heterostructures, while the difference in the bulk moduli of the two materials is relatively large ($\Delta/\beta = -0.012$; $B_{\text{ZnSe}} = 595$ kbar; $B_{\text{GaAs}} = 747$ kbar, $B'_{\text{ZnSe}} = 4.77$; $B'_{\text{GaAs}} = 4.67$ from Table I), a crossover condition is attained with $p_c < p_t$ (Fig. 2). It is predicted to occur at $p_c = 22.3, 22.0, 28.1,$ and 26.7 kbar using linear, quasilinear, quadratic, and exact theory, respectively, and has been seen experimentally by Tuchman *et al.*,⁴ Cui *et al.*,⁵ and Rockwell *et al.*⁶ A similar crossover with $p_c < p_t$ is predicted for GaSb/ZnTe (Ref. 5) ($\Delta/\beta = -0.007$) at $p_c = 12.4, 12.3, 14.2,$ and 13.9 kbar using linear, quasilinear, quadratic, and exact theory, respectively. Equation (8) can be used with Eq. (10) to examine the general trends for strain-free crossover in different-series heterostructures with $\Delta/\beta < 0$.

In some cases, linear and quasilinear theory predict crossover prior to the phase-transition pressure,⁵ while quadratic and exact theory indicate that these are expected to occur either after the phase transition, or not at all. Figure 3 indicates that for InAs/ZnTe heterostructures ($\Delta/\beta = -0.036$; $B_{\text{InAs}} = 579$ kbar; $B_{\text{ZnTe}} = 480$ kbar; $B'_{\text{InAs}} = 4.79$; $B'_{\text{ZnTe}} = 4.7$ from Table I), linear and quasilinear theory predict a crossover at 62.6 and 60.5 kbar, respectively. However, quadratic theory predicts that no crossover can occur, and indeed, actual crossover is expected to occur at 132 kbar—which is much greater than the phase-transition pressures of InAs (84 kbar) and ZnTe (95 kbar). For GaP/Si ($\Delta/\beta = -0.039$), despite the small initial mismatch ($\epsilon = -0.37\%$) and the rather high phase-transition pressures, quadratic and exact analysis indicate that no crossover can ever occur. Note that linear and quasilinear theory predict crossover at 104 and 100 kbar, respectively.

The example of InAs/ZnTe heterostructures in Fig. 3 illustrates the uncertain nature of strain predictions in heterostructures under hydrostatic pressure when B and B' are not accurately known, since $\epsilon(p)$ is sensitive to the exact choice of parameters. Using an alternate value of B (509 kbar) listed in Table I for ZnTe, and the value of B' used in the figure, p_c is predicted to be at 320 kbar using exact theory, instead of 132 kbar, which is still $\gg p_t$ for InAs and ZnTe. Moreover, if B' for ZnTe is changed to the alternate value listed in Table I (5.04), then for any of the listed values of B , a crossover will never occur. Usually, a change in B' is more significant than a change in B , and therefore only the exact and quadratic models are strongly affected by uncertainties in these parameters.

Although the examples provided in Figs. 1–3 refer to a thin epilayer on a substrate, similar conclusions can be drawn for all free-standing heterostructures of the corresponding materials. For example, though changes in biaxial strain with pressure are slower in superlattices than in epilayer-substrate structures, the crossover pressure p_c , at which there is no biaxial strain, is the same for all heterostructures of similar composition because the crossover condition is still $a_1(p_c) = a_2(p_c)$.

In closing, it should be noted that it may be possible to relate the condition for pressure-induced crossover through a strain-free condition in semiconductor hetero-

structures [Eq. (10)] with the phase-transition pressures of its bulk semiconductor constituents. There is evidence that the pressure at which the first phase transition occurs can be predicted fairly well by using the modified Born criterion,²⁷ which states that a phase transition occurs when the ratio of a shear modulus to the bulk modulus, $\eta = C_t(p)/B(p)$, where C_t is the smaller of C_{44} and $(C_{11} - C_{22})/2$, decreases below a critical value. [For zinc-blende semiconductors, $(C_{11} - C_{22})/2$ is the smaller of the two.] This is a revision of the original Born criterion which stated that $\eta_{\text{critical}} = 0$ at $p = p_t$. For alkali halides, it has been found that $\eta_{\text{critical}} \sim 0.15 - 0.20$.²⁷ For many II-VI and III-V zinc-blende semiconductors $\eta_{\text{critical}} \sim 0.17 - 0.23$, with smaller values for II-VI compounds than for III-V compounds,²⁸ while for Si and Ge, η_{critical} is closer to 0.30. Though it is known that η_{critical} tends to decrease with increasing ionicity,²⁸ there is no accurate information on how it varies over an entire semiconductor series. Nonetheless, within a group of similar bulk semiconductors (e.g., ZnS, ZnSe, and ZnTe) p_t could, in principle, be determined by when $C_t(p)/B(p)$ reaches the given critical value for that group.

It has further been shown²⁷ that one may extrapolate values of $\eta = C_t(p)/B(p)$ to high pressure by using low-pressure values and their derivatives. For the bulk modulus, $B(p) \sim B + B'p$ is determined by knowing the general form of B , say from Eq. (7), and $B' = dB/dp$, where B and B' are evaluated at 1 bar. For these semiconductors B' typically ranges from 4–5 (Table I). Moreover, it can be seen that B' is either nearly independent of the lattice constant a or increases very slowly with a . Keyes¹³ has shown that C_{44} and $(C_{11} - C_{22})/2$ both decrease as A/a^4 for semiconductors, where A decreases faster with ionicity¹⁹ than does the corresponding factor for the bulk modulus [Eq. (7)]. However, the general variation of dC_t/dp with lattice constant is not clear. For example, while in many materials dC_{44}/dp is typically 0.5–1.5, in some materials it is even negative.²⁸

Though these general trends between the strain crossover pressure p_c and the phase-transition pressures p_t of

the individual bulk materials can be established, the above analysis suggests that this is not of great importance since in most cases it is clear that $p_c > p_t$. It should also be noted that the thickness of a layer and the strain in that layer can affect to some degree the pressure at which the phase transition occurs, as has been shown by Weinstein *et al.*²⁹

V. CONCLUSIONS

In summary, the application of hydrostatic pressure to semiconductor heterostructures composed of semiconductors from the same series usually decreases the magnitude of biaxial in-plane strain in each layer. However, these systems will never cross over from compressive to tensile strain, and vice versa, through a strain-free condition. For strained layers composed of semiconductors from different series, the application of pressure may or may not decrease the magnitude of strains. When it does, crossover through a strain-free condition can only occur when the materials are very nearly lattice matched and yet have very different bulk moduli (possibly because of differing ionicity). This is true for a few II-VI/III-V, group-IV/II-VI, and group-IV/III-V combinations.

Finally, the pitfalls of using linear or quasilinear theory in heterostructure strain analysis have been demonstrated. Keeping terms quadratic in pressure does, however, improve the analysis somewhat. Exact theory confirms that there will be a crossover, prior to a phase transition, only when predicted by quadratic theory. However, only an exact strain analysis using Murnaghan's equation produces accurate numerical results.

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