

Pressure tuning of strains in semiconductor heterostructures: (ZnSe epilayer)/(GaAs epilayer)

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The heavy-hole and light-hole excitons of a pseudomorphic ZnSe film grown on a GaAs epilayer by molecular-beam epitaxy, are studied as a function of applied hydrostatic pressure using photomodulated reflectance spectroscopy. At ambient pressure, the signature in the spectrum due to the heavy-hole exciton occurs at an energy lower than that of the light-hole exciton, a consequence of the compressive biaxial strain in ZnSe due to its lattice mismatch with GaAs. As the pressure is increased, the two signatures approach each other in energy and coalesce at 36.2 kbar. The difference in the compressibility of ZnSe from that of GaAs generates a tensile strain that progressively compensates the lattice-mismatch-induced compressive strain and finally, at 36.2 kbar, the heterostructure is strain free. Beyond this pressure, the strain in ZnSe transforms from biaxial compression to biaxial tension, the light-hole signature now occurring at the lower energy. The transformation of strains via pressure tuning is continuous and reversible. The separation between the heavy-hole and light-hole signatures is superlinear in pressure, suggestive of a pressure-dependent shear-deformation-potential constant.

I. INTRODUCTION

The growth of high-quality epilayers and quantum wells of wide-band-gap II-VI materials, in particular ZnSe on GaAs, is especially interesting due to their application in optoelectronic devices with response in the blue such as blue-light emitting diodes and lasers. This system is also of interest because of reproducible growth of high-quality epilayers by molecular-beam epitaxy (MBE) and metal-organic chemical-vapor deposition. In addition, the growth of II-VI materials in combination with III-V materials is appealing because of the difficulty in doping the II-VI materials. Due to the lattice mismatch between the epilayer and the substrate, it is crucial to know the limiting conditions leading to a pseudomorphic growth by the accommodation of the strains due to lattice mismatch rather than the formation of misfit dislocations. The latter have a debilitating effect on the optical and electronic properties of a device. The compressibilities and/or thermal expansion coefficients of the materials forming the epilayer and the substrate are usually different. As a function of pressure and/or temperature, the lattice constants of the two constituent materials change differently leading to modifications in the biaxial strain. Systems that are lattice matched at a certain pressure or temperature may become lattice mismatched as these parameters are changed. The converse is also possible.

In this paper, we present a study of the excitonic signatures in the photomodulated reflectivity spectrum of a ZnSe epilayer grown on GaAs homoepitaxial epilayer

which exhibits these effects in a dramatic way under externally applied pressure. At a certain pressure, the biaxial compressive strain due to lattice mismatch is completely compensated by the pressure-induced strain. At higher pressures the biaxial strain becomes tensile leading to a light-hole-derived band gap. To our knowledge, this is the first direct observation of the reversible lattice-mismatch-induced crossover from a compressive to tensile strain in the same sample. The pressure dependence of the light- and heavy-hole gaps is accurately determined. The splitting of the heavy- and light-hole gaps is superlinear in pressure and suggests a pressure dependence of the uniaxial deformation potential b .

II. EXPERIMENT

The sample under study is a 0.1- μm epilayer of ZnSe grown on the (001) surface of a 1.5- μm -thick GaAs homoepitaxial epilayer by MBE at a growth temperature of 300°C employing a [Zn]:[Se] flux ratio of 1:1. The high-resistivity ZnSe was grown in a chamber separated from that in which the GaAs epilayer was grown; the transfer was implemented under high vacuum. In spite of the 0.25% lattice mismatch at room temperature, cross-sectional transmission electron microscopy measurements show no dislocations or stacking faults in the film and its interface.¹ The absence of dislocations in the presence of lattice mismatch is characteristic of "pseudomorphic" growth in which the lattice mismatch is accommodated by the deformation of the lattice constant of the epilayer while maintaining registry between successively grown

layers. For the ZnSe/GaAs epilayer system it has been found that coherent pseudomorphic growth is possible up to about $0.15 \mu\text{m}$ (Refs. 2 and 3) and for films thicker than this, there are dislocations introduced and the film has a lattice constant which approaches that of bulk ZnSe for increasing epilayer thickness.

The photomodulated reflectivity (PR) spectra were measured on a McPherson spectrometer set for a dispersion of 3.2 \AA . A 6-mW He-Ne laser or a 20-W Ar^+ laser was used for photomodulation with powers of about 0.02 mW for a spot size of $200 \mu\text{m}$ diameter. The modulation frequency was 200 Hz. The detector was a photomultiplier tube for both PR and ruby calibration. A variable temperature, high-pressure diamond anvil cell with argon as the pressure medium was used. Pressure was determined *in situ* using the ruby fluorescence technique. Details are available elsewhere.⁴

III. THEORETICAL CONSIDERATIONS

A. Strains due to lattice mismatch

The built-in strains in the epilayer due to the lattice mismatch are characterized by

$$\begin{aligned} \varepsilon = \varepsilon_{xx} = \varepsilon_{yy} &= \frac{a_s - a_e}{a_e}, \\ \varepsilon_{zz} &= \frac{2s_{12}}{s_{11} + s_{12}} \varepsilon, \\ \varepsilon_{xy} = \varepsilon_{yz} = \varepsilon_{zx} &= 0, \end{aligned} \quad (1)$$

where a_s and a_e are the lattice constants of the substrate and the epilayer, respectively, and s_{11} and s_{12} are the elastic compliance constants. The direction of growth of the epilayer is taken as the z axis and $\varepsilon = \varepsilon_{xx} = \varepsilon_{yy}$ is referred to as the biaxial strain.

The effects of biaxial strain on the direct ($\mathbf{k}=0$) band of zinc-blende semiconductors are as follows.^{5,6} In the absence of strain, the maxima of the heavy- and light-hole valence bands are degenerate with the fundamental gap designated E_g as in Fig. 1. The biaxial strain shifts and splits the heavy- and light-hole bands. The heavy- and light-hole band gaps E_g^{hh} and E_g^{lh} are given by

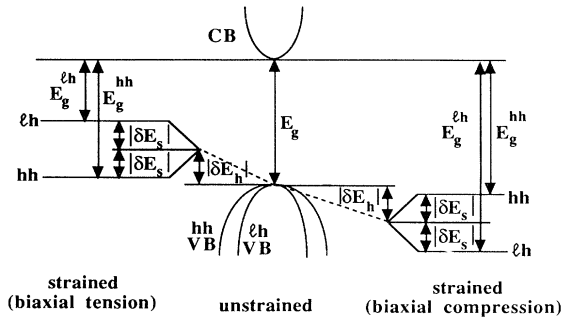


FIG. 1. The Γ_6 conduction-band minimum and the Γ_8 valence-band maximum in a zinc-blende semiconductor under a biaxial strain.

$$E_g^{\text{hh}} = E_g + (\delta E_h + \delta E_s), \quad (2a)$$

$$E_g^{\text{lh}} = E_g + (\delta E_h - \delta E_s) - \frac{2(\delta E_s)^2}{\Delta}, \quad (2b)$$

where

$$\delta E_h = 2a_{cv} \left[\frac{c_{11} - c_{12}}{c_{11}} \right] \varepsilon = 2a_{cv} \left[\frac{s_{11} + 2s_{12}}{s_{11} + s_{12}} \right] \varepsilon, \quad (2c)$$

$$\delta E_s = -b \left[\frac{c_{11} + 2c_{12}}{c_{11}} \right] \varepsilon = -b \left[\frac{s_{11} - s_{12}}{s_{11} + s_{12}} \right] \varepsilon. \quad (2d)$$

The effects on the band structure from Eqs. (2a)–(2d) are shown schematically in Fig. 1. Here, $|\delta E_h|$ and $|\delta E_s|$ are the magnitudes of the hydrostatic and the shear contributions of the gap energy, respectively. a_{cv} is the combined hydrostatic deformation potential for transitions between the conduction and valence bands, b is the shear deformation-potential constant characterizing the splitting of the Γ_8 valence band for tension or compression along [001]. Δ is the energy separation of the spin-orbit split Γ_6 valence-band maximum from the Γ_8 valence-band maximum. The c_{ij} are the elastic stiffness coefficients. For an epilayer which has a lattice constant larger than that of the substrate, as is the case in ZnSe/GaAs, the biaxial strain is compressive and a corresponding band-gap expansion occurs with the heavy-hole-derived band gap. Note that ε is defined negative for biaxial compressive strain. In contrast, for biaxial tension, the fundamental gap shrinks and is light-hole related. This can be an advantage for devices with increased hole mobilities which accompany this light mass. It should be noted that under strain the valence-band masses are anisotropic. Since the measurements here are related to the mass along the \mathbf{k}_z direction, the valence bands are called appropriately “heavy hole” and “light hole” for the ($J = \frac{3}{2}, m_j = \pm \frac{3}{2}$) and ($J = \frac{3}{2}, m_j = \pm \frac{1}{2}$) bands, respectively.

B. Strains due to applied pressure

Hydrostatic pressure decreases the lattice constants of a material. Since the compressibilities of different semiconductors vary, there can be pressure-induced biaxial strains between semiconductors that share a common interface. The strain thus generated in a heterostructure can be formulated quantitatively from expressions for the amount of change of the respective lattice constants. For bulk materials the elastic constants are related to the change in volume by $\Delta V/V = 3P/(c_{11} + 2c_{12})$ and the change in lattice constant is related to the change in volume by $3\Delta a/a = \Delta V/V$. Therefore we can write the normalized change in lattice constant as $\Delta a/a = P/(c_{11} + 2c_{12})$. Thus the strain in the epilayer as a function of pressure is given by

$$\varepsilon(P) = \frac{P}{(c_{11} + 2c_{12})_e} - \frac{P}{(c_{11} + 2c_{12})_s}, \quad (3)$$

where $\varepsilon(P)$ is the pressure induced strain, P is the applied hydrostatic pressure, and the c_{ij} 's are the elastic stiffness

coefficients for the epilayer (e) and substrate (s). The total strain on a strained layer under pressure is the sum of the strain induced by the initial lattice mismatch and that from Eq. (3).

The pressure coefficients α for the light- and heavy-hole band gaps can be found from Eqs. (2) and (3) as

$$\left. \begin{array}{l} \alpha_g^{\text{lh}} \\ \alpha_g^{\text{hh}} \end{array} \right\} = \alpha_{\text{bulk}} + \left[2a_{cv} \frac{(c_{11} - c_{12})}{c_{11}} \pm b \frac{(c_{11} + 2c_{12})}{c_{11}} \right] \times \left[\frac{1}{(c_{11} + 2c_{12})_e} - \frac{1}{(c_{11} + 2c_{12})_s} \right], \quad (4)$$

where the $+$ ($-$) sign in the second term is for light-hole (heavy-hole) band edges. The pressure coefficient, of the material forming the epilayer in its bulk state α_{bulk} , is $[-3a_{cv}/(c_{11} + 2c_{12})]$.

If the compressibility of an epilayer material is less than that of the substrate then the strain in Eq. (3) is negative and hence biaxially compressive. On the other hand, if the compressibility is greater, there will be a pressure dependent biaxial tensile strain, as is the case of the present study. These strains affect the band edges as shown in Fig. 1.

IV. RESULTS AND DISCUSSION

Figure 2 shows the photomodulated reflectivity spectra for the ZnSe/GaAs epilayer under study at 80 K with no externally applied pressure. Three transitions are seen. The most prominent signature at 2.7992 eV corresponds to the exciton associated with the heavy-hole valence- to conduction-band transition.² The signature at 2.8107 eV is due to the light-hole exciton. The intensity of the latter is approximately one-third the intensity of the heavy-hole-related transition, which is expected from comparison of the optical matrix elements for these transitions.⁷ The transition at 2.819 eV has been attributed to the $n=2$ light-hole-free exciton.¹

It should be noted here that the reflectivity for these samples was photomodulated with a laser line with a photon energy lower than that of the band gap of ZnSe. Therefore the mechanism typical in photomodulation ex-

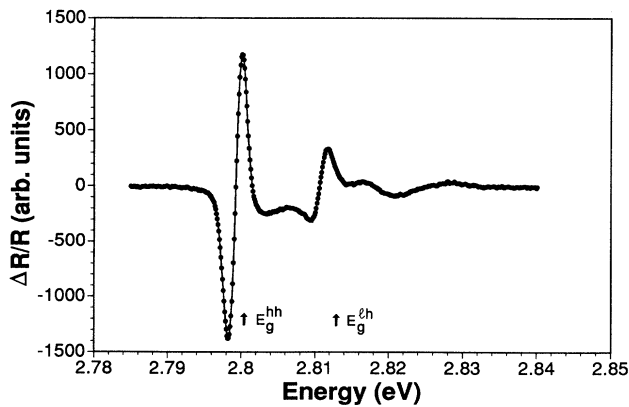


FIG. 2. The photomodulated reflectivity spectrum for the ZnSe/GaAs epilayer at 1 bar, 80 K.

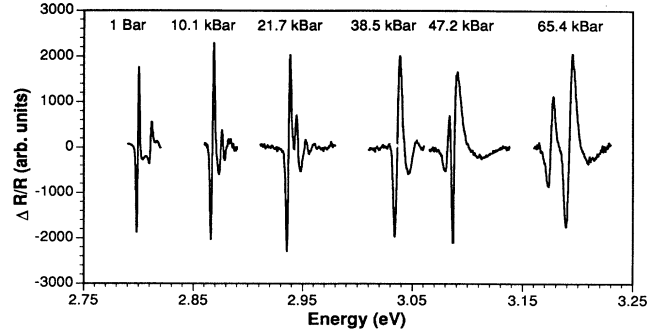


FIG. 3. The photomodulated reflectivity spectra for the ZnSe/GaAs epilayer at various pressures.

periments in which the modulation occurs at the front surface of the epilayer is not possible, rather the modulation appears to occur at the ZnSe-GaAs interface.¹ Further confirmation of this conjecture comes in the pressure studies reported here.

Figure 3 shows the evolution of the PR spectra of the ZnSe/GaAs heterostructure with increasing pressure. The spectra are fitted to the functional form⁸

$$\frac{\Delta R}{R}(E) = \sum_j \text{Re}[C_j e^{i\theta_j} (E - E_j + i\Gamma_j)^{-n}], \quad (5)$$

where C_j and θ_j are the amplitude and asymmetry of the line shape, and E_j and Γ_j are the energy and width of the transitions. The exponent n is characteristic of the type of the critical point. We have used $n=2$, which simulates two-dimensional excitonic line shapes.⁹ The above expression is convenient for numerical fits and yields line positions and widths which are in excellent agreement with other functions available in the literature. We have constructed a “pseudoabsorption” spectrum¹⁰ from the fitted parameters by calculating the integrated intensity I_j of j th peak,

$$I_j = \int |\text{Re}[C_j e^{i\theta_j} (E - E_j + i\Gamma_j)^{-n}]| dE, \quad (6)$$

where the energy is summed over the entire range of the spectrum of interest. Figure 4 is constructed from a sum

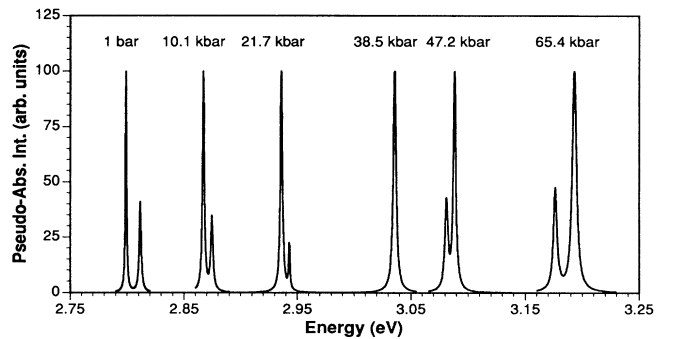


FIG. 4. The “pseudoabsorption” spectra obtained from the data of Fig. 3. Notice the signature associated with the heavy hole approaches that of the light hole and crosses it at ≈ 36 kbar. At higher pressures, the band gap is light-hole derived.

of Lorentzians with the energy positions E_j , width Γ_j , and intensity I_j , respectively. It should be remembered that such a representation is a convenient display of fitted parameters and is easier to visualize than the PR spectra which have complicated line shapes due to their derivative nature. In general, the phase angles are substantially different for different oscillators and also vary with pressure. Hence the amplitude factor C_j alone will not be enough to accurately represent the peak intensities which are given by the area under the curve for each oscillator. Equation (6) yields exactly that information.

Note as the applied pressure is increased, the heavy- and light-hole transitions approach each another and cross at 36.2 kbar. Beyond 36.2 kbar, the character of the fundamental gap of the sample changes from heavy-hole related to light-hole related. This is the first report of such behavior in a single sample.

The behavior displayed in Fig. 4 can be understood in terms of the strain evolution under pressure. To begin with, the strain in the epilayer is biaxial compressive due to the larger lattice constant of ZnSe compared to that of GaAs. Since the compressibility of ZnSe is larger than that of GaAs, there will be a pressure-dependent biaxial tensile strain superimposed on the initial compressive strain. As enough hydrostatic pressure is applied, the additional tensile strain at 36.2-kbar pressure equals the initial compressive strain. At this point the epilayer has the same lattice constant as the substrate and there are no strains in the epilayer and therefore no splitting of the Γ_8 valence-band maximum. As further pressure is applied, the pressure-dependent biaxial tensile strain is larger than the initial compressive strain and the epilayer experiences a net tensile strain and the light hole is at a lower energy. Therefore the phenomenon of heavy-hole–light-hole crossing is expected.

The phases and relative amplitudes of the oscillators remain constant with pressure, which indicates that the mixing between the heavy- and light-hole states is small. The widths of the transitions increase slightly from 3 meV at 1 bar to 5 meV at 65.4 kbar. This could be due to small nonhydrostatic components of pressure above 60 kbar or other factors.

The PR signals could be observed only up to 43.6 kbar from the 6328-Å radiation of the He-Ne laser, beyond which the 5145-Å radiation from an argon laser was used. The band gap of GaAs increases with pressure at a

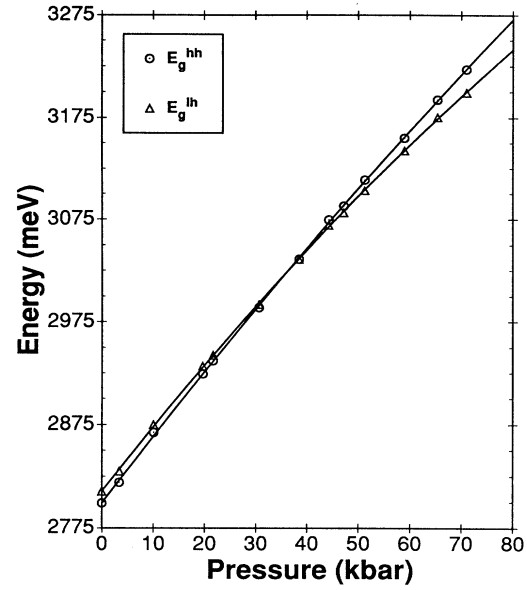


FIG. 5. The heavy- and light-hole transition energies vs pressure.

rate of 10.7 meV/kbar (Ref. 11) and exceeds the photon energy of the 6328-Å radiation of the He-Ne laser at 43 kbar. This observation confirms that the electric-field modulation occurs at the ZnSe-GaAs interface.

Figure 5 shows the transition energies from the PR data as a function of pressure. Both the E_g^{hh} and E_g^{lh} transitions have a small sublinear behavior. The lines shown are second-order polynomial fits from which the first- and second-order pressure coefficients can be found. As expected, from Eq. (4) for this material combination, the measured first-order pressure coefficient is smaller for E_g^{lh} . This is the first reported measurement of the pressure dependence for E_g^{lh} for the ZnSe/GaAs epilayer. These values are shown in Table I. Table II lists the material parameters used in this paper.¹² The first-order pressure coefficient of E_g^{hh} ($\alpha_{\text{hh}}=6.48\pm 0.2$ meV/kbar) can be compared to the photoluminescence measurements of Tuchman *et al.*¹³ on a similar sample (9 K). The second-order pressure coefficients β deduced from the present work can be compared to those found by Ves *et*

TABLE I. Linear and quadratic coefficients of the heavy- and light-hole gaps of ZnSe from the data of Figs. 5 and 7.

	α_{hh} (meV/kbar)	α_{lh} (meV/kbar)	β_{hh} (meV/kbar ²)	β_{lh} (meV/kbar ²)	ρ_{hh} (eV)	ρ_{lh} (eV)	γ_{hh} (eV)	γ_{lh} (eV)
Present work (80 K)	6.48 ± 0.2	6.33 ± 0.2	-0.007 ± 0.001	-0.012 ± 0.001	15.4 ± 0.5	15.3 ± 0.5	66	19.4
Tuchman <i>et al.</i> (Ref. 13) (9 K)	6.48 ± 0.21		0					
Ves <i>et al.</i> (Ref. 14) (bulk, 300 K)		7.2 ± 0.2		-0.015 ± 0.001		14.4 ± 0.4		6.2 ± 0.4

TABLE II. Elastic stiffness coefficients, bulk moduli, and their pressure derivatives at 80 K for ZnSe and GaAs.

	ZnSe	GaAs
c_{11} (kbar)	929 ^a	1221 ^d
c_{12} (kbar)	562 ^a	566 ^d
B (kbar)	684	784
B'	4.77 ^b	4.67 ^c
dc_{11}/dP	4.63 ^c	

^aReference 13.

^bReference 14.

^cReference 12.

^dReference 12.

^eReference 20.

*al.*¹⁴ for bulk ZnSe at room temperature. From the average of the α 's from Eq. (4), we can compute the hydrostatic deformation potential a_{cv} as

$$a_{cv} = -\frac{\alpha_{hh} + \alpha_{lh}}{2} \times \left[\frac{3}{(c_{11} + 2c_{12})_e} - \frac{2(c_{11} - c_{12})_e}{(c_{11})_e} \left(\frac{1}{(c_{11} + 2c_{12})_e} - \frac{1}{(c_{11} + 2c_{12})_s} \right) \right]^{-1}, \quad (7)$$

where the subscript *e* is for the epilayer and *s* is for the substrate. Using Eq. (7) and the values for the α 's from above we calculate the hydrostatic deformation potential for ZnSe to be $a_{cv} = -4.53$ eV. This can be compared to values which range from -3.0 to -5.4 eV,¹⁵ Lee *et al.*¹ obtained from the piezomodulated reflectivity data $a_{cv} = -5.26$ eV at ~ 20 K, whereas Gunshor *et al.*² obtain $a_{cv} = -4.87$ eV from photoluminescence measurements at 8K. The present value for a_{cv} depends only upon the measured pressure coefficients and elastic stiffness constants for the substrate and the epilayer. Hence this value is probably more reliable than the values which depend upon a detailed knowledge of the lattice constants at various temperatures.

In order to gain further insight into the dependence of the shear deformation potential b on hydrostatic pressure it is useful to plot the splitting between the heavy- and light-hole transitions ($E_g^{hh} - E_g^{lh}$) as a function of pressure, noting

$$E_g^{hh} - E_g^{lh} = 2\delta E_s + \frac{2(\delta E_s)^2}{\Delta}. \quad (8)$$

Figure 6 shows ($E_g^{hh} - E_g^{lh}$) as a function of pressure. Again, the initial splitting is negative, progressively diminishes and becomes zero at 36.2 kbar (beyond which it is positive and increases with pressure). The pressure dependence is clearly strongly superlinear. The strain induced mixing of the light-hole band and the spin-orbit split band leads to a nonlinear term in Eq. (8). However,

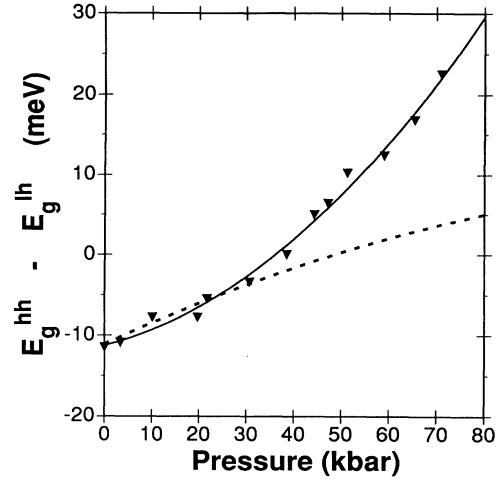


FIG. 6. The separation between the heavy- and light-hole transitions from Fig. 5 are plotted vs pressure. The solid line is a guide to the eye. The dashed line is a fit using the pressure dependence of the various parameters described in the text.

this term is only 1.3% of the linear term and is too small to account for the measured superlinearity.

Using the experimental data we can deduce an accurate value for b with the knowledge of only the elastic stiffness constants. First, we note that at 36.2 kbar the splitting between the heavy- and light-hole band edges is zero. This means that the compressive strain due to lattice mismatch at ambient pressure is exactly canceled by the tensile strain induced by the applied pressure, given by Eq. (3), leading to a strain-free epilayer at 36.2 kbar. From Eq. (3), we thus find that the strain at zero applied pressure is 2.25×10^{-3} . From the splitting of the heavy- and light-hole bands ($E_g^{hh} - E_g^{lh}$), which is -11.5 meV at 1 bar, and the lattice-mismatch strain with no applied pressure, we find $b = -1.17 \pm 0.03$ eV from Eq. (2d). Here the error bar in b is due to the uncertainty in the pressure measurement which is ± 1 kbar; Lee *et al.*¹ and Gunshor *et al.*² obtain the value of b to be -1.27 and -1.05 eV, respectively.

The pressure dependence of E_g^{hh} and E_g^{lh} in Fig. 5 is sublinear, whereas that of ($E_g^{hh} - E_g^{lh}$) in Fig. 6 is superlinear. The Murnaghan equation of state¹⁶ for the dependence of lattice constants with applied pressure is used to explain the sublinear behavior of the pressure coefficients of the band gap in bulk semiconductors. Murnaghan equation can be written

$$\frac{a(P)}{a_0} = \left[\frac{B'_0}{B_0} P + 1 \right]^{-1/3B'_0}, \quad (9)$$

where $a(P)$ is the lattice constant as a function of pressure, a_0 is the static lattice constant, B_0 is the bulk modulus, and B'_0 is the pressure derivative of the bulk modulus. Using this equation, Ves *et al.*¹⁴ found that the sublinear behavior for the band gap of bulk ZnSe was reduced when plotted versus $-\Delta a/a$. Figure 7 shows such an analysis of our data and a similar trend is seen. We can fit the transition energies in Fig. 7 to a second-order

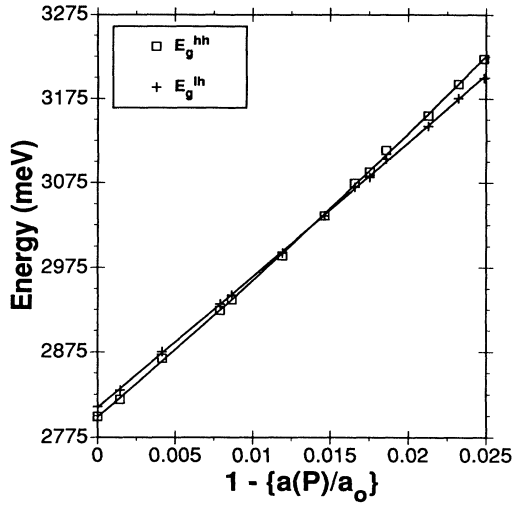


FIG. 7. The transition energies from the excitonic signatures in the photomodulated reflectivity spectrum of the ZnSe/GaAs epilayer plotted as a function of the normalized change in the lattice constant. A comparison of this figure with Fig. 5 shows a reduced nonlinearity in the variation in the excitonic energies.

polynomial in $(\Delta a/a)$ with the linear and quadratic coefficients, ρ and γ , respectively. These coefficients are shown in Table I and are compared with the data for bulk ZnSe; while the values of ρ are comparable, those for γ_{hh} and γ_{lh} are substantially larger for the ZnSe epilayer. The Murnaghan equation reduces the sublinearity in the data of Fig. 5, but does not fully account for the superlinear behavior of $(E_g^{hh} - E_g^{lh})$ as a function of pressure manifested in Fig. 6.

We have also calculated $(E_g^{hh} - E_g^{lh})$ taking into account the pressure dependence of the lattice constants, bulk moduli, and the elastic stiffness constants from Eqs. (8) and (2d). The dashed line in Fig. 6 is the result of this calculation. As can be seen, the agreement is not very good and the calculated dependence is slightly sublinear instead of being strongly superlinear.

In addition, we have considered the pressure dependence of the shear deformation potential, b . Figure 8 shows b versus the lattice spacing a_0 , for all group-IV, III-V, and II-VI materials.¹⁷ The trend in these materials is that the materials have larger negative deformation potentials as their lattice constants get smaller. It may be suspected, although not reported previously, that the deformation potential will get more negative as we apply pressure since the average lattice constant gets smaller.

In Fig. 9 the fit to $(E_g^{hh} - E_g^{lh})$ for the data assuming a pressure-dependent shear deformation potential b is shown. The value for b is then found to be $(b = -1.14 \pm 0.03)$ eV; labeling the pressure-dependent deformation potential db/dP as b' , its value is found to be $(b' = -0.017 \pm 0.002)$ eV/kbar. This analysis is consistent with the trend in Fig. 8. It is of interest to investigate if such a behavior is observed in other semiconductors for which both the shear and hydrostatic components of strain can be independently changed. A 20-

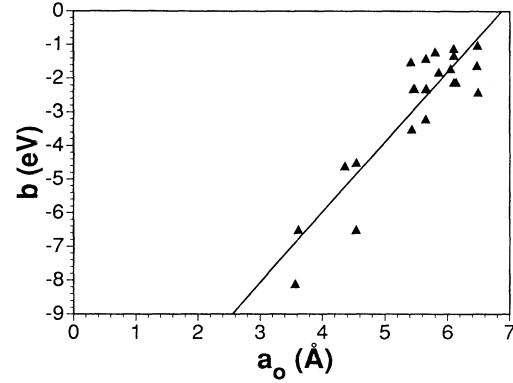


FIG. 8. The shear-deformation-potential constant b vs the lattice constant for group-IV, III-V, and II-VI semiconductors. The line is a guide to the eye showing the trend toward larger negative values of b with a decrease in the lattice constant.

band empirical tight-binding model (ETBM), which incorporates the spin-orbit splitting as well as a six-band $\mathbf{k} \cdot \mathbf{p}$ theory, predicts a value of $b = -1.2$ eV and fits the present data up to the crossover pressure but for higher pressures; the superlinear dependence of Fig. 6 is not produced by these calculations.¹⁸ However, good agreement can be obtained by introducing a pressure dependence for the coefficients of strain in the ETBM. A detailed theoretical calculation is in progress and will be published elsewhere.¹⁸

A situation similar to the pressure-induced biaxial strain above can occur for semiconductor systems where the thermal expansion coefficients for materials vary greatly. At each temperature, the lattice constant of pseudomorphic film in the (001) plane must adjust to that of GaAs in order to maintain registry. The strain thus associated with the differential thermal expansion or compression $\epsilon(T)$ can be expressed in terms of the thermal expansion coefficients α_{th} as

$$\epsilon(T) = (\alpha_{th}^{epilayer} - \alpha_{th}^{substrate})(T_G - T), \quad (10)$$

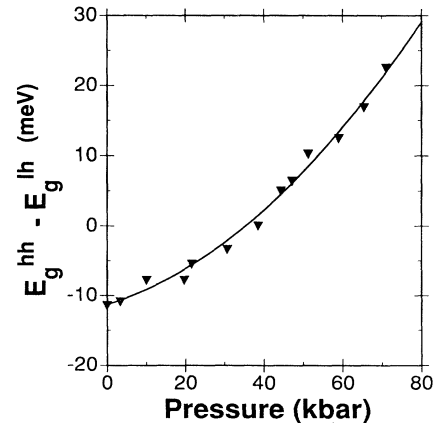


FIG. 9. The heavy-hole–light-hole splitting vs pressure. The fit is made allowing the shear-deformation-potential constant, b to be pressure dependent.

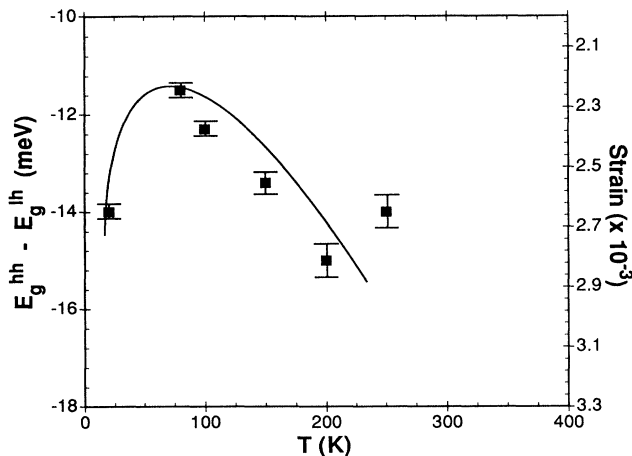


FIG. 10. The heavy-hole-light-hole splitting in the ZnSe/GaAs epilayer vs temperature. The curve through the data is a guide to the eye.

where T_G is the sample growth temperature.¹⁵ Note the α_{th} are highly temperature dependent as well. The observed splitting between the heavy- and light-hole transitions ($E_g^{hh} - E_g^{lh}$) is shown in Fig. 10 for various temperatures at ambient pressure. The data suggest that the total strain is most compressive at very low temperatures. It reaches a minimum at 80–100 K and gets slightly more compressive at higher temperatures. This behavior can be qualitatively understood from the temperature dependence¹⁹ of α_{th} and Eq. (10). Below 80 K, $\alpha_{th}^{ZnSe} < \alpha_{th}^{GaAs}$, they are equal at 80 K and at higher temperatures, $\alpha_{th}^{ZnSe} > \alpha_{th}^{GaAs}$. The additional temperature-dependent compressive strain and the lattice-mismatch strain make the total strain most compressive below 80 K. Around 80 K, $\epsilon(T)$ is zero and becomes slightly tensile at higher temperatures leading to a decrease in the total strain. As the temperature approaches T_G , the effect from Eq. (10)

decreases and the total strain approaches that obtained from Eq. (1).

V. CONCLUSIONS

The present work demonstrates how externally applied hydrostatic pressure can be exploited in the context of characterizing the built-in strains in the constituents of a heterostructure. The strain in an epilayer of ZnSe on GaAs, initially biaxial compressive, could thus be reduced to zero and transformed to biaxial tensile, in a continuous and reversible manner. Accurate values of the deformation-potential constants and their variation with pressure have emerged from the study.

Another closely related system is CdTe epilayer on an InSb substrate where a closer lattice matching prevails at ambient pressure: Lee *et al.*¹ reported the results of a piezomodulated reflectivity. ZnTe/AlSb/GaSb (Ref. 21) and ZnTe/InAs epilayers have been fabricated with MBE by us.²² These systems offer further interesting opportunities to explore analogous effects.

A recent Raman scattering study by Cui *et al.* compares the pressure coefficients of a ZnSe epilayer on GaAs with that of a bulk ZnSe sample and shows that the ZnSe epilayer becomes strain free at 21 kbar and 300 K.²³

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