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FINAL TECHNICAL REPORT

Spectroscopic Studies of $GaAs/Al_x Ga_{1-x} As$ Superlattices under Hydrostatic and Uniaxial Pressures at 8 to 300K.

GRANT NUMBER DAAL03-86-K-0083
ARMY RESEARCH OFFICE,
PHYSICS DIVISION

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July 1990

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ABSTRACT

We report on our spectroscopic investigations of bulk semiconductors and quantum well heterostructures under hydrostatic pressures at low temperatures (5 to 300K). We have studied several semiconducting materials: bulk AlGaAs, GaAs/AlGaAs quantum well heterostructures (QWH), GaSb/AlSb QWH, and the II-VI alloys, CdMnTe. The motivating factor in all the studies was to use pressure as a tool to uncover fundamental properties of the materials that were directly of value in the design of devices. In order to conduct these studies we have become, to our knowledge, the only group in the world that conducts photoreflectance measurements under pressure in a diamond anvil cell. We are also known for our photoluminescence studies at low temperatures and high pressures.

In the GaAs/AlGaAs QWH we made a *direct* measurement of the valence band offset via an elegant pressure measurement, settling a controversy that was ten years old when we reported it in 1986. The VB offset is the single most important quantity that determines the design of GaAs/AlGaAs devices. On the same material, we conducted the *first* measurements of the effects of pressure on quantum confinement: we established that well widths and quantum numbers affect pressure coefficients, a study that has motivated several theoretical calculations. We have used these studies to determine Γ–X scattering deformation potentials, initiating the most accurate method of measuring them. Our most recent discovery in this family of materials has been a *new center* in AlGaAs, which we have observed both in bulk AlGaAs and in QWH. This may well turn out to be the dominant trap for electrons in high-x $Al_xGa_{1-x}As$.

More recently we have studied quantum confinement in GaSb/AlSb QWH, a material of interest for 1.5 μm devices. We find huge pressure induced effects in the quantum confined levels and large deviations from the bulk. These effects are currently being calculated by theorists.

Another material of current interest has been the II–VI alloy $Cd_{1-x}Mn_xTe$, which of interest for lasers and optical devices in the red region. We have obtained accurate and systematic pressure coefficients in the alloys. These systematic *and* precise data are more important now than previously: these band edge deformation potentials are used to calculate shifts in valence bands and VB offsets in QWH. A 15% inaccuracy may not be of importance in the bulk alone, but it can give rise to drastic errors in strained layer heterostructure calculations. Our experiments on CdMnTe under pressure have also produced a surprising result: that the magnetic interactions and the exchange integrals, which are usually regarded as constant, change with pressure. This phenomenon may lead to revised thinking about how exchange integrals are handled in the diluted magnetic semiconductor alloys.

I. SUMMARY OF RESEARCH CONDUCTED DURING THE GRANT PERIOD

INTRODUCTION

The last decade has seen numerous breakthroughs in optoelectronic and microwave devices, fueled by the development of high quality ternary semiconductors[1]. Laser diodes, bipolar transistors, charge coupled devices, superlattice photodetectors and picosecond photodetectors are a few of many examples. The alloys and their quantum well heterostructures (QWH) are versatile: their band gaps can be tailored by changing the alloy compositon or the well widths in the QWH, and tuned to match a specific application.

Pressure, coupled with optical techniques has long been recognized as an indispensible tool in the study of semiconductors[2]. This powerful and fundamental thermodynamic tool has the advantage of providing a 'clean' technique for changing bond distances, and consequently the electronic properties. An interesting example of the predictive power of pressure was seen in the development of high T_c materials. The fact that a smaller atom was needed to increase T_c was inferred after a pressure measurement[3] showed that squeezing the atoms closer together increased T_c. Another example is seen in the frequently used (Ga,Al)As alloys, where changes in the conduction bands (CB's) due to alloying are mimiced by pressure: the direct Γ CB *increases in energy and crosses the* X CB, both with increasing pressure and with increasing Al content. The advantage with pressure is that the studies can be made on ***one single sample***, without the vagaries of dopant concentration, alloy disorder effects, etc., which can occur for samples of different compositions.

The PI has developed considerable experience in high pressure studies of quantum well systems using low temperature photoluminescence (PL) and photoreflectance (PR) in a diamond anvil cell. The two techniques are complementary: PL enhances the lowest confined transitons in QWH and is excellent for impurity related transitions. PR is ideal to study higher quantized levels in the QWH. Ours is the *first* laboratory to use PR under pressure in the QWH, and, to our knowledge, we are unique in this capability. In the past few years, we have studied the GaAs/AlGaAs, GaSb/AlSb and GaAs/InGaAs systems (Sec. III, Publications). We have used pressure to obtain the valence band offset[4]. We

[1] See, for example, A.Y. Cho, *The Technology and Physics of Molecular Beam Epitaxy*, ed. E.H.C. Parker, Plenum (1985), p. 1., and references therein.

[2] A. Jayaraman, Rev. Mod. Phys. 55, 65 (1983), and references therein.

[3] M.K. Wu, J.R. Ashburn, C.J. Torng, P.H. Hor, R.L. Meng, L. Gao, Z.J. Huang, Y.Q. Wang, and C.W. Chu, Phys. Rev. Lett. 58, 908, (1987).

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were the *first* to show that the pressure coefficients of the confined transitions depend on the well width (using PL) and on the quantum number[5,6] of the transition (using PR). These works have had tremendous impact on the field. They have motivated several theoretical calculations and experiments in the area of high pressure studies of quantum wells. Our most recent important discovery has been that of a *new trapping center* in AlGaAs, which we believe may be the most important trap in high-x AlGaAs.

This technical report is divided into six subsections (A – F), where we describe the work we have conducted under the auspices of this grant. The subsections are divided, for the sake of convenience, by the material studied. Sec. A describes our work on bulk AlGaAs; Sec. B on doped GaAs/AlGaAs quantum wells; Sec. C on Γ–X mixing in GaAs/AlGaAs quantum wells; Sec. D on the quantum confinement in GaAs/AlGaAs QWH; Sec. E on GaSb/AlSb quantum wells; and Sec. F on CdMnTe. A considerable fraction of this work is now in the process of being submitted for publication and is included in the Ph.D. thesis of W.P. Roach, which will be sent to the ARO in Aug. 1990. Recent manuscripts that have not yet been sent to the ARO are attached as appendices.

A. BULK AlGaAs

A.1 The new trapping center in AlGaAs

Substitutional group IV and group VI dopants in $Al_xGa_{1-x}As$ give rise to two types of electronic states[7] : a shallow effective mass level and a more localized level, DX, arising from lattice distortion near the donor. The DX center, which acts as an electron trap in devices, has been the subject of several optical and electrical studies in recent years. Most of the deep levels of common dopants such as Si are not within the direct gap, but are above the minimum of the Γ CB (e.g., the DX level in GaAs is about 170 meV above Γ). These non-effective mass like levels are highly localized states, and therefore do not see the translational invariance of the crystal. Hence they do not follow a particular CB, as the shallow levels do. Some of these levels have been studied as a function of alloy composition[8], and are found to have a binding energy that changes as the CB minima change as a function of x. However, one runs into the problem of differing sample quality, dopants, and doping levels for samples of different compositions. This is particulary important at high x's, where the gap is indirect, and signal levels are low. Since the major influence on the levels is the position of the CB minima, moving the CB's in a *single* sample and in a systematic manner with hydrostatic pressure provides a 'clean' method of

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studying the levels.

We report the observation of a *new* localized state in $Al_{0.3}Ga_{0.7}As$ which we have uncovered using hydrostatic pressure. It is higher in energy than DX, and should be active at ambient pressures at $x \approx 0.7$. It is in some ways reminiscent of the DX center. It is metastable, with an energy above the X CB at pressures below 40 kbar. At higher pressures it becomes stable and captures all electrons that are photoexcited into the X CB, causing ***a sharp drop in the intensity*** of radiative transitions by about two orders of magnitude. Upon reducing the pressure, the intensity of the radiative transitions does ***not recover*** despite thermal cycling to room temperature, indicating an ***unusually deep emission barrier***, much deeper than that of DX. The intensity finally recovers at very low pressures (~ 10 kbar).

The significance of the new center lies in that it may be the dominant electron trap in $Al_xGa_{1-x}As$ at high x-values. The pressure at which this new center becomes active is equivalent to about $x \approx 0.7$. It is well known that[9] the refractive index of $Al_xGa_{1-x}As$ decreases with increasing x, making high-x material desirable as cladding in GaAs/AlGaAs lasers. Electron traps caused by Si and Zn (the usual dopants) for x>0.4 have caused serious problems of degradation in device performance.

The understanding of this new center is vital to the growth and applications of good quality high-x $Al_xGa_{1-x}As$. If the energy of the metastable level and the chemical species that causes it are well known, device engineers and growers can choose the appropriate dopant for a given x, lending a degree of predictability to high-x material. In the rest of this section we will briefly describe the experiment we have performed, the questions it has raised, and then describe the experiments we have proposed to answer the questions.

Our Experiment

$Al_{0.3}Ga_{0.7}As$ is a direct gap semiconductor. Under pressure, the energy of the direct Γ CB increases while that of the indirect X CB decreases, crossing around 13 kbar. Well below the $\Gamma - X$ crossing, the PL spectrum consists of a sharp, intense peak due to the neutral donor bound exciton BE^{Γ}, and weaker peaks due to donor-acceptor recombination, DA^{Γ}, at lower energies. Around 9 kbar, new peaks appear below BE^{Γ} (Fig. 1). The high energy peak labelled A is the exciton bound to the X CB, while the broad peaks labelled B,C and D are due to donor-acceptor (DA) recombination. These peaks show considerable bowing around crossover[10], indicative of Γ-L-X mixing, and then move downward in energy with pressure with a pressure coefficient of –1.6 meV/kbar. The energies of all observed transitions under pressure are shown in Fig. 2. The peaks are quite intense till about 45 kbar. Beyond 45 kbar, the intensity drops steeply, decreasing by more than two

[9] G.A. Samara, Phys. Rev. **B 27**, 3494, (1983); R.E. Fern and A. Onton, J. Appl. Phys. **42**, 3499 (1971).

[10] W.P. Roach, M. Chandrasekhar, H.R. Chandrasekhar, F.A. Chambers and J.M. Meese, Semicond. Sci. and Technol. **4**, 290 (1989).

orders of magnitude at ~ 65 kbar (Figs. 3 and 4).

The unusual feature occurs when the pressure is reduced. The intensity of the PL spectrum *does not recover* at the same pressure at which it declined. An example is seen in panels (d) and(e) of Fig. 3, where we show the spectrum at almost the same pressures as in panels (a) and (b), but for *decreasing* pressure (downstroke). Pressurizing the sample to 65 kbar and decreasing the pressure reduced the intensity by a factor of 17 at 44 kbar, though the peak positions and PL lineshape remain similar. The ratio improves to a factor of six at 31 kbar, and is about a factor of two at very low pressures of ~ 10 kbar (for BE^{Γ}).

A decrease in PL intensity due to level crossings is a common feature. When the Γ and X CBs cross, and electrons are scattered preferentially to the X CB and Γ VB recombination intensity decreases by several orders of magnitude as in the 10–15 kbar region of Fig. 4a. Another example is the crossing of the nitrogen deep levels in GaAs[11] with the X CB near 70 kbar. When the N-levels become resonant with the X CB, their intensity drops. In both cases, however, the transitions reappear upon decreasing the pressure with the same intensity and at the same pressure as in the upstroke, unlike the behavior we observe. The *hysteresis* in the intensity, then, rules out a simple level crossing.

Yet another cause for a decrease in PL intensity is dislocations occuring near a structural phase transition, seen in several direct gap materials such as CdS[12] and CdTe[13]. In AlGaAs, the phase transition takes place at ~150 kbar[14], and is too far away to cause dislocations at 70 kbar. Another characteristic of dislocations is that releasing the pressure does not allow the PL intensity to recover: since we find near total recovery near 10 kbar, we conclude that dislocations do not cause of the effect we observe.

The simplest model that describes the effect we observe is a trapping center with lattice relaxation. Since the hysteresis is so large, we use the model for a large lattice relaxation. A schematic model is shown on a configuration coordinate diagram in Fig. 5. The minimum in the potential energy for the center (U_T) is displaced from that of the X CB (U_X). Scattering to U_T can occur thermally (via the capture barrier E_B) or via an intermediate state, as has been suggested for the DX center[15]. A detailed discussion is given in Appendix I, which we are submitting to Physical Review Letters.

We have observed evidence for the new center in two samples: bulk $Al_{0.3}Ga_{0.7}As$(10^{15} cm^{-3} Si) and a multiple quantum well (MQW) of GaAs/ $Al_{0.3}Ga_{0.7}As$

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[15] P.M. Mooney, N.S. Caswell and S.L. Wright, J. Appl. Phys. **62**, 4786 (1987).

(40Å/80Å). In the MQW, the hysteresis is seen for the indirect X- like staggered transition from the X–CB of $Al_{0.3}Ga_{0.7}As$ to the VB of GaAs, which arises from the same conduction band state as in the bulk sample. The effect, therefore, is undeniably tied to the crossing of a the center with the X–CB of $Al_{0.3}Ga_{0.7}As$.

The energy behavior (discussed in Appendix I) is consistent with the hysteresis in the intensity, and suggests that a donor is involved in the trapping process. The center has an energy that is above than the X CB at ambient pressures, and crosses to come below it at high pressures. The center is not the DX center: DX is below the X CB at all pressures[16], and its emission barrier E_e is sufficient to empty[17] it at 300K. E_e for this new center is > 300K at high pressures. A level that does cross X at high pressures is the recently observed SD level[18,19]. However, its E_e is less than that of the DX center, which rules it out as this new center.

The conclusions of the experiment are as follows:

(a) The decline and hysteresis in the intensity occurs due to a *new* trapping center, which could be the dominant electron trap in high-x $Al_xGa_{1-x}As$.

(b) The center is active above 45 kbar for x = 0.3. This translates to a zero pressure equivalent of $x \approx 0.7$.

(c) The center is an electron trap caused by donors whose chemical species is not known at present.

(d) The center has an unusually high thermal emission barrier, whose value is not known at present.

We will perform annealing experiments to determine the thermal and optical emission barriers. These experiments are vital to determining whether the center has large or small lattice relaxation. Studies will also be conducted on GaAs and $Al_xGa_{1-x}As$ of various x values between 0.0 and 1.0 to determine the x value at which the center is active at ambient pressures. Samples with various dopants will be used to determine the chemical species that causes the center. All these experiments are included in the proposal presently being submitted to ARO.

Activation energies of the deep donor levels.

We have obtained some of the most detailed information on the activation energies associated with the deep X- associated donor levels. Using PL under pressure, we have studied the temperature dependence of the radiative transitions at pressures typical of the Γ, Γ-L-X mixing and X-like regions. We vary the temperature from 15 to 125K, record PL

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[17] D.V. Lang, *Deep Centers in Semiconductors, ed. S.T. Pantelides,* (Gordon and Breach, New York, 1986) pp. 489-539 and references therein.

[18] Y.B. Jia, M.F. Li, et. al, J. Appl. Phys. **66**, 5632 (1989).

[19] S.B. Zhang and D.J. Chadi, Preprint.

spectra. The spectra are fit to lorentzian lineshapes in order to extract the intensities of the individual peaks. These integrated intensities are fit to an Arrhenius function to obtain activation energies E_a

$$I = \frac{I_o}{1 + \sum C_j \exp (E_{a,j}/k_B T)}$$

where j = 1,2 depending on the energy level and the temperature behavior. A sample Arrhenius plot is shown in Fig. 6(a). Fig. 6(b) shows a plot of the peak positions and the energy levels (dashed lines) corrected for the temperature shift of the energy levels.The activation energies and scattering processes we obtain are shown in Table I.

Table I. Activation Energies in $Al_{0.3}Ga_{0.7}As$ at selected pressures

Pressure	Transition	E_a(meV)	Scattering process
1 bar	BE^{Γ}	21 ± 5	To Γ CB
		101 ± 11	FE^{Γ} to L CB
	DA^{Γ}	23 ± 4	Ionization of acceptor
6 kbar	BE^{Γ}	21 ± 8	To Γ CB
		85 ± 20	FE^{Γ} to L CB
	DA^{Γ}	24 ± 10	Ionization of acceptor
		111 ± 5	Donor to L CB
26 kbar	BE^{X}(A)	9 ± 1	BE^{X} to FE^{X}
		73 ± 17	FE^{X} to L CB
	DA^{X} (B + C)	9 ± 2	To BE^{X}(A)
		56 ± 3	DA^{X} to X CB
	DA^{X} (D)	30 ± 5	Ionization of acceptor
		116 ± 9	DA^{X} (D) to X or E_m
33 kbar	BE^{X}(A)	11 ± 1	BE^{X} to FE^{X}
	DA^{X} (B + C)	9 ± 3	To BE^{X}(A)
		43 ± 5	DA^{X} to X CB
44 kbar	BE^{X}(A)	13 ± 4	BE^{X} to FE^{X}
		44 ± 13	FE^{X} to X CB
	DA^{X} (B + C)	19 ± 3	To FE^{X}(A)
		143 ± 32	To L CB
	DA^{X} (D)	29 ± 3	Ionization of acceptor

Coupling the information from the peak positions as a function of temperature with the activation energies above, and the scattering processes listed in Table I, we generate an energy level diagram (Fig. 7). We find that the presence of the trapping center is evident in these data as well: below 40 kbar, scattering processes prefer the X CB. Above it, the scattering changes radically, and scattering occurs to the L CB.

A.3 Pressure Coefficients of the radiative transitions

We have obtained a complete and accurate set of pressure coefficients for all the radiative transitions observed. This, as far as we know is the first such set, and if of vital importance in accurately calculating parameters, in particular VB offsets, associated with quantum well heterostructures. These pressure coefficients are obtained from the energy vs. pressure curves in Fig. 2.

Table II. Pressure coefficients of the peaks in $Al_{0.3}Ga_{0.7}As$, fit to $E(P) = E(0) + \alpha P$

Transition	E(0) (eV)	α (meV/kbar)	Pressure range (kbar)
BE^{Γ}	1.9001 ± 0.0033	9.47 ± 0.32	0 – 18
E^{Γ}(sh)	1.8905 ± 0.0002	10.28 ± 0.19	0 – 15
DA^{Γ}(1)	1.8731 ± 0.0025	8.76 ± 0.27	0 – 15
DA^{Γ}(2)	1.8637 ± 0.0015	8.56 ± 0.15	0 – 15
DA^{Γ}(3)	1.8398 ± 0.0018	6.64 ± 0.19	0 – 15
DA^{Γ}(4)	1.8125 ± 0.0045	6.43 ± 0.50	0 – 15
FE^{X}	2.0388 ± 0.0025	– 1.43 ± 0.09	15 – 40
BE^{X}	2.0300 ± 0.0022	– 1.65 ± 0.05	15 – 70
DA (B)		– 1.65 ± 0.06	20 – 70
DA (C)		– 1.68 ± 0.08	20 – 70
DA (D)		– 1.72 ± 0.12	20 – 50
Previous works (nominally x = 0.3)			
BE^{Γ}	1.872 ± 0.002	9.9 ± 0.1	0 – 20, 8K (Ref. a).
BE^{X}	2.013 ± 0.003	– 0.93 ± 0.09	15 – 42, 8K (Ref. a).
Band Gap (Γ)		10.8 ± 0.1	0 – 10, 300K (Ref. b).

a. M. Chandrasekhar, U. Venkateswaran, H.R. Chandrasekhar, B.A. Vojak, F.A. Chambers and J.M. Meese, *Proceedings of the XVIII International Conference on the Physics of Semiconductors, Stockholm* ed. O. Engström, (World Scientific 1987), p. 943; and U. Venkateswaran, unpublished results.

b. N. Lifshitz, A. Jayaraman, R.A. Logan, R.G. Maines, Phys. Rev. **B 20**, 2398 (1979).

Associated publications : Sec. III, #s 2, 4, 5, 6, 15, 20, 21.

Associated invited talk: Sec. IV, # 7.

Associated contributed talks: Sec. V, #s 1, 5, 7, 8, 10, 15, 18, 23.

B. DOPED QUANTUM WELL HETEROSTRUCTURES UNDER PRESSURE

Doped quantum wells are frequently used in devices. It is of vital importance to understand the deep donor levels and traps in these materials, which degrade device performance. We have studied a center doped GaAs/AlGaAs quantum well (40Å/80Å), doped in the center third of the well with 10^{18} Si/cm^3. We report new effects due to the trapping center described in Sec. I.A. We also observe interesting many-body and mixing effects via the lineshapes, which are currently under investigation.

Confirmation of the new center observed in AlGaAs

We expect to see effects due to the new center in this sample at pressures above the Γ – X crossover, since the indirect transition observed is from the X CB of AlGaAs to the VB of GaAs, and the initial state is the same as the one we observed in the bulk. As expected, we do observe the decline in the PL intensity and the hysteresis characteristic of the center (Fig. 8(a) and (b)). This provides confirmation that the center arises from AlGaAs, and is not limited to one sample, or merely to a surface effect in bulk AlGaAs.

In addition, we observe something more interesting: the energies of the staggered transitions also cycle in a way that is consistent with the trapping of electrons. Recall that the PL intensity declined on the upstroke at 45 kbar, and recovered on the downstroke at 30 kbar. The energies of the highest energy X-related transition are shown in Fig. 9 for temperatures of 15, 40 and 80K, open (solid) symbols for up(down)strokes. When the E_{1h}^{Γ} and AlGaAs X bands cross, staggered transitions are observed. At 15 and 40K (circles and triangles in Fig. 9) an X– related level, E_1 is observed, but only up to a pressure of ~ 40 kbar. Above 40 kbar E_1 abruptly disappears, and a new peak 12 meV higher in energy,which we label E_2 appears. This peak continues to shift at –1.6 meV/kbar, and is visible till about 50 kbar, beyond which it is masked by the GaAs:N levels. When the pressure was increased to 70 kbar and then reduced, downstroke, the E_2 peak once again emerged from the GaAs:N levels near 50 kbar. Instead of following the upstroke path and switching to E_1 at 40 kbar, it *continues* to follow the E_2 path to pressures of 30 kbar. Recovery of E_1 was never observed, even at pressures at which it had been seen in the upstroke. In contrast, at a higher temperature of 80K, E_2 is the only level observed, both in up- and downstrokes (squares in Fig. 9).

It is reasonable to assume that at 80K E_2 is the free exciton associated with the confined level in the X CB. Its energy is consistent with previous studies[6] at 80K of other undoped MQW samples. When corrected for the temperature shift of the band gaps, E_1 at 15K is ≈24 meV lower in energy. The switching of radiative transitions at 15 and 40K from E_1 to E_2 at 40 kbar in the upstroke suggests that the effect is directly related to the trapping center. It is possible that the availability of a large number of electrons makes a lower energy transition viable in the upstroke below 40 kbar. When the electrons are trapped by the center beyond 40 kbar, the level is no longer available. Nor is it available in the downstroke, until recovery takes place (<30 kbar). The exact identification of E_1 is not clear at present, and its energy may involve screening effects due to 10^{18} electrons. At 80K, the thermal smearing of the Fermi sea makes the free exciton E_2 the only viable state both in the up- and downstrokes.

The energy behavior is consistent with the pressure induced hysteresis in the intensity, and suggests that a donor state is involved in the trapping process, both in bulk AlGaAs and in the MQW. Further investigations of this center were discussed in Sec. A.1. and Appendix I.

Lineshapes

The doping of the quantum well produces broadened lineshapes due to the large Fermi sea. The lineshapes are shown in Fig. 10 for a series of pressures. At low pressures, the lineshape is broad, about 40 meV, due to the transitions from the impurity band in the CB. In order to understand these lineshapes, a many-body calculation is in progress in collaboration with one of the theorists in our department, Giovanni Vignale. The interesting feature in this data is the abrupt change in lineshape that occurs between 19 and 21 kbar, panels (b) and (c) in Fig. 10. Due to the crossing of the X CB of AlGaAs with the Γ confined state in the GaAs well, the electrons are dumped into the X CB, and the Γ confined state now exhibits its intrinsic linewidth (18 meV). This transformation from a broad to a narrow linewidth allows to determine *exactly* the width and shape that has to be deconvoluted from the low pressure spectrum in order to calculate the many-body effects, since it is the *same* sample, with and without electrons in the well. Previous studies on doped quantum wells have had to assume intrinsic lineshapes and widths, which we do not have to.

At pressures above the crossover, we observe asymmetric and broadened lineshapes, with a steady increase in the broadening of the E_{1h}^{Γ} confined state. This occurs due to mixing of the Γ wavefunction with that of the X CB, allowing us to obtain the deformation potentials associated with the scattering process, $D_{\Gamma X}$. This feature will be discussed in the Sec. C.

Pressure coefficients

We have obtained pressure coefficients of all observed transitions, listed in the Table III below:

Table III. Pressure coefficients of transitions in GaAs/AlGaAs (40Å/80Å) Multiple Quantum Well

Transition	E(0) (eV)	α (meV/kbar)	β (meV/kbar^2)	Pressure range (kbar)
15K				
E^{Γ}_{1h}	1.6850 ± 0.0019	10.36 ± 0.14	−0.014 ± 0.002	0 – 65
$E^{\Gamma}_{1h}(2)$	1.6613 ± 0.0030	9.94 ± 0.25		0 – 21
$E^{\Gamma}_{1h}(3)$	1.6510 ± 0.0021	9.98 ± 0.20		0 – 19
$E^{\Gamma}_{1h}(4)$	1.6138 ± 0.0027	9.90 ± 0.26		0 – 19
E^{Γ}(1,GaAs)	1.5152 ± 0.0011	11.10 ± 0.10		0 – 21
E^{Γ}(1,GaAs)	1.4965 ± 0.0021	11.07 ± 0.18		0 – 21
FE(X)(stag.)	1.9368 ± 0.0035	−1.74 ± 0.08		26 – 52
BE(X)(stag.)	1.9255 ± 0.0030	−1.81 ± 0.10		23 – 38
Level B(stag.)	1.9030 ± 0.0042	−1.81 ± 0.13		23 – 44
Level C(stag.)	1.8937 ± 0.0068	−1.91 ± 0.22		23 – 38
40K				
FE(X)(stag.)	1.9321 ± 0.0021	−1.62 ± 0.05		28 – 50
BE(X)(stag.)	1.9144 ± 0.0041	−1.43 ± 0.12		29 – 38
Level B(stag.)	1.8827 ± 0.0120	−1.27 ± 0.37		28 – 38
80K				
E(X)(stag.)	1.9376 ± 0.0011	−1.78 ± 0.02		29 – 65
Level B(stag.)	1.8821 ± 0.0056	−1.23 ± 0.13		29 – 59

Associated publications: Sec. III, #s 20 and 21.

Associated contributed talks: Sec. V, # 23.

C. CALCULATION OF SCATTERING DEFORMATION POTENTIALS FROM FANO LINESHAPES IN GaAs/AlGaAs QUANTUM WELLS

As mentioned in Sec. B, the lineshape of the E_{1h}^{Γ} transition in GaAs/AlGaAs quantum wells beyond the $\Gamma - X$ crossover is broadened and asymmetric. This occurs due to scattering of the electrons from Γ to X, and the mixing of wavefunctions associated with it. An analysis of the lineshapes allows us to calculate the scattering deformation potential, $D_{\Gamma X}$ to be equal to 6.4 eV. This may well be the most accurate method of determining the deformation potential. Further details are described in Appendix II.

Associated publications: Sec. III, #s 12 and 17.

Associated contributed talks: Sec. V, #s 11 and 20.

D. GaAs/AlGaAs QUANTUM WELLS UNDER PRESSURE

We have already described some of our more recent results on GaAs/AlGaAs quantum wells under pressure, such as the discovery of the new trapping center, many body effects and measurement of scattering deformation potentials. In this section we will summarize the experiments that started the whole process, our seminal work on undoped quantum wells under pressure. This work is well known and well quoted in the literature, therefore we will briefly list the salient results and the impact this work has had on the field.

Determination of Valence Band Offsets

The question of valence band offsets in GaAs/AlGaAs was outstanding in 1986. We established it with an elegant measurement under pressure. When the Γ CB is driven to higher energies with pressure, it crosses the X CB. Because of the band lineups, it is the AlGaAs X CB that is lower than that of the X CB in GaAs, causing radiative transitions to occur *across* the heterointerface from the AlGaAs X CB to the GaAs VB (Fig. 11). We can now determine the VB offset *directly*: it is the difference in energy between the staggered transition and the energy of the X CB in bulk AlGaAs at the same pressure. This work was done simultaneously with a similar measurement by another group[20].

Since we have measured the X CB energy in bulk AlGaAs under pressure as well, we have an accurate determination of the VB offset. The ratio of CB to VB offsets, $Q_c:Q_v$ is 70:30. We are currently using the same technique to obtain VB offsets in InGaAs/GaAs quantum wells. Here the situation is more complicated, because the interlayer strains change with pressure due to the different compressibilities of the well and substrate.

[20] D.J. Wolford, T.F. Kuech and J.A. Bradley, et. al, J. Vac. Sci. Technol. B 4 1043 (1986).

Quantum confinement under pressure

In our previous studies of the GaAs/AlGaAs and, GaSb/AlSb systems under pressure, we have used both PL (to study the lowest quantized transition) and PR (to study several quantized levels). We have found that there is a *systematic decrease* of the pressure coefficients of the allowed quantized transitions both with decreasing well width, and increasing quantum number n. Our work has spawned several theoretical calculations, notably the ones in Ref. 21. The increase in the CB effective mass is found to play a dominant role for low n's and wide wells, while wavefunction mixing with the barrier is a major contributor for large n's and narrow wells.

The effect of changing well widths was studied using PL at 80K. Our PL spectra under pressure are shown in Fig. 12a. The lowest quantized levels in GaAs/AlGaAs quantum wells, the n = 1 heavy and light hole excitons, E_{1h} and E_{1l}, respectively, are observed in a sample with four different well widths. The pressure coefficients are shown along with theoretical calculations[21] using a one band Wannier orbital model in Fig. 12b. The agreement is excellent.

The work on quantum confinement was followed up by photoreflectance measurements under pressure in GaAs/AlGaAs and GaSb/AlSb quantum wells (Sec. E.) by other members of our group.

Associated Publications: Sec. III, #s 1, 3, 7, 8, 14.

Associated Invited talks: 1, 2, 3, 4, 5, 6, 8, 9, 10.

Associated contributed talks: 2, 3, 4, 6, 9.

E. GaSb/AlSb UNDER PRESSURE USING PHOTOREFLECTANCE

Strained-layer superlattices are composed of semiconductors of significantly different lattice constants and have new device applications. The axial strain between the layers of two semiconductors splits the degeneracy of the light and heavy hole zone center states. This could lead to the light hole derived sub-band to be the ground state as in the case of GaSb / AlSb quantum wells of well width greater than 100Å. Devices based on such structures have the advantage of high hole mobilities.

Using photoreflectance and photoluminescence under pressure, we have studied the confined transitions in GaSb/AlSb quantum wells. These materials are of interest because of their infrared bandgap (0.7 eV), a low-loss spectral region of importance in fiber optic

[21] D.Z.-Y. Ting and Y.C. Chang, Phys. Rev. **B 36**, 4359 (1987); P. Lefebvre, B. Gil, and H. Mattieu, Phys. Rev. **B 35**, 5630 (1987).

technology. Using photoreflectance, we have studied upto the eighth heavy hole confined transition (Fig. 13). We find that the pressure coefficient is markedly dependent on the quantum number of the transition: the highest transition observed has upto 30% smaller pressure coefficient than the first heavy hole transition. This is seen in Fig. 14. Previous calculations by Ting and Chang predicted this trend in the GaAs/AlGaAs quantum wells, but the effect was of the order of a few percent. Calculations are not available for the GaSb/AlSb system, where the small band gap and intralayer strain are expected to play a role.

The substrate on which the epilayers are grown also plays a significant role. For pseudomorphic structures, below a critical thickness the in-plane lattice constants of a *thin* epilayer will be forced to that of the substrate by accommodating the elastic strains in the axial direction. The effect of pressure on an epilayer grown on a substrate has an additional feature. If the substrate has a different compressibility, the epilayer may experience a different amount of pressure than the *applied* pressure and may have a uniaxial component as well. The former effect leads to a change in the pressure coefficient and the latter will alter the separation between the heavy and light hole derived sub-bands.

In our PR experiments, (Appendix III) we have show that the pressure coefficients of the ground state excitons in GaSb–AlSb MQW's grown on a GaAs substrate are lower (10-15%) than those grown on a GaSb substrate. This is due to the lower compressibility of GaAs than that of GaSb or AlSb. Additionally a uniaxial deformation alters the splitting of light and heavy hole sub-bands with pressure. The quantum confinement effects have an added contribution which is greater for narrow wells or higher sub-band states.

Associated publications: Sec. III, #s 9, 11, 14, 18.

Associated invited talk: Sec. IV, # 10.

Associated contributed talks: Sec. V, #s 12, 14, 16, 21.

F. CdMnTe UNDER PRESSURE

Quantum well heterostructures of the II-VI binary and ternary compounds offer an exciting array of bandgaps and physical properties. The bandgaps range from the deep red 1.6 eV to the near UV 3 eV region by using Cd and Zn for the Group II and Se, Te and S for the Group VI material. Continuous tuning of the band gap is achieved by means of ternary alloys or by replacing the Group II with a magnetic ion such as Mn or Fe, which produces interesting magnetic effects in these diluted magnetic semiconductor (DMS) alloys.

Applications of the II-VI heterostructures range from blue-green lasers, modulators, nonlinear devices, optical memories and flat panel high resolution displays and screens (manufactured by Sharp, Japan). The shorter wavelengths are favored because the lower diffraction allows better focusability. Laser layouts have been made with 2 million lasers/cm^2, triggered with blue light. The phenomenon of giant Faraday rotation in DMS alloys has been used in devices that measure fringe magnetic fields, fast transient magnetic fields at GHz frequencies and as Faraday isolators in fiber optic cables.

QWH such as $Zn_{1-x}Mn_xSe/Zn_{1-x}Cd_xSe$, $Cd_{1-x}Mn_xTe$ / $Cd_{1-y}Mn_yTe$ and various other combinations have been successfully grown by MBE. They have been studied via photoluminescence, piezo-, electro-, and photo-modulated reflectivity spectra[22]. Most of them are strain layered structures[23], grown on a GaAs substrate. The band offset, often small or near zero[24], is controlled by strain, which depends on the interlayer lattice constants, the buffer layer and the substrate.

It is vitally important to know how the band offset changes with strain. The present technique is to grow several samples with different buffers, substrates and layer compositions. The strain is predicted from the lattice constants and the band offsets estimated from experimental measurements. The drawback of this approach, apart from the necessity of growing a large number of samples, is that interlayer defects vary from sample to sample, and excitons bound to defect states can mislead the interpretation.

Review of our recent work

In the last two years, we have obtained some of the most detailed and accurate data on $Cd_{1-x}Mn_xTe$ for $x = 0.0$ to 0.20. Previous experiments under pressure[25] have focussed on studying the band gap and the intraionic Mn^{2+} d-d transitions. Most of the studies were done at 300K, and a few at 77K, primarily using optical absorption. We have performed all our studies at 5 and 15K. With PL we see much sharper excitonic peaks and impurity levels such as the e-A^o, which are not observed otherwise. So far ours have been the first studies of magnetic effects under pressure.

A typical spectrum for one of these samples at 15K is shown in Fig. 15. These spectra are for CdTe under pressure. We see similar features for the CdMnTe alloy. The dominant high energy peak is the exciton (A^oX, bound to neutral acceptors, or X, the free

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22 R.L. Harper, R.N. Bicknell, D.K. Blanks, N.C., Giles, J.F. Schetzina, Y.R. Lee, and A.K. Ramdas, J. Appl. Phys. **65**, 624 (1989).

23 N. Bottka, J. Stankiewicz, and W. Giriat, J. Appl. Phys. **52**, 4189 (1981).

24 S.K. Chang, A. Nurmikko, J.W. Wu, L.A. Koldziejski and R.L. Gunshor, Phys. Rev. B 37, 1191 (1988).

25 G.A. Babonas, R.A. Bendoryus, A. Yu. Shileika, Sov. Phys. Semicond. **5**, 392 (1971); G. Abrazevicius, G. Babonas, S. Marcinkevicius, V.D. Prochukhan, and V. Yu. Rud, Sol. State. Commun., **49**, 651 (1984); Wei Shan, S.C. Shen, H.R. Zhu, Sol. State. Commun. **55**, 475 (1985); E. Müller, W. Gebhardt, and W. Rehwald, J. Phys. C, **16**, L1141 (1983); S. Ves, K. Strössner, W. Gebhardt, and M. Cardona, Phys. Rev. **B 33**, 4077 (1986).

exciton, depending on the level of doping). At lower energies is the e-A^o transition. At still lower energies are donor-acceptor (DA) recombination peaks. By studying these transitions under pressure we have established the following:

(a) Accurate pressure coefficients of all the observed radiative transitions, listed in Table IV. The energy vs. pressure curves are shown in Fig. 16. These systematic *and* precise data are of particular importance now: these band edge deformation potentials are used to calculate shifts in valence bands and VB offsets in QWH. A 15% inaccuracy may not be of importance otherwise, but it can give rise to drastic errors in strained layer heterostructure calculations[26] (Appendix IV).

We propose to apply the results of the pressure coefficients to studies of interlayer strains in heterostructures, as detailed in the proposal we are currently submitting to ARO.

(b) We have performed the *first* studies of the effect of pressure on the magnetic interactions in $Cd_{1-x}Mn_xTe$. We find that the exchange integrals, which are normally assumed to be constant for a given material, are in fact *not* a constant with pressure. In most magnetic phenomena, the exchange interaction appears as a product of the exchange integral and $\bar{x}$, the effective concentration. Since they cannot be disentangled, all variations in the exchange interaction are usually lumped into $\bar{x}$. Our experiments show that this simplistic picture may have to be abandoned (Appendix V).

Under pressure, the variation of $\bar{x}$ depends only on the volume change. All further changes in the magnetic effects have to be due to the exchange integral. This is what we have done in our experiments. In $Cd_{1-x}Mn_xTe$, the magnetic effect, manifest via the acceptor bound magnetic polaron (BMP), is seen in the energy separation between the A^oX and e-A^o transitions. By an analysis of the shift of A^oX relative to e-A^o, we see how the binding energies change with pressure (Fig. 17). In CdTe, the changes can be explained by a Coulombic picture (Ref. 27). In $Cd_{1-x}Mn_xTe$, BMP effects account for the changes. Recent calculations by Prof. L.R. Ram-Mohan have shown that the exchange integrals have to change with pressure in order to explain our results[27].

[26] M. Prakash, M. Chandrasekhar, H.R. Chandrasekhar, A.K. Ramdas and I. Miotkowski, *Phys. Rev*, to appear Aug 15, 1990. In this paper, where we report on CdTe, we have shown how important it is to obtain accurate pressure coefficients.

[27] M. Prakash, M. Chandrasekhar, H. R. Chandrasekhar, A.K. Ramdas, I. Miotkowski, and L.R. Ram-Mohan, to appear in *Proc. of the XX Int'l Conf. on Physics of Semiconductors*, Thessaloniki, Greece, Aug. 1990.

Table IV. Pressure coefficients of the peaks in $Cd_{1-x}Mn_xTe$, fit to $E(P) = E(0) + \alpha P + \beta P^2$
All data at 15K unless otherwise noted.

x	Transition	E(0) (eV)	α (meV/kbar)	β (meV/kbar^2)	Comments
0.0	A^oX	1.594 ± 0.002	7.59 ± 0.19	− 0.029 ± 0.007	
	A^oX–LO	1.572 ± 0.002	7.74 ± 0.20	− 0.038 ± 0.007	5K
	e-A^o	1.556 ± 0.002	7.91 ± 0.18	− 0.038 ± 0.005	
	e-A^o– LO	1.536 ± 0.002	7.78 ± 0.24	− 0.034 ± 0.007	
	DA 1	1.477 ± 0.002	6.39 ± 0.09		
	DA 2	1.452 ± 0.002	6.60 ± 0.08		
	DA 3	1.432 ± 0.002	6.52 ± 0.07		
	DA 4	1.407 ± 0.002	6.57 ± 0.06		
0.05	A^oX	1.663 ± 0.001	7.91 ± 0.17	− 0.036 ± 0.005	
	L1	1.648 ± 0.002	8.17 ± 0.30	− 0.05 ± 0.01	
	e-A^o	1.616 ± 0.001	8.44 ± 0.14	− 0.044 ± 0.004	
	e-A^o–LO	1.595 ± 0.001	8.01 ± 0.20	− 0.035 ± 0.005	
0.15	A^oX	1.826 ± 0.001	7.66 ± 0.20	− 0.032 ± 0.007	
	L1	1.806 ± 0.002	7.92 ± 0.26	− 0.041 ± 0.009	
	e-A^o	1.742 ± 0.001	7.53 ± 0.18	− 0.033 ± 0.006	
0.20	A^oX	1.902 ± 0.001	7.95 ± 0.17	− 0.033 ± 0.005	
	L1	1.880 ± 0.001	7.20 ± 0.10		
	e-A^o	1.801 ± 0.001	7.45 ± 0.19	− 0.024 ± 0.006	
	DA	1.624 ± 0.002	7.03 ± 0.16		
Previous works					
0.0	Band Edge[a]		8.0 ± 0.2		77K, absorption & reflectivity
	Band Edge[b]		7.9 ± 0.2		300K, reflectivity
	Band Edge[c]	1.483	8.3	− 0.004	300K, absorption
	Exciton[d]		6.5 ± 0.2		2K, PL
0.1	Band Edge[c]	1.618	7.7	− 0.039	300K, absorption

[a] D. Langer, *Proc. of the VII Intl. Conf. on the Physics of Semiconductors*, Paris 1964 (Dunod, Paris, 1964), p. 241.

[b] G.A. Babonas, R.A. Bendoryus, and A. Yu. Shileika, Fiz. Tekh. Poluprovodn. 5, 449 (1971) (Sov. Phys. Semicond. 5, 392 (1971)).

[c] W. Shan, S.C. Shen, and H.R. Zhu, Solid State Commun. 55, 475 (1985).

[d] D.J. Dunstan, B. Gil, and K.P. Homewood, Phys. Rev. B 38, 7862 (1988).

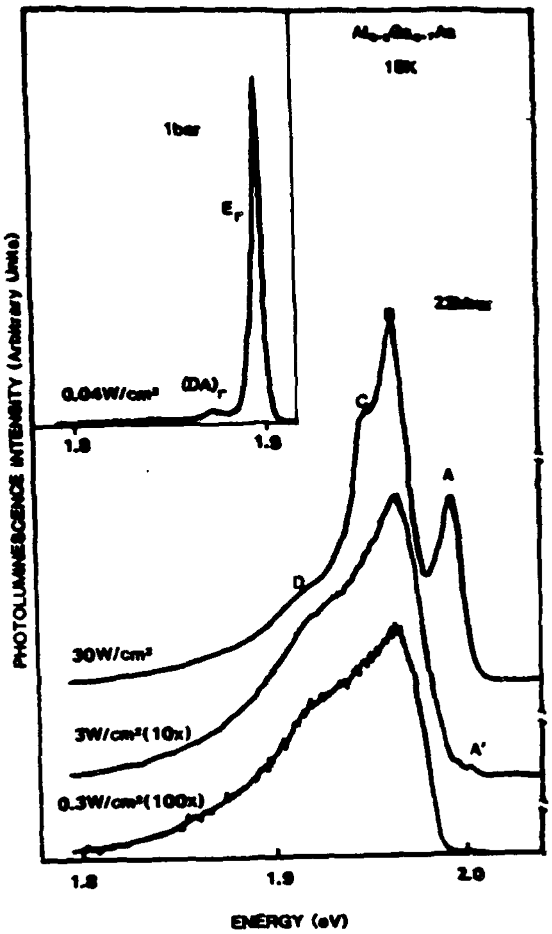


Fig. 1. Photoluminescence spectra of $Al_{0.3}Ga_{0.7}As$ under hydrostatic pressure at 15 K. At atmospheric pressure (inset), the principal feature is the bound exciton, accompanied by a few weak peaks due to donor-acceptor recombination. These features give way to deep level spectra shown at 14.3 kbar (lower panel), where we show the spectra for different exciting intensities (Roach, Chandrasekhar et.al., Ref. 10).

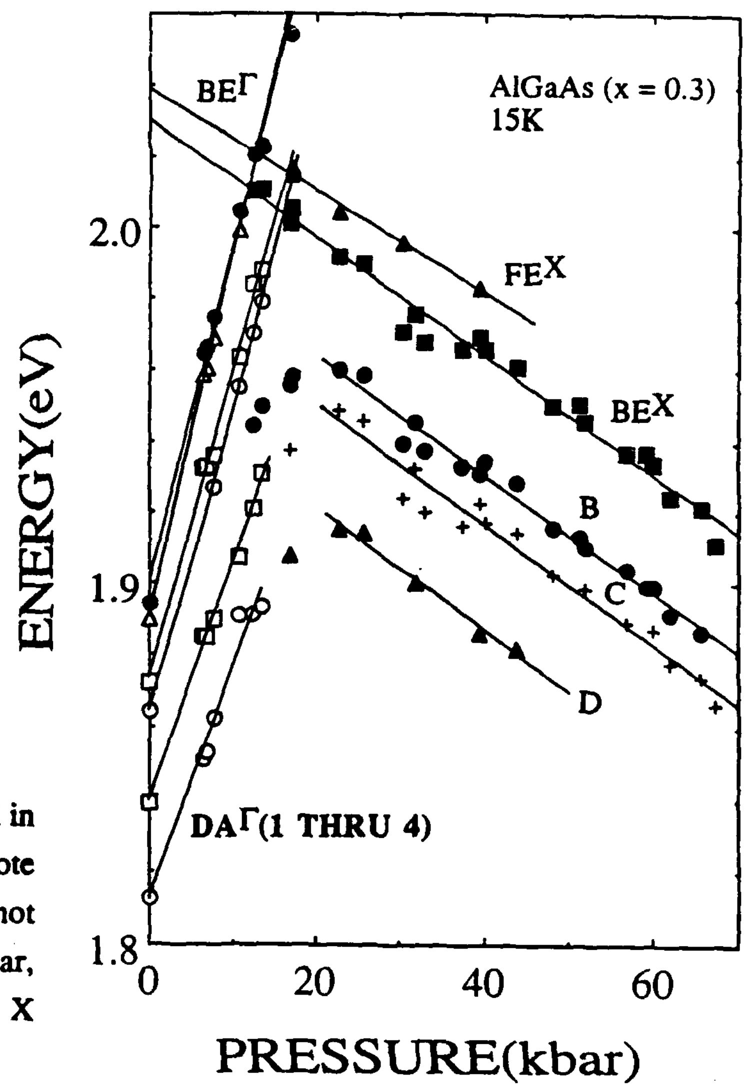


Fig. 2. The energies of the levels observed in $Al_{0.3}Ga_{0.7}As$ as a function of pressure. Note how the deep levels (B, C, and D) do not follow any conduction band in particular, except at high pressures, where they are X CB-like(Ref. 10).

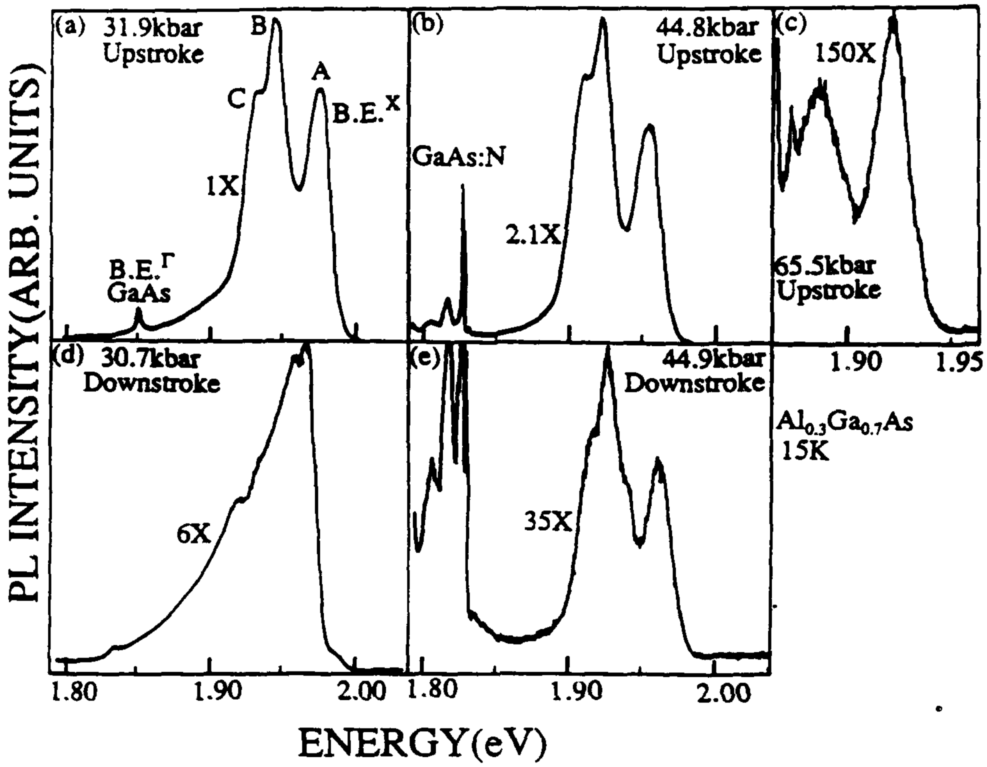


Fig. 3 PL spectra of $Al_{0.3}Ga_{0.7}As$ for a few selected pressures. Panels (a – c) show the spectra for increasing pressure (upstroke). The intensity drops sharply between 44 and 65 kbar. Panels (d) and (e) show spectra at the same pressures as (a) and (b), but for *decreasing* pressure (downstroke). PL intensities are considerably lower, but recovering as the pressure is lowered. (W.P. Roach, Ph.D. thesis, University of Missouri 1990)

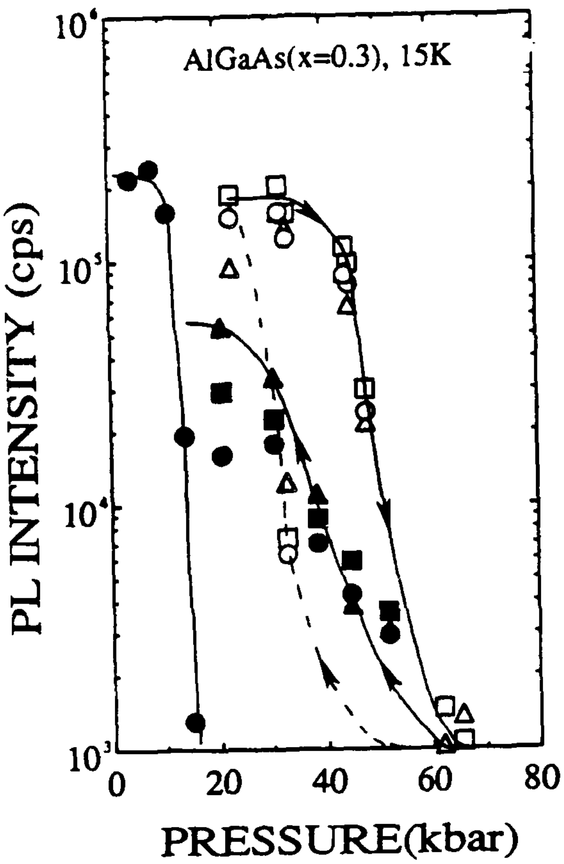
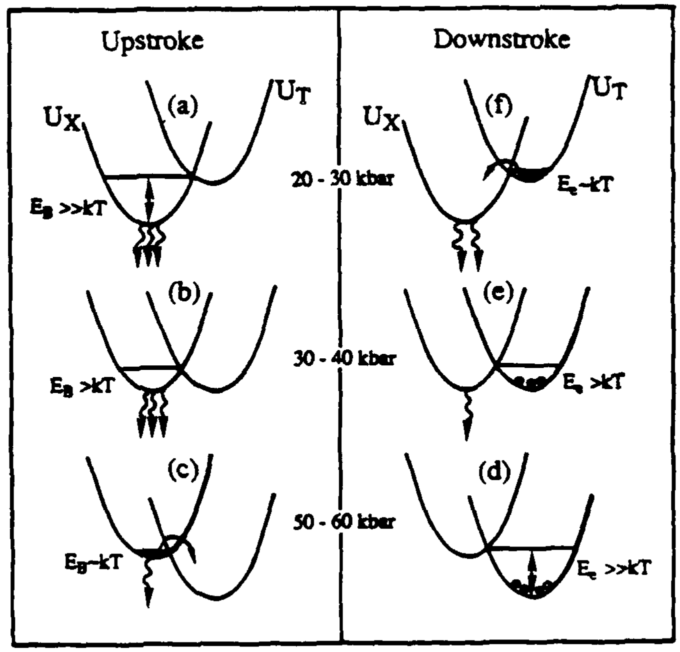


Fig. 4. The PL intensity of the peaks in $Al_{0.3}Ga_{0.7}As$ as a function of pressure. The intensity decreases around 45 kbar in the upstroke: it shows a hysteresis, finally recovering around 10 kbar. The dashed lines indicate the recovery postulated if the sample was held at 15K while the pressure was decreased. (W.P. Roach, Ph.D. thesis, University of Missouri 1990).

Fig. 5. Configuration coordinate diagram for large lattice relaxation. In the upstroke (left panels), electrons transfer to the center only when $E_B \approx kT$ (at 15K) as in panel (c), causing a sharp decline in PL intensity. Upon reducing the pressure (downstroke), the electrons do not transfer back to the CB until the emission barrier $E_e \approx kT$ (at 300K), which occurs at very low pressures, panel (f). This causes a hysteresis in the PL intensity. (Appendix I and W.P. Roach, Ph.D. thesis, University of Missouri 1990).



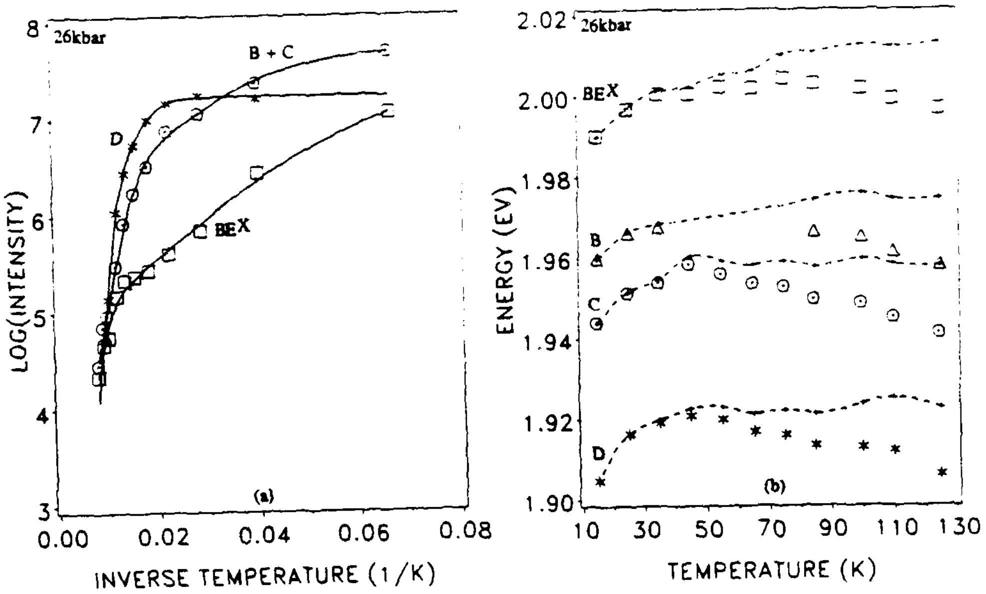


Fig. 6. (a) Arrhenius plots for the intensities of the X- related transitions in bulk AlGaAs. (b) Energies of the X- related transitions in bulk AlGaAs as a function of temperature. The dashed lines represent the temperature shifted energies, so that they are relative to the CB edge.

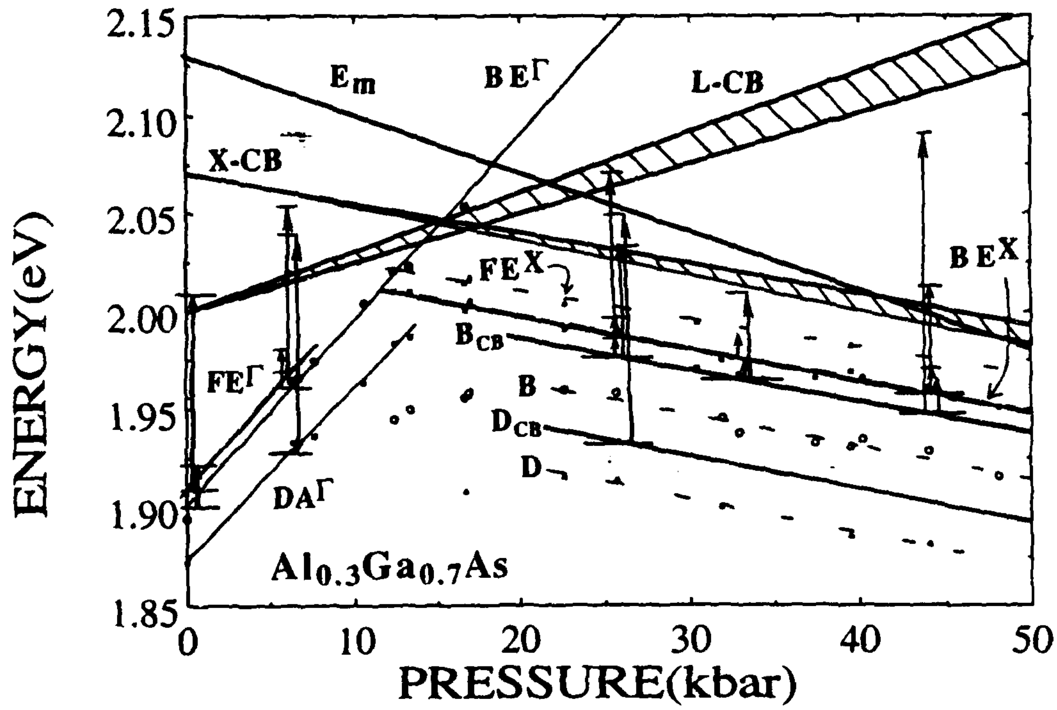


Fig. 7. Energy level diagram showing the scattering processes at several pressures, obtained from figures such as Fig. 6, and Table I. The arrows indicate the scattering processes.

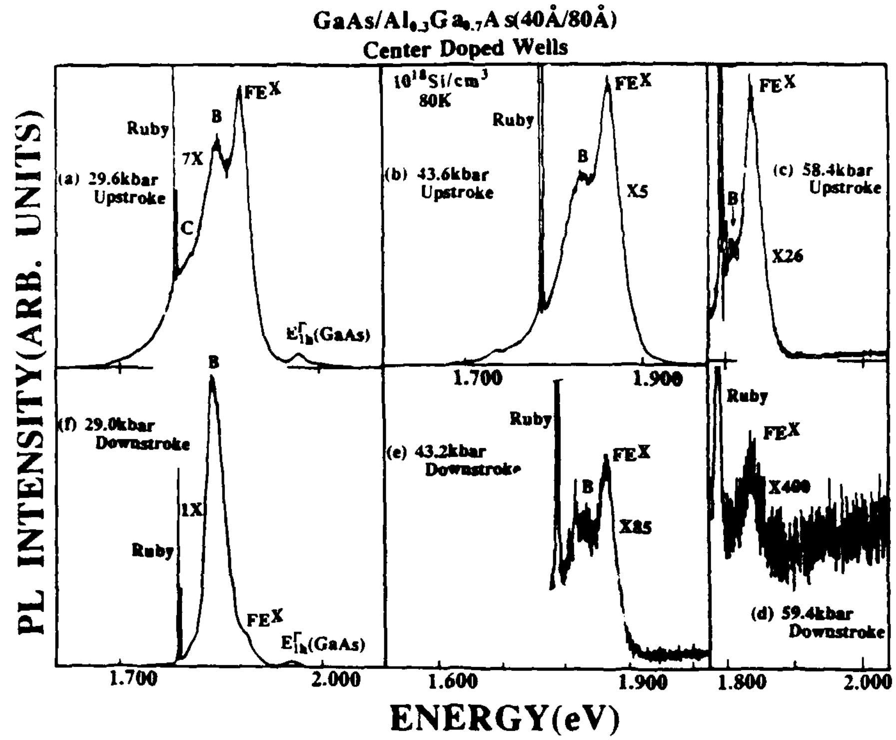


Fig. 8(a). PL spectra of the MQW staggered transitions under pressure, showing the decline in PL intensity in the upstroke, hysteresis in the downstroke and recovery at 29 kbar (downstroke). This behavior is similar to that observed in the bulk AlGaAs sample, Fig. 3. (Roach, Chandrasekhar, et. al, to appear in *Proc. of the 4th International Conference on High Pressure in Semiconductor Physics*, Porto Carras, Greece, Aug. 1990).

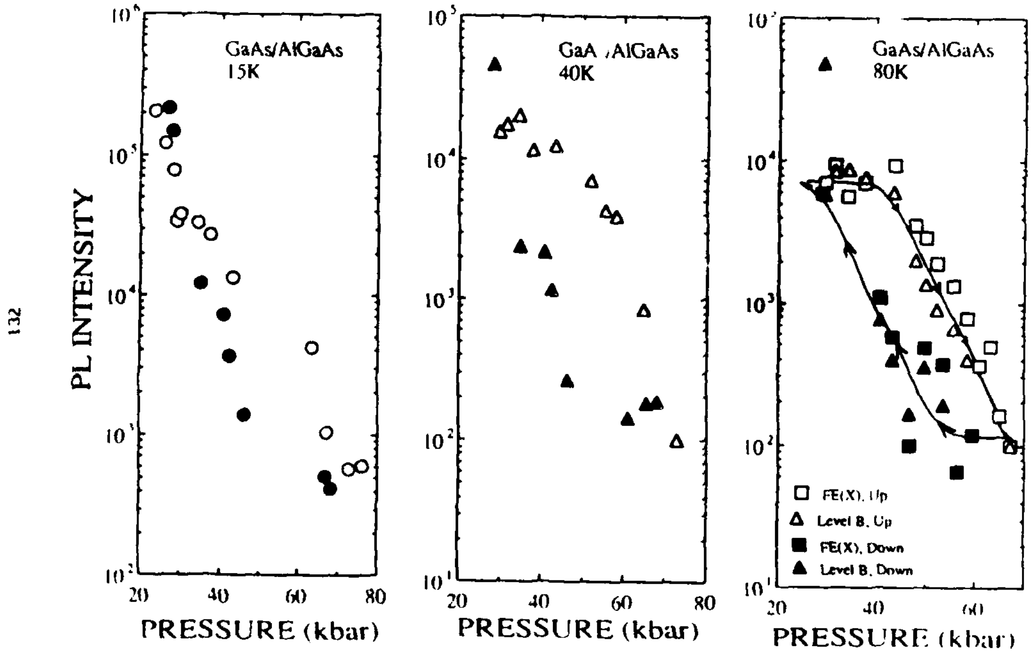


Fig. 8(b). Hysteresis curves of the intensity in the MQW sample.

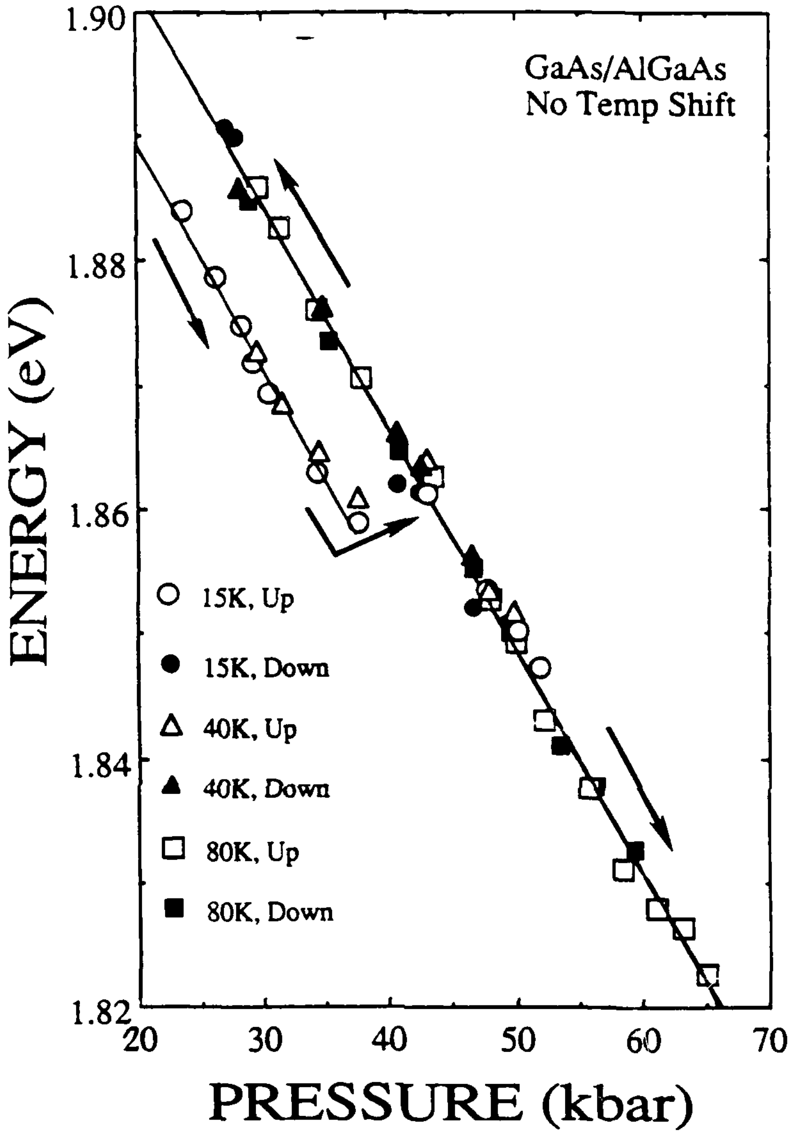


Fig. 9. Energies of the dominant staggered transition in the MQW sampleas a function of pressure. Note the switching of the energies from E_1 to E_2 at 40 kbar, for the 15 and 40K data. On the downstroke, the energies follow the shifted line.

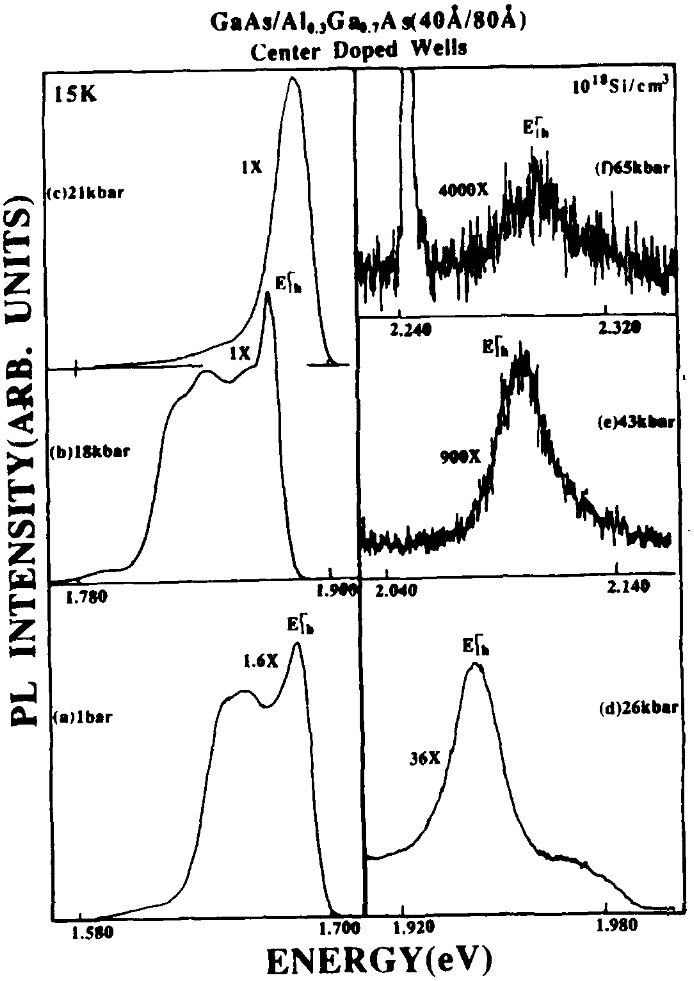


Fig. 10. Lineshapes of the direct quantum well transitions under pressure. At low pressures, the Fermi sea causes a broadening of the E^{Γ}_{1h} line. At 21 kbar, the crossing of the X CB causes all electrons to be dumped into the barrier, narrowing the E^{Γ}_{1h} line. At still higher pressures, the line broadens becauuse of mixing with the X CB.

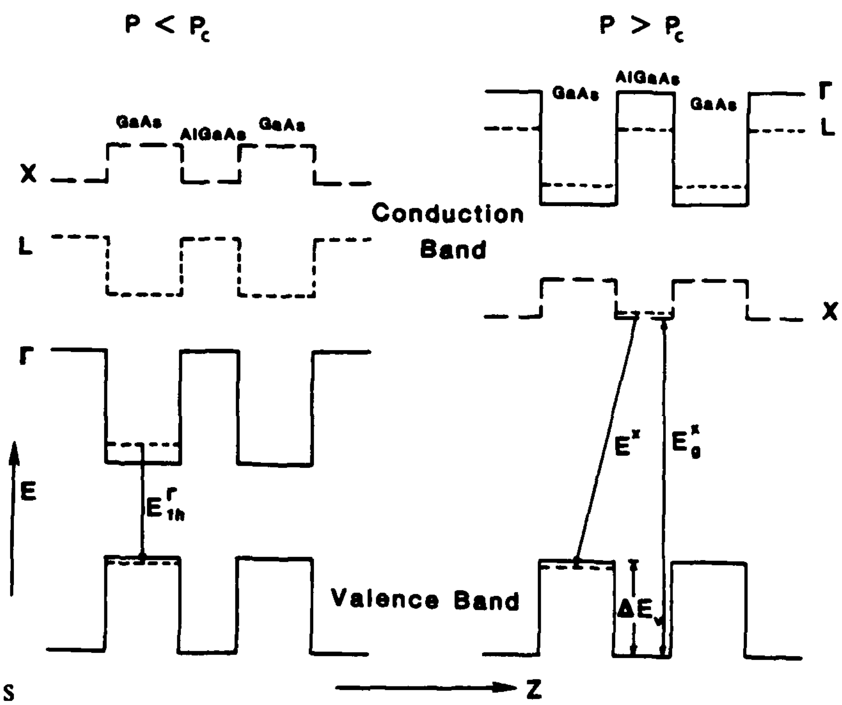


Fig. 11. Band lineups in GaAs/AlGaAs quantum wells at low pressures and above the $\Gamma - X$ crossover.

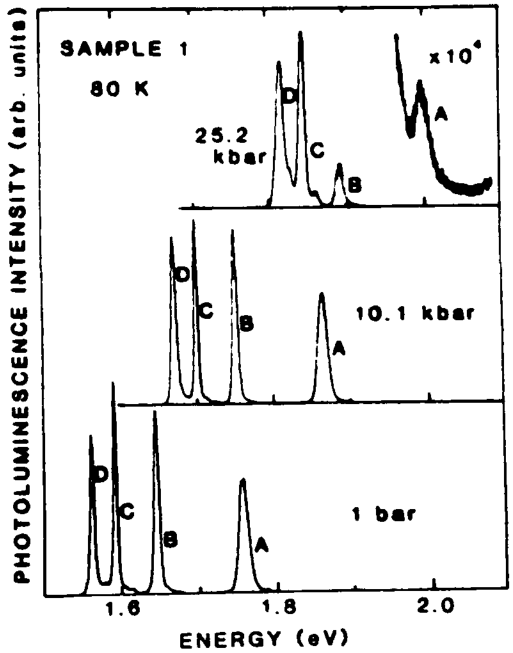


Fig. 12(a). PL spectra of GaAs/GaAlAs quantum wells at several pressures. The four major peaks correspond to heavy hole excitons (E_{1h}) in the GaAs wells, which vary in width between 26 to 150Å. (Venkateswaran, Chandrasekhar et.al., Ref. 4).

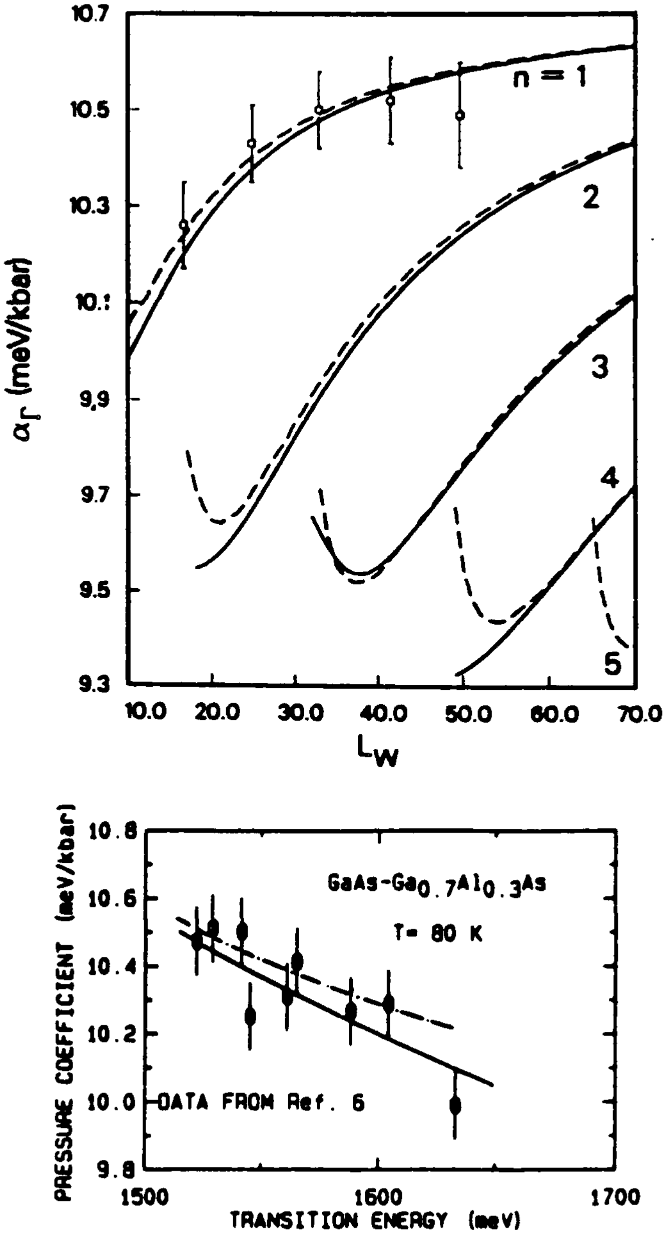
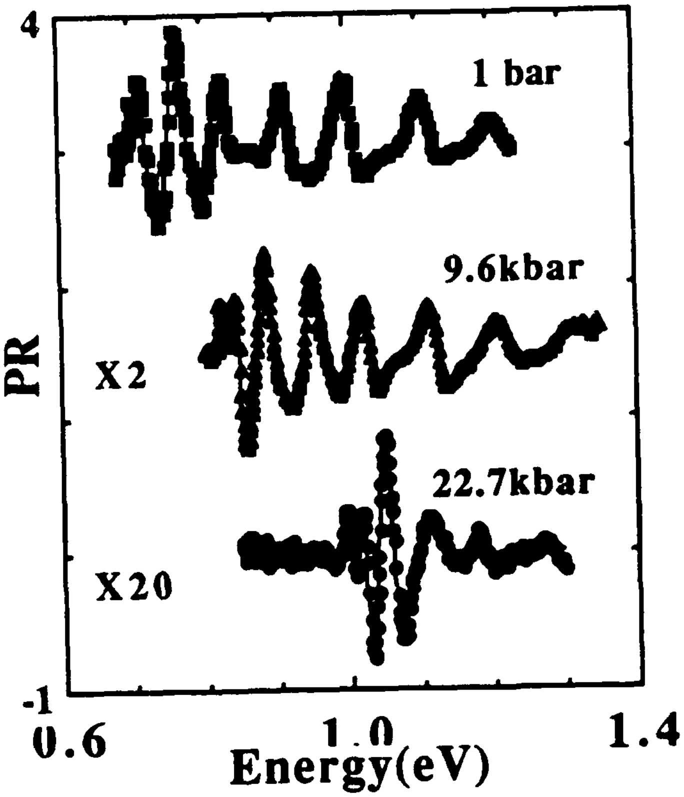
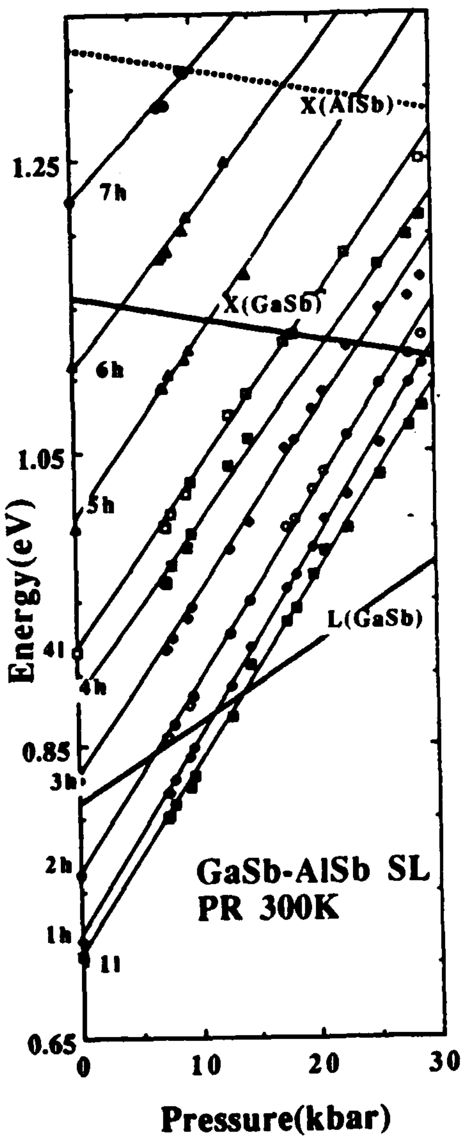


Fig. 12(b). Our experimentally obtained pressure coefficients for the E_{1h} and E_{1l} transitions in GaAs/AlGaAs (data points) are compared with theoretically calculated values using a one band Wannier orbital model (upper panel, Ting and Chang, Ref. 21); and to the calculations of Lefebvre, Gil and Matthieu (lower panel, Ref. 21). Note the decrease in the pressure coefficient with well width, and with quantum number.

Fig. 13. Photoreflectance spectra in GaSb/AlSb (Rockwell, Chandrasekhar, et.al., Ref. 6).





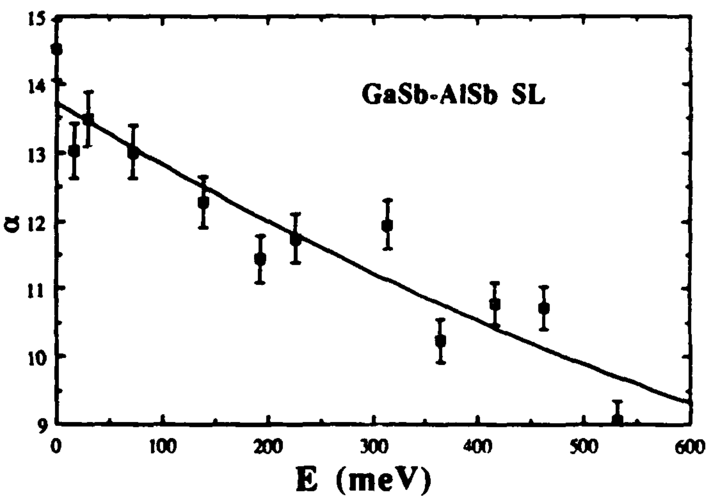


Fig. 14. Energies of quantized transitions in GaSb/AlSb as a function of pressure (left). Note the markedly lower slope of the higher quantized transitions (right), in agreement with the general trend predicted by Ting and Chang (Ref. 21) for the GaAs/AlGaAs system. (Rockwell, Chandrasekhar, et.al., Ref. 6).

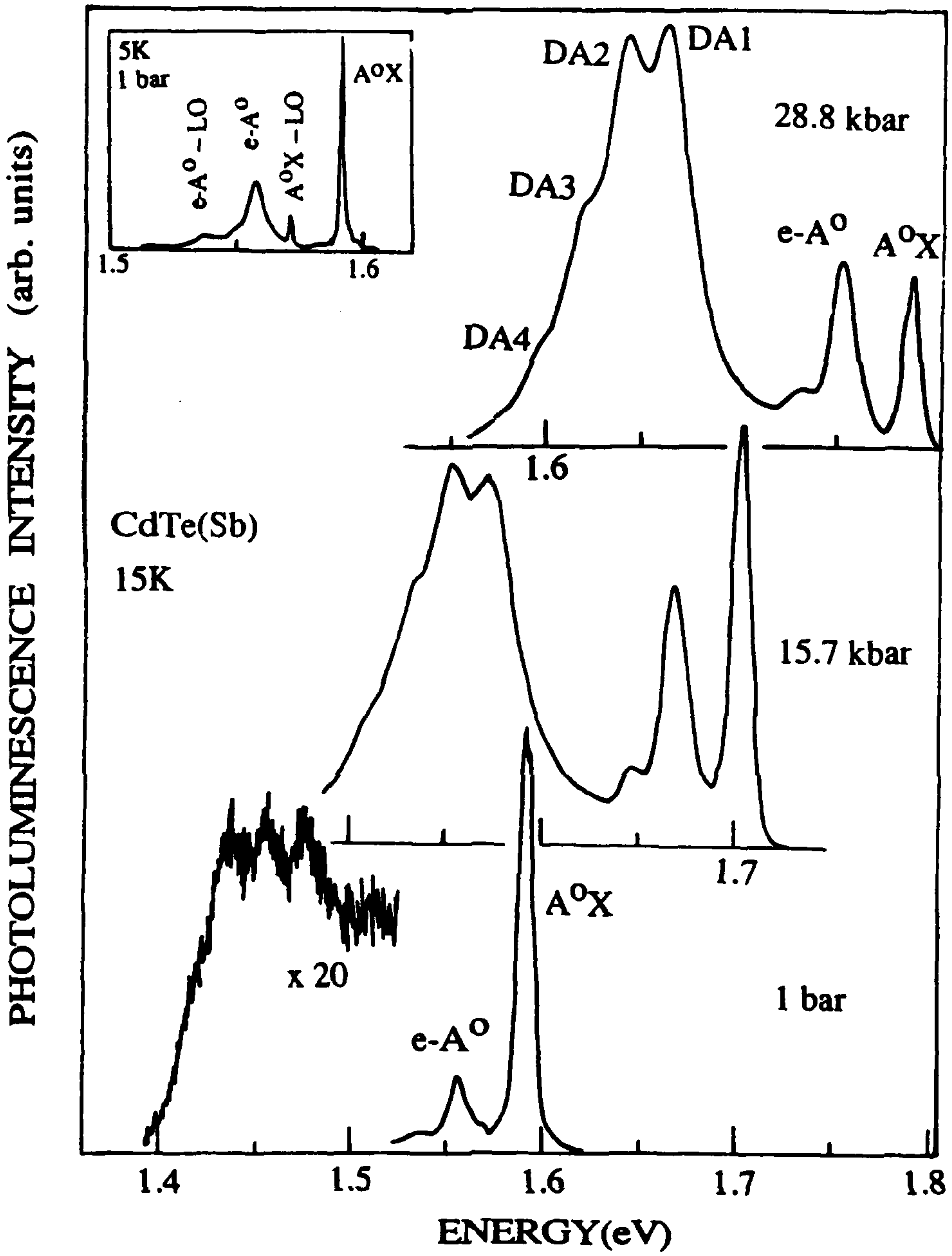


Fig. 15. PL spectra of CdTe, shown under hydrostatic pressure. The exciton ($A^{O}X$), electron to acceptor ($e\text{-}A^{O}$) and donor-acceptor (DA) transitions are typical of $Cd_{1-x}Mn_xTe$ alloys as well. (M. Prakash, M. Chandrasekhar, et. al., Phys. Rev. B, Aug 1990).

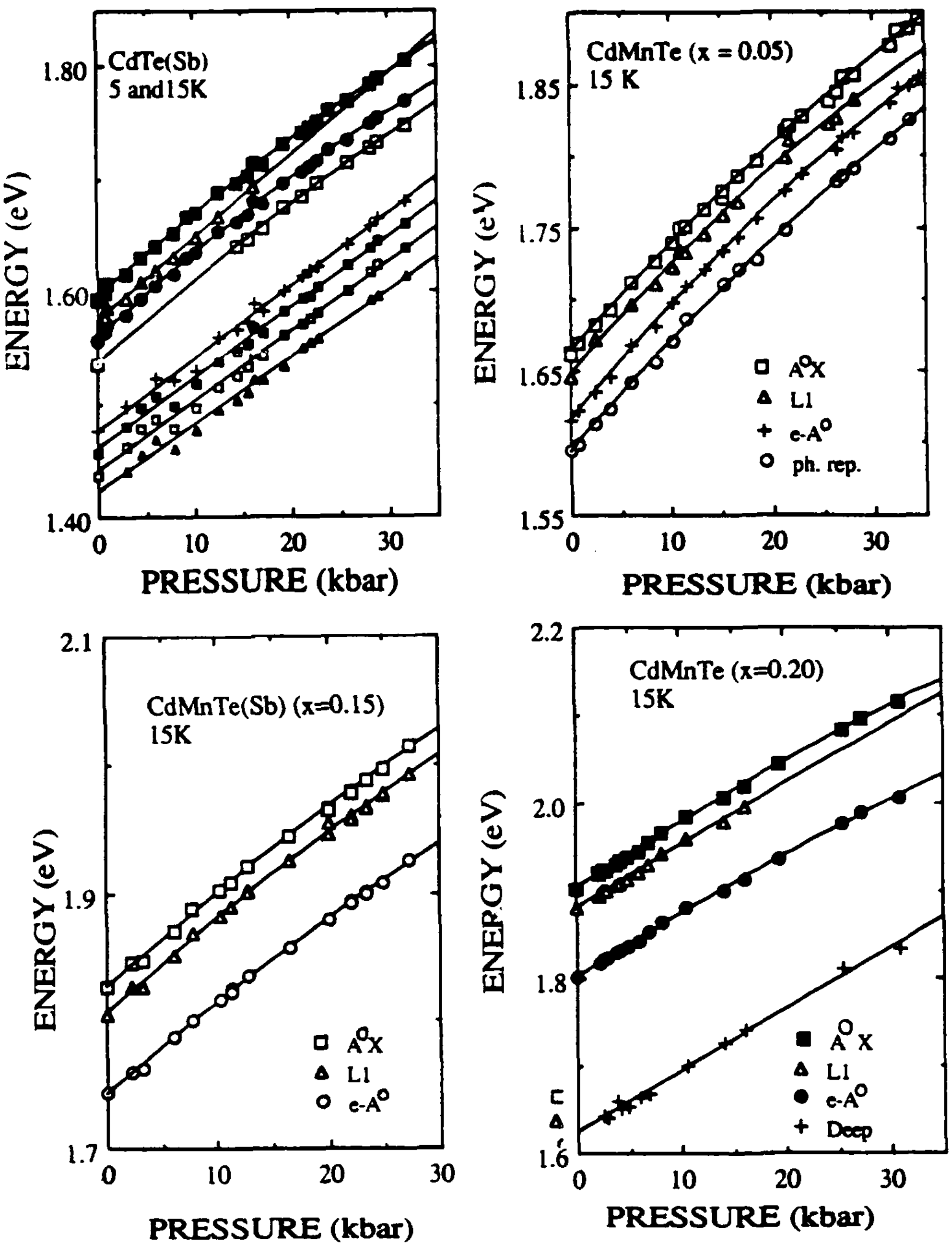


Fig. 16. Energy vs. pressure curves for $Cd_{1-x}Mn_xTe$ for x = 0.0, 0.05, 0.15, and 0.20. (M. Prakash, M. Chandrasekhar, et. al, Refs. 13, 28 and unpublished).

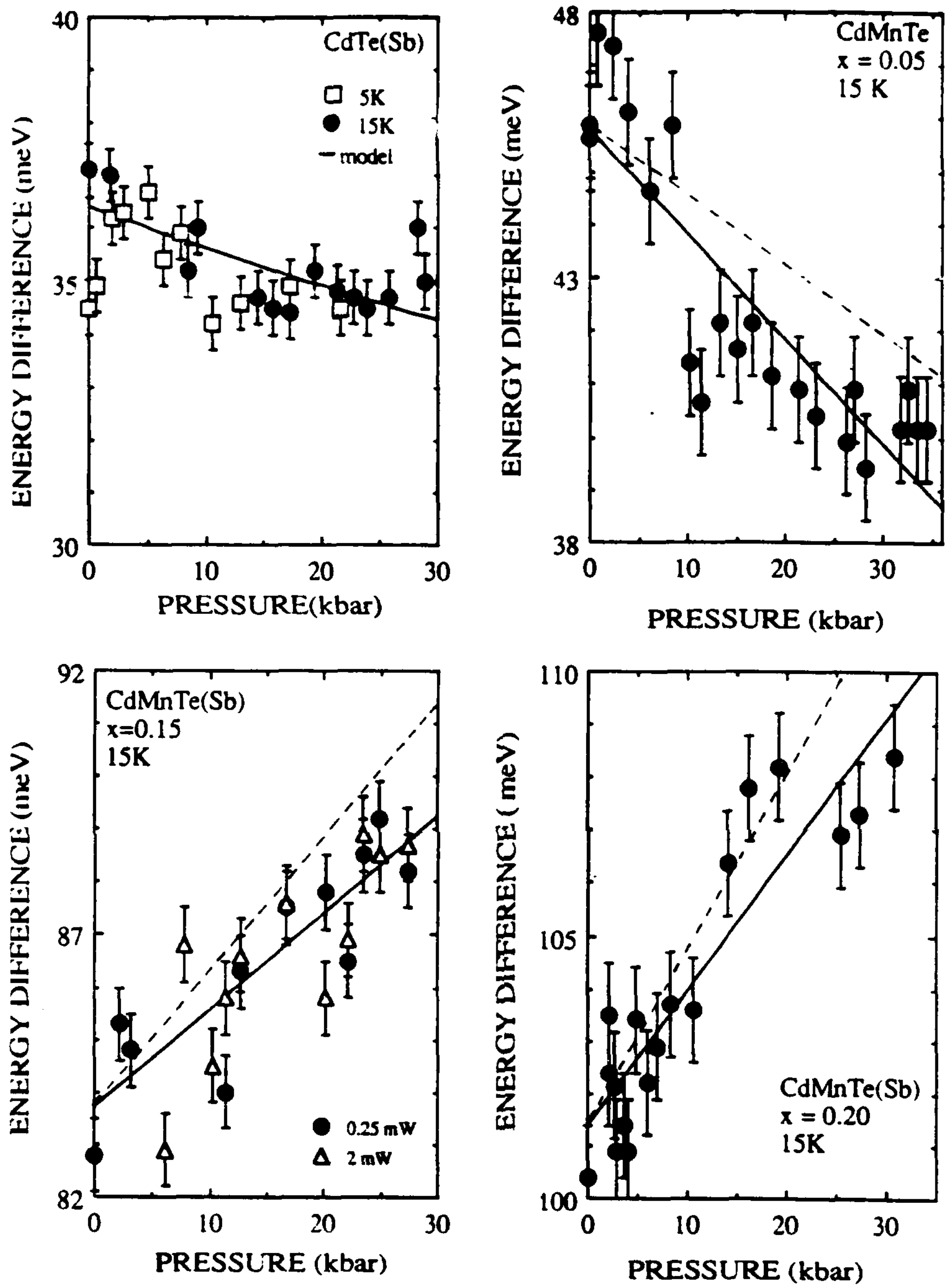


Fig. 17. Energy difference between A^0X and $e\text{-}A^0$ transitions for $Cd_{1-x}Mn_xTe$. For x = 0.0, the difference is due to Coulombic binding energies and can be accounted for via the change in the electron effective mass with pressure (solid line for x = 0.0). For the three samples with Mn, the difference energy has both Coulombic and magnetic binding energies due to the acceptor bound magnetic polaron. The magnetic parts are explained in terms of changing exchange integrals. (M. Prakash, M. Chandrasekhar, et. al., to appear in the *Proc. of the XX Intl Conf. on Phys. of Semiconductors*, Greece, Aug. 1990).

II. PERSONNEL SUPPORTED BY THE ARO GRANT

STUDENTS

William Patrick Roach, Ph.D. Aug. 1990. (supported Jan. 1987-Aug. 1990).
Thesis title: " Deep levels in semiconductors under hydrostatic pressure"
Mr. Roach conducted pressure studies on bulk GaAlAs and GaAs/AlGaAs quantum wells. He is leaving to work for the U.S. Air Force as a research biophysicist at Brooks Air Force Base, San Antonio, Texas.

John R. Whitlock, Undergraduate Research Assistant, Sep. 1988-Aug. 1989. Mr. Whitlock is spending a year in Japan as an exchange scholar, and expects to return Sep. 1990 to complete his B.S. degree.

Albert Mungo, Research Assistant, June 1, 1986 - June 30, 1987.

Erlandy Villarama, Undergraduate Research Assistant, (September 1989 - May 1990

POSTDOCTORAL FELLOW

Dr. Maneesha Prakash, Jan. 1988 - June 1990. Dr. Prakash conducted pressure studies on CdMnTe, and has left for a position as a medical physicist.

Dr. Uma Venkateswaran, June 1, 1986 - June 30, 1986.

PI

Major parts of the PI's summer salary during the summers of 1986, 1987, 1988 and 1989 were paid from the ARO grant.

III. PAPERS PUBLISHED WITH THE SUPPORT OF ARO GRANT

1. "High Pressure Study of GaAs-$Al_xGa_{1-x}As$ Quantum Wells at Low Temperatures," U. Venkateswaran, M. Chandrasekhar, H.R. Chandrasekhar, B.A. Vojak, F.A. Chambers and J.M. Meese, Superlattices and Microstructures 3, 217 (1987).

2. "Shallow and Deep Donors Related to Indirect Conduction Bands in $Al_xGa_{1-x}As$," M. Chandrasekhar, U. Venkateswaran, H.R. Chandrasekhar, B.A. Vojak, F.A. Chambers and J.M. Meese, *Proc. of the 18th International conference on the Physics of Semiconductors*, Stockholm, Aug. 1986. (Ed. O. Engstrom, World Scientific 1987) p. 943.

3. "Hydrostatic Pressure Study of GaAs-$Al_xGa_{1-x}As$ Quantum Wells at Low Temperatures," U. Venkateswaran, M. Chandrasekhar, H.R. Chandrasekhar, B.A. Vojak, F.A. Chambers and J.M. Meese, *Proc. of the 18th International Conference on the Physics of Semiconductors*, Stockholm, Aug. 1986. (Ed. O. Engstrom, World Scientific 1987) p. 621.

4. "Quantum Wells and Deep Impurity Levels Under Hydrostatic Pressure," M. Chandrasekhar, H.R. Chandrasekhar, A. Kangarlu, U. Venkateswaran, F.A. Chambers and J.M. Meese, Superlattices and Microstructures 4, 107 (1988).

5. "Pressure Studies of Impurity Levels in $Al_xGa_{1-x}As$," W.P. Roach, M. Chandrasekhar, H.R. Chandrasekhar, F.A. Chambers and J.M. Meese, Semicond. Sci. and Technol. 4, 290 (1989).

6. "Deep Levels in $Al_{0.3}Ga_{0.7}As$ Under Hydrostatic Pressure," W.P. Roach, M. Chandrasekhar, H.R. Chandrasekhar, F.A. Chambers and J.M. Meese, *Proc. of the 19th International Conference on the Physics of Semiconductors*, ed. W. Zawadski, (Institute of Physics,Warsaw, 1988) p. 1055.

7. "Spectroscopic Studies of GaAs-$Ga_{1-x}Al_xAs$ Quantum Wells Under Hydrostatic Pressure," H.R. Chandrasekhar, M. Chandrasekhar, A. Kangarlu, F.A. Chambers, B.A. Vojak and J.M. Meese, *Proc. of the 19th International Conference on the Physics of Semiconductors*, ed. W. Zawadski (Institute of Physics, Warsaw, 1988).p. 275.

8. "Electronic Transitions in Quantum Wells Under Pressure," M. Chandrasekhar, and H.R. Chandrasekhar, review article in High Pressure Research, Vol. II, ed. by M. Ross, J.M.

Besson and N. Mori (Gordon and Breach, 1989) (in preparation).

9. "High Pressure optical studies of GaSb/AlSb multiple quantum wells", B. Rockwell, H.R. Chandrasekhar, M. Chandrasekhar, F.H. Pollak, H. Shen, L.L. Chang, W.I. Wang, and L. Esaki, Surf. Sci. **228**, 322 (1990).

10. "Photoluminescence Studies of diluted magnetic semiconductors under hydrostatic pressure: CdMnTe", M. Prakash, M. Chandrasekhar, H.R. Chandrasekhar, I. Miotkowski and A.K. Ramdas, Mat. Res. Soc. Symp. Proceedings 1989 (accepted for publication).

11. "High pressure studies of GaSb/AlSb superlattices", B. Rockwell, H.R. Chandrasekhar, M. Chandrasekhar, H. Shen, F. Pollak, L.L. Chang, W.I. Wang and L. Esaki, Mat. Res. Soc. Symp. Proceedings, **160**, 751 (1989).

12. Pressure-induced Fano resonance broadening of excitons in semiconductors, S. Satpathy, M. Chandrasekhar and H.R. Chandrasekhar, submitted to Phys. Rev. Lett.

13. Electronic transitions in CdTe under pressure, M. Prakash, M. Chandrasekhar, H.R. Chandrasekhar, I. Miotkowski and A.K. Ramdas, to appear in Phys. Rev., Aug. 1990.

14. Invited paper: "Photoreflectance studies of electronic transitions in quantum well structures under high pressure", H.R. Chandrasekhar and M. Chandrasekhar, Proceedings of the SPIE Conference on Modulation Spectroscopy, San Diego, March 1990. (in press).

15. A new deep center in $Al_{0.3}Ga_{0.7}As$, W.P. Roach, M. Chandrasekhar, H.R. Chandrasekhar, and F.A. Chambers, to appear in *Proc. of the 20th International Conference on the Physics of Semiconductors*, Thessaloniki, Aug. 1990.

16. The bound magnetic polaron in CdMnTe under pressure, M. Prakash, M. Chandrasekhar, H.R. Chandrasekhar, I. Miotkowski, A.K. Ramdas, and L.R. Ram-Mohan, to appear in *Proc. of the 20th International Conference on the Physics of Semiconductors*, Thessaloniki, Aug. 1990.

17. Pressure-Induced Fano resonance of excitons in semiconductors, S. Satpathy, M. Chandrasekhar and H.R. Chandrasekhar, to appear in *Proc. of the 20th International Conference on the Physics of Semiconductors*, Thessaloniki, Aug. 1990.

18. How strain affects the valence band discontinuity in GaSb/AlSb Quantum wells, B. Rockwell, H.R. Chandrasekhar, M. Chandrasekhar, H. Shen, F. Pollak, L.L. Chang,

W.I. Wang and L. Esaki, to appear in *Proc. of the 20th International Conference on the Physics of Semiconductors*, Thessaloniki, Aug. 1990.

19. Pressure tuning of magnetic interactions in CdMnTe, M. Prakash, M. Chandrasekhar, H.R. Chandrasekhar, I. Miotkowski, A.K. Ramdas, and L.R. Ram-Mohan, to appear in *Proc. of the 4th International Conference on the High Pressure in Semiconductor Physics*, Porto Carras, Greece, Aug. 1990.

20. A pressure activated center in AlGaAs and GaAs/AlGaAs, W.P. Roach, M. Chandrasekhar, H.R. Chandrasekhar, and F.A. Chambers, to appear in *Proc. of the 4th International Conference on the High Pressure in Semiconductor Physics*, Porto Carras, Greece, Aug. 1990.

21. A new deep center in AlGaAs, W.P. Roach, M. Chandrasekhar, H.R. Chandrasekhar, and F.A. Chambers, submitted to Phys. Rev. Lett.

MANUSCRIPTS IN PREPARATION (to be submitted before Dec. 1990.)

1. Photoluminescence studies in AlGaAs under pressure (Phys. Rev.). This paper will describe part of the thesis work of W.P. Roach.

2. GaAs/AlGaAs doped quantum wells under pressure (Phys. Rev.). This paper will describe part of the thesis work of W.P. Roach.

3. The band offset in InGaAs/GaAs measured using pressure techniques (Phys. Rev. Rapid Commun.).

4. Pressure effects on the band structure and bound magnetic polarons in CdMnTe (Phys. Rev.). Experiments have been concluded and calculations for this work are in progress.

IV. HONORS AND INVITED TALKS DURING THE PERIOD OF THE GRANT

Honors

Meera Chandrasekhar: 1990 Chancellor's Award for Outstanding Research and Creativity in the Physical and Mathematical Sciences (chosen from among 200 faculty in the Physical Sciences and Engineering).

Meera Chandrasekhar: 1987 Purple Chalk Award presented for excellence in teaching by the Arts and Science Science Student Government.

W. Patrick Roach: 1990 Superior Graduate Student Award, presented by the Graduate Student Association of the University of Missouri.

Invited Talks

1. "Semiconductor Superlattices Under Pressure," Physics Department Colloquium, Kansas State University, Manhattan, KS, Sept. 18, 1986.
2. "Superlattices, Heterostructures and $Al_xGa_{1-x}As$ Under Pressure," Condensed Matter Seminar, Physics Department, Kansas State University, Manhattan, KS, Sept. 19, 1986.
3. "GaAs-$Al_xGa_{1-x}As$ Quantum Wells and $Al_xGa_{1-x}As$ Under Pressure - A Study Using Optical Techniques," Solid State Seminar, Physics Department, University of Illinois at Urbana-Champaign, Sept. 26, 1986.
4. "Effect of Hydrostatic Pressure on the Excitonic Transitions in GaAs-$Ga_{1-x}Al_xAs$ Quantum Wells," March Meeting of the American Physical Society, New York, March 16-20, 1987, Bull. Am. Phys. Soc. **32**, 458 (1987).
5. "Quantum Wells Under Hydrostatic Pressure," Third International Conference on Superlattices, Microstructures and Microdevices, Chicago, August 1987.
6. "Pressure Dependence of Electronic Transitions in Quantum Wells," Gordon Conference on High Pressure, June 27-July 1, 1988. Meriden, N.H.
7. Member of special panel on deep levels in A_3B_5 semiconductors, International Conference on High pressure in Semiconductors, Warsaw, Poland, August 1988.
8. "Semiconductor Heterostructures under pressure", Colloquium at the Physics Department, University of Notre Dame, Dec 1, 1988.
9. "Semiconductors and their heterostructures under pressure", Condensed Matter Seminar, Physics Department, Purdue University, Oct 6, 1989.
10. "Photoreflectance studies of electronic transitions in quantum well structures under high pressure", H.R. Chandrasekhar and M. Chandrasekhar, SPIE Conference on Modulation Spectroscopy, San Diego, March 1990.

V. CONTRIBUTED PRESENTATIONS SUPPORTED BY ARO GRANT

1. "Shallow and Deep Donors Related to Indirect Conduction Bands in $Al_xGa_{1-x}As$," M. Chandrasekhar, U. Venkateswaran, H.R. Chandrasekhar, B.A. Vojak, F.A. Chambers and J.M. Meese, 18th International Conference on the Physics of Semiconductors, Stockholm, Aug. 1986.

2. "High Pressure Study of GaAs-$Ga_{1-x}Al_xAs$ Quantum Wells at Low Temperatures," U. Venkateswaran, M. Chandrasekhar, H.R. Chandrasekhar, B.A. Vojak, F.A. Chambers and J.M. Meese, 18th International Conference on the Physics of Semiconductors, Stockholm, Aug. 1986, and the Second International Conference on Superlattices and Microstructures, Goteborg, Sweden, Aug. 1986.

3. "Photoreflectance Spectroscopy of GaAs-$Al_xGa_{1-x}As$ Quantum Wells Under Hydrostatic Pressure," A. Kangarlu, H.R. Chandrasekhar, M. Chandrasekhar, F.A. Chambers, B.A. Vojak and J.M. Meese, 18th International Conference on the Physics of Semiconductors, Stockholm, Aug. 1986, and the Second International Conference on Superlattices and Microstructures, Goteborg, Sweden, Aug. 1986.

4. "Photoreflectance Studies of GaAs-$Al_xGa_{1-x}As$ Quantum Wells Under High Pressure,"A. Kangarlu, H.R. Chandrasekhar, M. Chandrasekhar, Y.M. Kapoor, B.A. Vojak, F.A. Chambers, J.M. Meese, March Meeting of the American Physical Society, New York, 1987, Bull. Am. Phys. Soc. **32**, 471 (1987).

5. "Deep Donor States in $Al_{0.3}Ga_{0.7}As$ Under Hydrostatic Pressure," W.P. Roach, M. Chandrasekhar, H.R. Chandrasekhar, F.A. Chambers and J.M. Meese, March Meeting of the American Physical Society, New Orleans, LA, 21-25 March, 1988, Bull. Am. Phys. Soc. **33**, 424 (1988).

6. "High Pressure Photoreflectance Studies of GaAs-$Ga_{1-x}Al_xAs$ Quantum Wells," H.R. Chandrasekhar, M. Chandrasekhar, A. Kangarlu, Y.M. Kapoor, B.A. Vojak, F.A. Chambers and J.M. Meese, March Meeting of the American Physical Society, New Orleans, LA, 21-25 March, 1988, Bull. Am. Phys. Soc. 33, 424 (1988).

7. "Pressure Studies of Impurity Levels in $Al_xGa_{1-x}As$," W.P. Roach, M. Chandrasekhar, H.R. Chandrasekhar, F.A. Chambers and J.M. Meese, International Conference on High Pressures in Semiconductor Physics, Warsaw, August 1988.

8. "Deep Levels in $Al_{0.3}Ga_{0.7}As$ Under Hydrostatic Pressure," W.P. Roach, M. Chandrasekhar, H.R. Chandrasekhar, F.A. Chambers and J.M. Meese, 19th International Conference on the Physics of Semiconductors, Warsaw, August 1988.

9. "Spectroscopic Studies of GaAs-$Ga_{1-x}Al_xAs$ Quantum Wells Under Hydrostatic Pressure," H.R. Chandrasekhar, M. Chandrasekhar, A. Kangarlu, F.A. Chambers, B.A. Vojak and J.M. Meese, 19th International Conference on the Physics of Semiconductors, Warsaw, August 1988.

10. "A hydrostatic pressure study of deep donor states in $Al_{0.3}Ga_{0.7}As$" W. P. Roach, M. Chandrasekhar, H.R. Chandrasekhar, F.A. Chambers and J.M. Meese, March Meeting of the American Physical Society, St. Louis, Bull. Am. Phys. Soc., **34**, 683 (1989).

11. "Fano Resonance Broadening of Quantum Well levels in GaAs/GaAlAs", S. Satpathy, M. Chandrasekhar, and H.R. Chandrasekhar, March Meeting of the American Physical Society, St. Louis, Bull. Am. Phys. Soc., **34**, 682 (1989).

12. "Photoreflectance Spectroscopy of Strained layer GaSb/AlSb superlattices", B. Rockwell, H.R. Chandrasekhar, M. Chandrasekhar, F.H. Pollak, H. Shen, L.L. Chang, W.I. Wang, L. Esaki, March Meeting of the American Physical Society, St. Louis, Bull. Am. Phys. Soc., **34**, 830 (1989).

13 "Photoluminescence Studies of diluted magnetic semiconductors under hydrostatic pressure: CdMnTe", M. Prakash, M. Chandrasekhar, H.R. Chandrasekhar, I. Miotkowski and A.K. Ramdas, Fall Meeting of the Materials Research Society, Boston, Nov. 26 - Dec 1, 1989.

14. "High pressure studies of GaSb/AlSb superlattices", B. Rockwell, H.R. Chandrasekhar, M. Chandrasekhar, H. Shen, F. Pollak, L.L. Chang, W.I. Wang and L. Esaki, Fall Meeting of the Materials Research Society, Boston, Nov. 26 - Dec 1, 1989.

15. "Deep donor states in AlGaAs under hydrostatic pressure", W.P. Roach, M. Chandrasekhar, H.R. Chandrasekhar and F.A. Chambers, March Meeting of the American Physical Society, Anaheim, Bull. Am. Phys. Soc. **35**, 414 (1990).

16. "Does the valence band discontinuity in GaSb/AlSb Multiple Quantum Wells depend on strain?", B. Rockwell, H.R. Chandrasekhar, M. Chandrasekhar, H. Shen, F. Pollak, L.L. Chang, W.I. Wang and L. Esaki, March Meeting of the American Physical Society, Anaheim, Bull. Am. Phys. Soc. **35**, 212 (1990).

17. "Photoluminescence Studies of Diluted Magnetic Semiconductors under Hydrostatic Pressure: $Cd_{1-x}Mn_xTe$", M. Prakash, M. Chandrasekhar, H.R. Chandrasekhar, I. Miotkowski and A.K. Ramdas, March Meeting of the American Physical Society, Anaheim, Bull. Am. Phys. Soc. **35**, 662 (1990).

18. A new deep center in $Al_{0.3}Ga_{0.7}As$, W.P. Roach, M. Chandrasekhar, H.R. Chandrasekhar, and F.A. Chambers, *20th International Conference on the Physics of Semiconductors*, Thessaloniki, Aug. 1990.

19. The bound magnetic polaron in CdMnTe under pressure, M Prakash, M. Chandrasekhar, H.R. Chandrasekhar, I. Miotkowski, A.K. Ramdas, and L.R. Ram-Mohan, *20th International Conference on the Physics of Semiconductors*, Thessaloniki, Aug. 1990.

20. Pressure-Induced Fano resonance of excitons in semiconductors, S. Satpathy, M. Chandrasekhar and H.R. Chandrasekhar, *20th International Conference on the Physics of Semiconductors*, Thessaloniki, Aug. 1990.

21. How strain affects the valence band discontinuity in GaSb/AlSb Quantum wells, B. Rockwell, H.R. Chandrasekhar, M. Chandrasekhar, H. Shen, F. Pollak, L.L. Chang, W.I. Wang and L. Esaki, *20th International Conference on the Physics of Semiconductors*, Thessaloniki, Aug. 1990.

22. Pressure tuning of magnetic interactions in CdMnTe, M. Prakash, M. Chandrasekhar, H.R. Chandrasekhar, I. Miotkowski, A.K. Ramdas, and L.R. Ram-Mohan, *4th International Conference on the High Pressure in Semiconductor Physics*, Porto Carras, Greece, Aug. 1990.

23. A pressure activated center in AlGaAs and GaAs/AlGaAs, W.P. Roach, M. Chandrasekhar, H.R. Chandrasekhar, and F.A. Chambers,*4th International Conference on the High Pressure in Semiconductor Physics*, Porto Carras, Greece, Aug. 1990.

VIII. APPENDIX I

A NEW DEEP CENTER IN $Al_{0.3}Ga_{0.7}As$

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Amoco Technology Corporation, Naperville, IL 60566

ABSTRACT

We report the observation of a new trapping center in $Al_{0.3}Ga_{0.7}As$, which becomes active under hydrostatic pressure. The center becomes active at ~45 kbar, has an unusually deep emission barrier. It quenches all radiative transitions and causes a hysteresis in the intensity which we interpret via a lattice relaxation model. It is neither the DX nor the SD center, and is probably related to a donor.

Manuscript submitted to Phys. Rev. Lett.

Substitutional group IV and group VI dopants in $Al_xGa_{1-x}As$ give rise to two types of electronic states: a shallow effective mass level and a more localized level, labelled DX, arising from lattice distortion near the donor. The relative stability of the two states depends on alloy composition. Below $x = 0.22$, the localized level is a resonance above the conduction band minimum (CBM). Above $x = 0.22$ DX becomes a bound state, more stable than the shallow donor state. The application of hydrostatic pressure for $x<0.22$ can move DX from a resonant to a stable state. This shallow-deep transition occurs between 20 and 30 kbar in GaAs.

We report the observation of a *new* localized state in $Al_{0.3}Ga_{0.7}As$ under hydrostatic pressure, which is in some ways reminiscent of the DX center. It is resonant above the X - CBM at pressures below 40 kbar. At higher pressures it becomes stable and captures all electrons that are photoexcited into the X - CBM, causing a *sharp drop in the intensity* of radiative transitions. Upon reducing the pressure, the intensity does *not recover* despite thermal cycling to room temperature, indicating an *unusually deep emission barrier*, much deeper than that of DX. The intensity finally recovers at very low pressures (~ 10 kbar).

We have repeatedly seen both the decline in intensity and the hysteresis in bulk $Al_{0.3}Ga_{0.7}As$(~2×10^{15} Si/cm^{-3}) and in a GaAs / $Al_{0.3}Ga_{0.7}As$ (40Å/80Å) multiple quantum well (MQW) sample. At pressures above the Γ-X crossover, radiative recombination is observed from the X- CB of AlGaAs barriers to the VB of the GaAs wells. The initial states of the electron are the same for this staggered transition as in bulk AlGaAs, and, as expected, they show behavior similar to the bulk.

Both samples were MBE grown on a GaAs substrate. Photoluminescence (PL) at 15K was excited using principally 5145Å radiation from an Ar^+ laser. Measurements under pressure were made in a diamond anvil cell with argon as the pressure transmitting medium. Ruby flourescence was used as the in-situ manometer.

$Al_{0.3}Ga_{0.7}As$ is a direct gap semiconductor. Under pressure, the energy of the Γ – CBM increases while that of the X CBM decreases, crossing around 13 kbar. Well below the Γ – X crossing, the PL spectrum consists of a sharp, intense peak due to the neutral donor bound exciton D^oX, and weaker peaks due to donor-acceptor recombination, DA^Γ, at lower energies. Around 9 kbar, new peaks appear below D^oX. These peaks show considerable bowing around crossover, indicative of Γ-L-X mixing, and then move downward in energy with pressure with a pressure coefficient of –1.6 meV/kbar. The energies of all observed under pressure are shown in Fig. 1(f). A typical spectrum beyond the Γ–X crossover is shown in Fig. 1(a) at 31 kbar. The high energy peak labelled A is the exciton bound to the X CB BE^X, while the broad peaks labelled B,C and D are due to donor-acceptor recombination. The peaks are quite intense till about 45 kbar. Beyond 45 kbar, the intensity drops steeply, decreasing by more than two orders of magnitude at ~ 65 kbar (Fig. 2).

The unusual feature occurs when the pressure is reduced. The intensity of the PL spectrum *does not recover* at the same pressure at which it declined. An example is seen in panels (d) and(e) of Fig. 1, where we show the spectum at almost the same pressures as in panels (a) and (b), but for *decreasing* pressure (downstroke). Pressurizing the sample to 65 kbar and decreasing the pressure reduced the intensity by a factor of 17 at 44 kbar, though the peak positions and PL lineshape remain similar. The ratio improves to a factor of six at 31 kbar, and is about a factor of two at very low pressures of ~ 6 kbar (for BE^{Γ}). In the MQW sample, the E^{Γ}_{1h} transition also loses intensity at 70 kbar, but recovers its intensity on the same path, while the staggered transitions show a hysteresis.

A decrease in PL intensity due to level crossings is a common feature. In GaAs it was used to establish the Γ–X crossover pressure: when the bands cross, electrons scatter preferentially to the X CB, and Γ–VB recombination intensity decreases by several orders of magnitude. We see this process when the Γ and X CB's cross in AlGaAs in the low pressure region of Fig. 2. Another example is the crossing of the nitrogen deep levels in GaAs with the X CB near 70 kbar. When the N-levels become resonant with the X CB, their intensity drops. In both cases, however, the transitions reappear upon decreasing the pressure with the same intensity and at the same pressure as in the upstroke, unlike the levels we observe. The hysteresis in the intensity, then, rules out a simple level crossing.

Another cause for a decrease in PL intensity is dislocations occuring near a structural phase transition, seen in several direct gap materials such as CdS and CdTe. In AlGaAs, the phase transition takes place at ~150 kbar, and is too far away to cause dislocations at 70 kbar. Another characteristic of dislocations is that releasing the pressure does not allow the PL intensity to recover: since we find near total recovery near 10 kbar, we conclude that dislocations are not the cause of the effect we observe.

The simplest model that describes the effect we observe is a trapping center with lattice relaxation. Since the hysteresis is so large, we use the model for a large lattice relaxation. A schematic model is shown on a configuration coordinate diagram in Fig. 3. The minimum in the potential energy for the center (U_T) is displaced from that of the X CB (U_X). We assume that the X CB is the feeder level for the deep levels B, C, and D in bulk AlGaAs and for the staggered MQW transitions. Scattering to U_T can occur thermally (via E_B) or via an intermediate state as has been postulated for the DX center. Our data does not make it possible to differentiate between the two. For simplicity, therefore, we will assume a level E_m which is the level mediating the transfer of electrons from U_X to U_T (either the intermediate state or the energy defining E_B), whose separation ΔE from the bottom of U_X varies linearly with pressure.

At low pressures (20 to 30 kbar) the U_T is high above the X CB, as is E_I. ΔE >> kT (at 15K, the temperature at which electrons are photoexcited into X), no electrons scatter to the trap and strong recombination is seen (Fig. 3(a)). At slightly higher pressures (say, ~ 40 kbar), although the bottoms of the potential energy curves line up, a situation akin to level crossing if there were no lattice relaxation, there is still no transfer of electrons into the trap because $\Delta E > kT$ (Fig. 3(b)). At still higher pressures (~ 50 kbar), U_T is well below U_X, $\Delta E \approx kT$, and electrons transfer to the trap and PL intensity decreases sharply (Fig. 3(c)). At higher pressures of ~ 65 kbar, all electrons transfer to the trap, and PL intensities die below experimentally detectable levels.

We fit the upstroke PL intensity I as a function of pressure P to the function

$$I = \frac{I_o}{1 + A\, e^{\Delta E / kT}} + I_{min} \qquad (1)$$

where $\Delta E = (\alpha_X - \alpha_m)(P - P_T)$ is the energy separation between the mediating level and the X CB, α_m and α_X are their respective pressure coefficients, P_T is the crossover pressure, defined by the pressure at which the energy difference between E_m and the bottom of $U_X \approx kT$. Fitting the upstroke data to this equation, we obtain $P_T = 45$ kbar, and $(\alpha_X - \alpha_m) = 0.8 \pm 0.1$ meV / kbar, giving $\alpha_m = -2.4 \pm 0.3$ meV/kbar, since $\alpha_X = -1.6 \pm 0.2$ meV / kbar. Similar fits to the MQW sample yield $P_T = 47 \pm 1$ kbar, and $\alpha_m = -3.5 \pm 0.3$ meV/kbar, values from two different samples that are within two standard deviations of each other.

On the downstroke, when the pressure is reduced back near 50 kbar where the intensity initially decreased (Fig. 3(d)), few electrons are present, making for low PL intensity. At lower pressures (say, ~ 40 kbar), where previously the PL intensity was high since the electrons could not enter the trap, now the reverse is true: most of the electrons are in the trap, and the emission barrier, E_e is still larger than kT, preventing strong recombination (Fig. 3(e)). Finally, at very low pressures (~ 10 – 20 kbar, Fig. 3(f)), $E_e \approx 26$ meV, the center empties out and PL intensity recovers to close to pre-pressurizing levels.

This scenario would yield a sharp recovery curve as indicated by the dashed lines if the temperature was held at 15K while the pressure was reduced. However, some trap emptying occurs because we cycle our temperature to 300K in order to change the pressure. Above 46 kbar, a few electrons transfer out of U_T into U_X and the VB. These electrons are photoexcited into U_X at 15K, where most of them transfer back to U_T, but a few undergo radiative recombination. This makes the downstroke curve smoother than the upstroke. Below 46 kbar, the photoexcited electrons do not transfer back to U_T since they have too high a barrier E_B to scatter into the trap, however, since some electrons are still in U_T, PL intensity has not yet recovered. Our data is not sensitive enough to separate the competing processes above 46 kbar, so we assume the dominant process and fit the downstroke data to Eq. (1), with $\Delta E = \Delta\alpha\,(P - P_R)$, and T =300K. We obtain a crossover pressure of 30 ± 3 kbar for the two samples, consistent with the qualitative picture of the hysteresis. Because of the competing processes, we do not believe that the $\Delta\alpha$'s are reliable. However, we get a rough idea by comparing the values of $\Delta\alpha/kT$. In the upstroke (T = 15K), $\Delta\alpha/kT = 15 \times 10^{-3}$, while it is 2×10^{-3} in the downstroke (T = 300K), indicating that the pressure dependence of the trapping process is ten times larger than the rocovery. It is possible, then, that recovery occurs via E_e, while trapping occurs via an intermediate state.

Keeping the trapping and recovery pressures of 45 and 30 kbar, respectively, in mind, We now look at the energies of the main peak in the staggered transition in the MQW sample. These are shown in Fig. 2(b) for temperatures of 15, 40 and 80K, open (filled) symbols for up(down)strokes. This sample had a center doped well ($2x10^{18}$ Si/cm^{3}). When the E^{Γ}_{1h} and AlGaAs X bands cross and the staggered transitions are observed, there are electrons spill into the AlGaAs and recombine with holes in GaAs via a staggered transition that we call E_1, but only up to ~40 kbar. Above 40 kbar E_1 abruptly disappears, and a new peak at a slightly higher energy, E_2, appears. E_2 continues to shift at –1.6 meV/kbar, and is visible till about 50 kbar,beyond which it is masked by the GaAs:N levels. Pressure was increased to 70 kbar and then reduced. On the downstroke, E_2 peak emerges from the GaAs:N levels near 50 kbar, but *continues* to follow the E_2 path to pressures of 30 kbar. E_1 was never recovered, even at pressures at which it had been seen in the upstroke. In contrast, at a higher temperature of 80K, E_1 is the only level that can be observed, both in the up- and downstrokes.

It is reasonable to assume that at 80K E_2 is the free exciton associated with the confined level in the X CB. Its energy is consistent with previous studies[5] at 80K of other undoped MQW samples. When corrected for the temperature shift of the band gaps, E_1 at 15K is ≈24 meV lower in energy. The switching of radiative transitions at 15 and 40K from E_1 to E_2 at 40 kbar in the upstroke suggests that the effect is directly related to the trapping center. It is possible that the availability of a large number of electrons makes a lower energy transition viable in the upstroke below 40 kbar. When the electrons are trapped by the center beyond 40 kbar, the level is no longer available. Nor is it available in the downstroke, until recovery takes place (<30 kbar). The exact identification of E_1 is not clear at present, and its energy may involve screening effects due to 10^{18} electrons. At 80K, the thermal smearing of the Fermi sea makes the free exciton E_2 the only viable state both in the up- and downstrokes.

The energy behavior is consistent with the hyteresis in the intensity, and suggests that a donor state is involved in the trapping process. This is reinforced by the fact that its crossing with the X CB determines the decline in intensity, both in bulk and MQW samples. It is an energy level that is *above* the X CB at ambient pressures, and crosses to come below it at higher pressures. (If it were below the X CB at low pressures, it would trap electrons efficiently, and PL intensity would rise when it crossed the X CB at high pressures, which is contrary to our experimental observations.) It is not the DX center: the DX is below the X CB at all pressures, and its emission barrier is sufficient to empty it at 300K. E_e for this new center is > 300K at high pressures. A level that does cross X at high pressures is the recently observed shallow donor SD level. However, its E_e is less than that of the DX center, which rules it out as this new center.

In conclusion, we have observed a new center in $Al_{0.3}Ga_{0.7}As$ under hydrostatic pressure. This center has lattice relaxation, and forms an efficient electron trap. It produces a hysteresis in the PL intensity, which does recover at low pressure. The hysteresis rules out a simple level crossing, and the recovery of PL rules out dislocations. The energy of the center is higher than that of the X CB at ambient pressures by about 60 ± 25 meV, and it is neither the DX or the SD center. The microscopic origin of the center is not known at present. Annealing experiments and investigations of samples with other Al compositions are currently under way.

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11. In fact, the N-levels from the GaAs substrate are seen in the 44 kbar spectra in Fig. 1, panels (b) and (c), and provide an internal calibration of the AlGaAs intensities. The AlGaAs levels overshadow them in the upstroke, while the reverse is true in the downstroke. This confirms that the intensity differences we observe are not due to problems of alignment in the pressure cell.
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17. That the recombination may be due to a few photoexcited carriers is borne out by the

shape of the spectrum. While the 44 kbar spectra for the up- and downstroke look alike, the ones at 32 kbar do not. We have seen previously (Ref. 1) that the A level is seen only for high exciting intensities, while the lower energy levels D and B are more pronounced for low intensities. This is due to a saturation effect for the lower energy levels. Though all spectra in Fig. 2 were taken at the same laser power (746 W/cm^2), the 32 kbar downstroke spectrum (Fig. 2 (d)) looks remarkably like a 32 kbar upstroke taken with a laser power of 75 W/cm^2. Here the A level was not seen, but the B, C and D were seen. This leads us to believe that at lower pressures, though the recovery of intensity is not complete, there are enough electrons that saturation effects similar to the upstroke are active, though the laser intensities required are about a factor of 10 more.

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FIGURE CAPTIONS

Fig. 1. PL spectra for selected pressures in $Al_{0.3}Ga_{0.7}As$ for both increasing and decreasing pressures. Note the decline in intensity in the downstroke. In the inset we show the energies of the radiative transitions as a function of pressure

Fig. 2(a). The intensity of radiative transitions in $Al_{0.3}Ga_{0.7}As$ for up- and downstrokes, showing the hysteresis in the intensity between 30 and 70 kbar. The fits are described in the text. (b) Energies of the staggered high energy X-related peaks in the MQW sample at 15, 40 and 80K for up- and downstroke. Inset is the intensity of the main peak as a function of pressure.

Fig. 3. A schematic configuration coordinate diagram of the X CB and the new center, U_T.

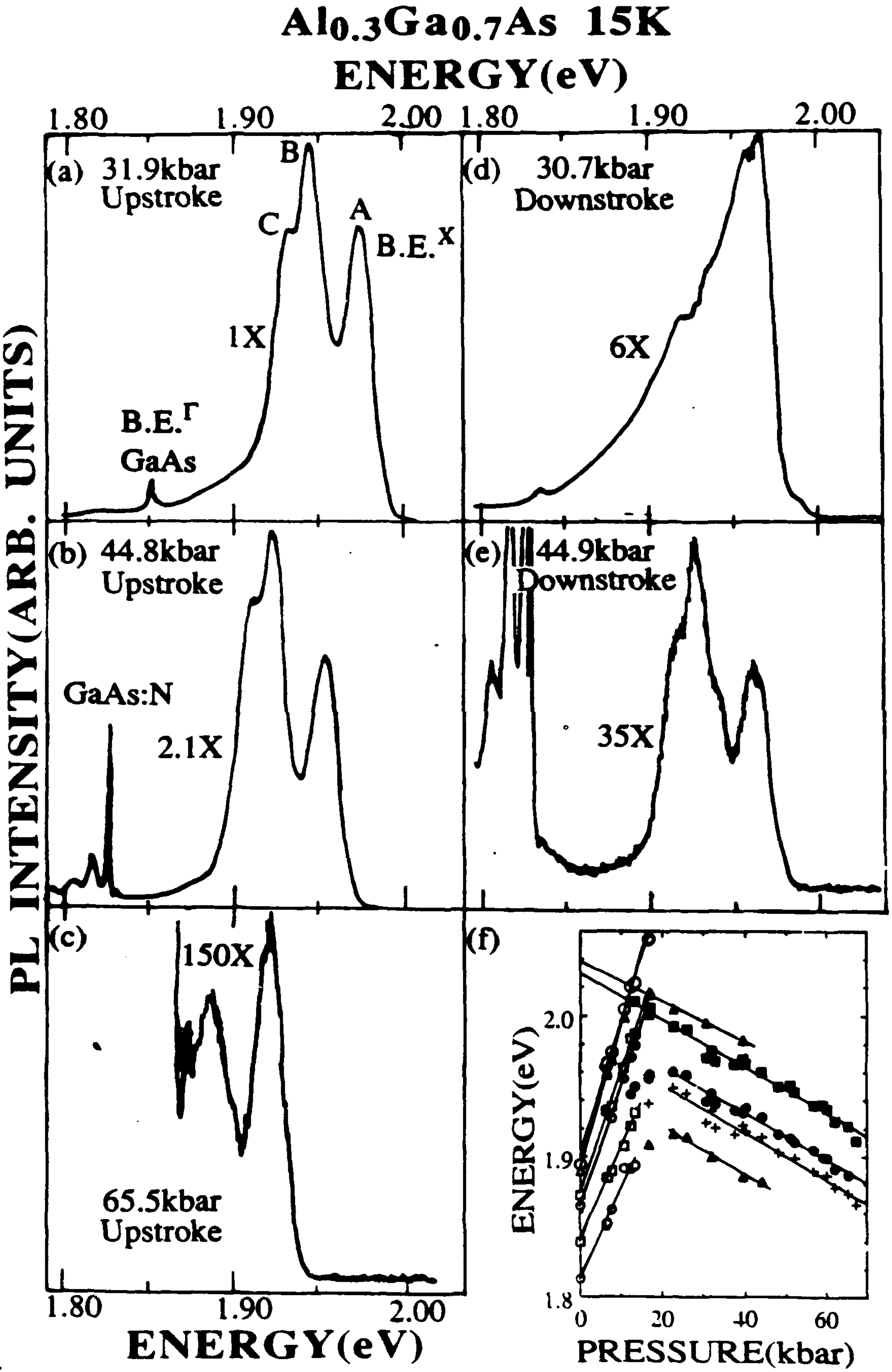
Al0.3Ga0.7As 15K
ENERGY(eV)
1.80
1.90
2.00
(a) 31.9kbar
Upstroke
B
C
A
B.E.X
1X
B.E.Γ
GaAs
(d) 30.7kbar
Downstroke
6X
(b) 44.8kbar
Upstroke
GaAs:N
2.1X
(e) 44.9kbar
Downstroke
35X
(c)
150X
65.5kbar
Upstroke
(f)
ENERGY(eV)
2.0
1.9
1.8
0
20
40
60
PRESSURE(kbar)
PL INTENSITY(ARB. UNITS)
ENERGY(eV)

Fig. 1.

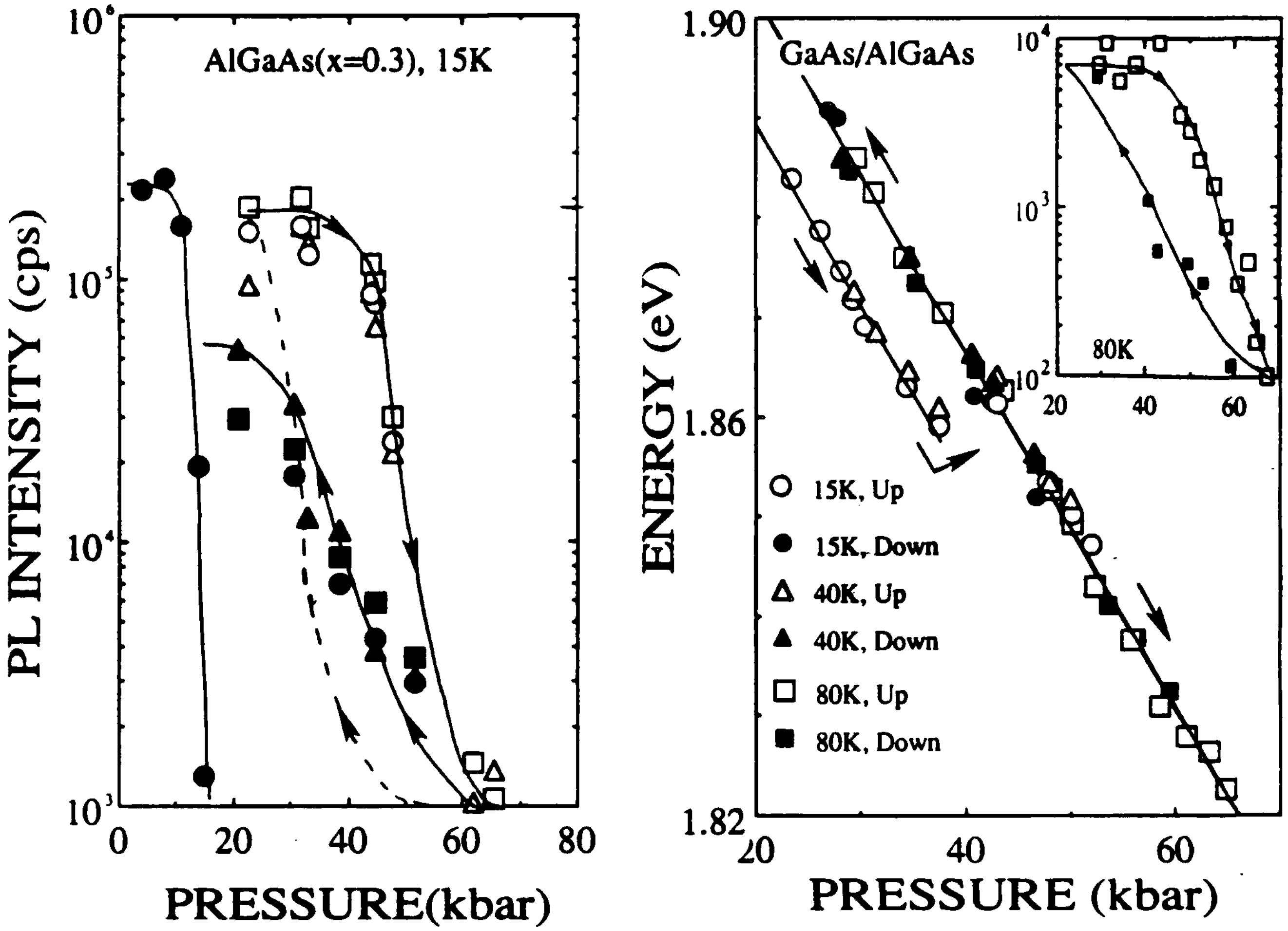

Fig 2(a) and (b)

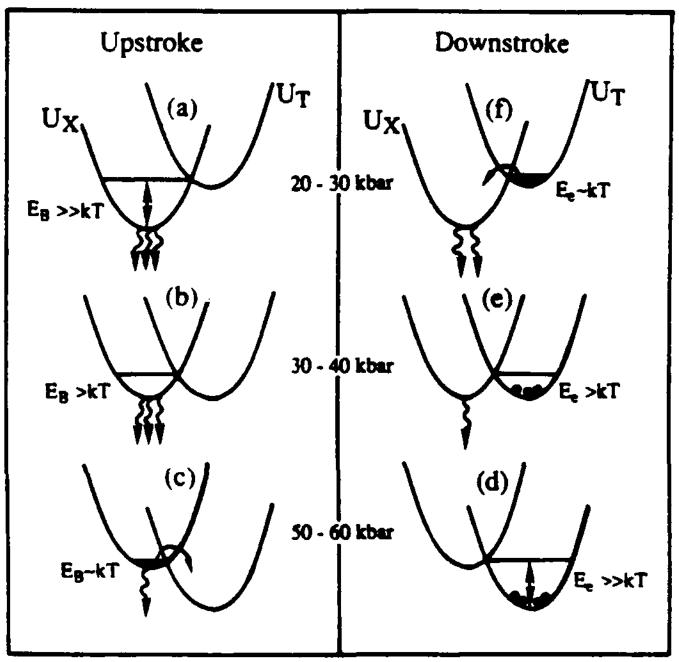

Fig. 3

To appear in *Proceedings of the 20th International Conference on the Physics of Semiconductors*, Thessaloniki, Greece, Aug. 1990.

APPENDIX II Pressure-induced Fano resonance of excitons: A new method for the determination of electron-phonon deformation potential*

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Intervalley scattering of electrons in the conduction band plays an important role in high-field transport properties, relaxation of photoexcited carriers, in processes such as light absorption in indirect semiconductors, and in a host of other phenomena such as the Gunn effect. Even though impurities, composition fluctuations, or even electron-hole scattering can sometimes affect the intervalley scattering rate of the electron, in most situations it is primarily governed by the phonon-assisted transition between the valleys. Thus the electron-phonon deformation potential D_{kq} which is a measure of the electron-phonon coupling strength:

$$H_{el\text{-}ph} = \sum_{kq} M_{kq} \left(a^{\dagger}_{-q} + a_q \right) c^{\dagger}_{k+q} c_k \qquad (1a)$$

with

$$M_{kq} = \sqrt{\frac{\hbar}{2 V \rho \Omega^{q}_{ph}}} \, D_{kq} \, . \qquad (1b)$$

is a quantity of fundamental interest. Here, a_q, $a_q^{\dagger}$ are the phonon annihilation, creation operators, c_k, $c_k^{\dagger}$ are the electron operators, V is the volume of the crystal, ρ is its density, and Ω^{q}_{ph} is the phonon frequency with momentum q.

In this paper we report the pressure-induced variation of the Fano[1] resonance broadening of the Γ exciton lineshape in GaAs, caused by the resonance hybridization with the X and the L continua via electron-phonon coupling, and use this effect to extract the electron-phonon deformation potential.

The pressure-induced Fano resonance effect is understood as follows. In many semiconductors there is a crossover from direct gap to indirect gap under the application of pressure. In this paper we focus on GaAs where there is a crossover from direct gap to indirect gap at the crossover pressure P_c of about 35 Kbar when both the X and the L conduction bands cross the bottom of the Γ band. For pressures larger than P_c, the Γ

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exciton overlaps in energy with the two-particle electron-hole continuum with electron states in the X conduction band and hole states in the Γ valence band. As a result, the photoluminescence (PL) peak of the Γ exciton takes the well-known Fano lineshape caused by interference with transitions from the continuum. Since under pressure the relative position of the exciton can be changed with respect to the continuum, the Fano resonance effect can be switched on and off depending on whether the applied pressure P exceeds P_C or not. Furthermore, the magnitude of the resonance broadening can be controlled by varying the energy of the exciton in the continuum with pressure. The net result is the pressure-tuning of the resonance effect.

The experiments were performed using quantum wells, since in bulk GaAs the donor-bound exciton dominating the PL spectrum looses intensity rapidly beyond P_C and is not observable in a sufficiently large pressure range. The quantum well used in the experiment (MQW-I) consisted of 40 periods of alternate layers of 150-Å GaAs and 100-Å $Al_{0.25}Ga_{0.75}As$. The experimental results reported here are at T = 80 K. In Fig. 1 we show the positions of the Γ, X, and the L conduction band bottoms as a function of pressure.[2] The data points on the Γ curve are energies of the n=1 heavy-hole exciton (1h). The X data points represent the staggered transition from the X conduction band in AlGaAs to the n=1 heavy-hole in GaAs.

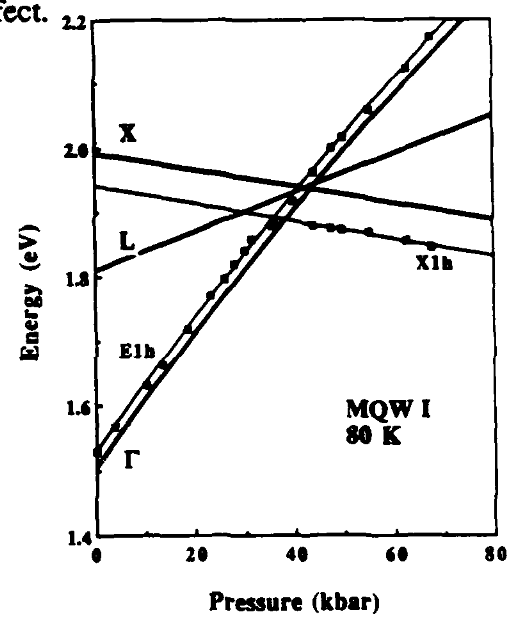

Fig. 1

Fig. 2 shows the PL spectrum for several pressures. At P = 1 bar, both the light-hole (1l) and the heavy-hole (1h) excitons with linewidths ~ 3-4 meV are seen. The PL spectrum remains virtually unchanged until P > P_C, when the dominant 1h exciton peak is progressively broadened because of the resonance effect and the 1l peak is no longer observable. The intensity

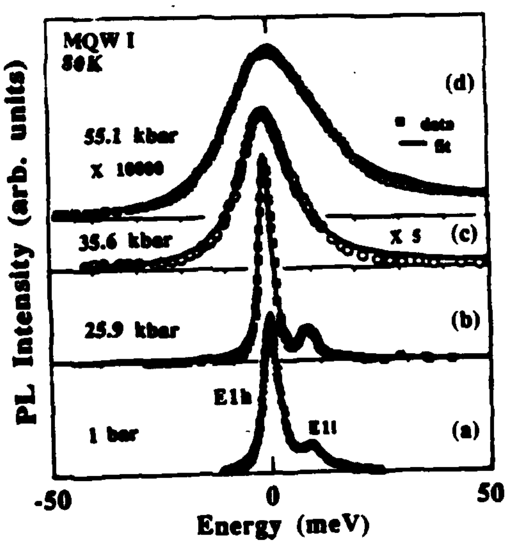

Fig. 2

of the Γ-exciton peak is at the same time drastically reduced since electrons are now scattered to the bottom of the X band.

The interaction of the exciton with the continuum via $H_{el\text{-}ph}$, Eq. (1), results in a self-energy, the imaginary part of which produces a broadening Δ of the exciton lineshape, which can be shown to be given by:

$$\Delta = \pi\ |M_{\Gamma \to X}|^2\ \rho_X(\varepsilon_d) + \pi\ |M_{\Gamma \to L}|^2\ \rho_L(\varepsilon_d)\ . \qquad (2)$$

Since the scattering mechanism does not induce a spin-flip of the electron, in Eq. (2) $\rho_X(\varepsilon_d)$ and $\rho_L(\varepsilon_d)$ are the DOS for one spin only but include contribution from all equivalent valleys:

$$\rho_X(\varepsilon_d) = N_X\ \frac{m_X^{3/2}\sqrt{\varepsilon_d - \varepsilon_{Xc}}}{\sqrt{2}\,\pi^2\,\hbar^3} \qquad (3)$$

where ε_{Xc} is the energy of the X conduction bottom, ε_d is the exciton energy and N_X is the number of X valleys, $N_X = 3$. Here we have used a free-electron like $\varepsilon^{1/2}$ DOS close to the band edge. Now, $\varepsilon_d - \varepsilon_{Xc}$, varies linearly with pressure (Fig. 1):

$$\varepsilon_d - \varepsilon_{Xc} = \alpha_{\Gamma \to X}\,(P - P_c), \qquad (4)$$

where $\alpha_{\Gamma \to X}$ is the pressure coefficient. The expression for $\rho_L(\varepsilon_d)$ is similar to Eqs. (3-4) with $N_L = 4$. From Eqs. (2-4) we find, neglecting the slight difference between the P_c's for the X and the L conduction bands, that the linewidth Δ should be proportional to $(P-P_c)^{1/2}$ for $P > P_c$. This is borne out by the experimental results (Fig. 3).

In addition to the broadening, the interference effect from the continuum leads to a characteristically asymmetric Fano lineshape. If T_Γ (T) denotes the transition

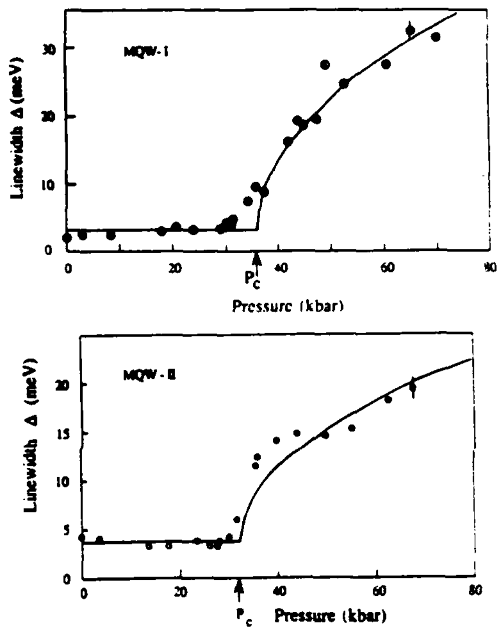

Fig. 3

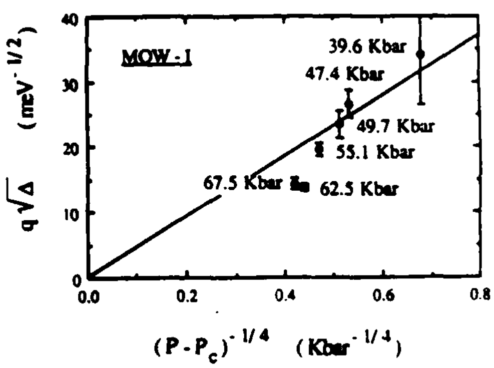

Fig. 4

matrix elements from the Γ (X or L continuum), then the PL lineshape is given by[1, 3]

$$L(\hbar\omega) = (\Delta / |M|^2)\, T^2 (q + \varepsilon)^2 / (1 + \varepsilon^2) \qquad (5)$$

where $\varepsilon = (\hbar\omega - \varepsilon_d) / \Delta$ and $q \approx |M|\ T_\Gamma / (T\Delta)$. Here Δ and q are, respectively, the linewidth and the asymmetry parameters and |M| is an average e-ph matrix element. Beyond P_c the lineshape becomes more and more asymmetric, roughly following the dependence $q\sqrt{\Delta} \sim (P - P_c)^{-1/4}$ which follows upon elimination of |M| in the expressions for q and Δ. This is shown in Fig. 4.

The experimental values reported earlier for the two deformation potentials, $D_{\Gamma\rightarrow X}$ and $D_{\Gamma\rightarrow L}$, vary between 1 and 10 eV/Å,[4] while calculations show[5] them to be approximately equal and in the range of 2.9 - 3.4 eV/Å. Taking $m_X = 0.85\ m_e$, $m_L = 0.56\ m_e$, $\alpha_{X\rightarrow\Gamma} = 12$ meV/ Kbar,[6,2] $\alpha_{X\rightarrow L} = 6$ meV/ Kbar,[14] and neglecting the small difference between the two deformation potentials, we find from the measured value of |M| that $D_{\Gamma\rightarrow X} \approx D_{\Gamma\rightarrow L} \approx 6.4 \pm 0.7$ eV/ Å. This compares extremely well with the $D_{\Gamma\rightarrow L}$ value of 6.4 ± 1.5 eV/ Å recently obtained[7] from picosecond luminescence measurements.

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APPENDIX III To appear in *Proceedings of the 20th International Conference on the Physics of Semiconductors*, Thessaloniki, Greece, Aug. 1990.

The effect of substrate on the pressure coefficients of GaSb-AlSb quantum wells

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The pressure coefficients of the excitons in GaSb–AlSb quantum wells are shown to depend strongly on the quantum confinement, the compressibility of the substrate and the pressure induced mixing of the light and heavy hole states.

Strained-layer superlattices are composed of semiconductors of significantly different lattice constants and have new device applications[1]. The axial strain between the layers of two semiconductors splits the degeneracy of the light and heavy hole zone center states. This could lead to the light hole derived sub-band to be the ground state as in the case of GaSb - AlSb quantum wells of well width greater than 100Å. Devices based on such structures have the advantage of high hole mobilities.

The substrate on which the epilayers are grown plays a significant role also. For pseudomorphic structures,below a critical thickness the in-plane lattice constants of the *thin* epilayer will be forced to that of the substrate on which it is grown by accommodating the elastic strains in the axial direction. The effect of pressure on an epilayer grown on a substrate has an additional feature. If the substrate has a different compressibility, the epilayer may experience a different amount of pressure than the *applied* pressure and may have a uniaxial component as well. The former effect leads to a change in the pressure coefficient and the latter will alter the separation between the heavy and light hole derived sub-bands. It can be easily shown[2] that the band gap energy shifts, $\delta E_g + \delta E_{\pm}$, with the externally applied pressure, P, are

$$\delta E_g = -3a_{cv}\, P(S_{11} + 2S_{12}) \qquad \text{(1a)}$$

$$\delta E_{\pm} = \left[2a_{cv}\left\{\frac{S_{11}+2S_{12}}{S_{11}+S_{12}}\right\} \pm b\left\{\frac{S_{11}-S_{12}}{S_{11}+S_{12}}\right\}\right]\{(S_{11}+2S_{12}) - (\sigma_{11}+2\sigma_{12})\}P \qquad \text{(1b)}$$

The +(-) sign correspond to light(heavy) hole valence bands. Eq.(1a) shows the hydrostatic shift of the band edge. The two terms in Eq.(1b) are due to the hydrostatic component of the strain and the tetragonal deformation. Here, "a_{cv}" is the combined hydrostatic deformation potential for the conduction and valence bands and "b" is the uniaxial deformation potential. $S_{ij}(\sigma_{ij})$ are the elastic compliance coefficients of the epilayer(substrate). The pressure coefficient,α, for the epilayer will be then different from that in its bulk form due to Eq.(1b).

We have performed PR and PL measurements under pressure[3] on GaSb-AlSb superlattices grown on thick substrates of GaAs and GaSb, respectively. Table I shows the relevant parameters. The lattice mismatch (0.65%) between GaSb and AlSb results in a biaxial tensile(compressive) strain in GaSb(AlSb) layers. The ground state excitons associated with the GaSb quantum well are split at 1bar due to the different confinement energies of the light and heavy hole sub-bands and the biaxial tensile stress in the well layers.

Table I

Parameter	units	Sample1	Sample2
well width	Å	260	100
barrier width	Å	280	100
buffer		AlSb	GaSb
substrate		GaAs	GaSb
$\alpha(E_{1l})$ measured	meV/kbar	13.1±0.2	14.5±0.2
$\alpha(E_{1l})$ calculated	meV/kbar	12.7±0.4	14.4±0.4
$\alpha(E_{1h})$ measured	meV/kbar	13.6±0.3	14.6±0.3
$\alpha(E_{1h})$ calculated	meV/kbar	14±0.4	14.7±0.4

Sample 1 was grown on a GaAs substrate with a fully relaxed AlSb buffer and sample 2 was grown on a GaSb substrate with a GaSb buffer layer. The pressure dependence for E_{1l} and E_{1h} is given by

$$\begin{matrix} E_{1l}(P) \\ E_{1h}(P) \end{matrix} = E_g(P) + \delta E_{\pm}(P) + \left[\Delta E_{1c}(P) + \begin{matrix} \Delta E_{1l}(P) \\ \Delta E_{1h}(P) \end{matrix} \right] \qquad (2)$$

The first term is the band gap of GaSb including the lattice mismatch strain.The second term is shown in Eq.(1b) and the third term (the electron, light and heavy hole confinement energies for n=1 sub-band) is also pressure dependent[4]. The relative contributions of the second and third terms in Eq.2 to the pressure coefficients of E_{1h} and E_{1l} can be estimated by comparing the data for our two samples. Sample 2 (grown on a GaSb substrate) will not be affected by the second term. Sample 1(grown on GaAs substrate) would contain both terms. However, the well width of this sample was very wide(260Å). Even though, the electron and light hole masses increase significantly with pressure due to the increase in band gap (15 meV/ kbar)[5,6], the confinement energies decrease by ~0.1 meV/kbar each for ΔE_{1c} and ΔE_{1l}. No change is expected for ΔE_{1h}. For sample 2 (well width 100Å) the decrease in ΔE_{1c} and ΔE_{1l} are 0.35 and 0 27 meV/kbar, respectively. Using the relevant elastic compliance coefficients, deformation potential constants and the lattice constants[7] of GaSb and GaAs, in Eq.(1b), the pressure derivatives of $\delta E_{\pm}$ for sample 1 are -2.1 and -0.9 meV/kbar, respectively. Hence Eq.2 would predict (12.7±0.4) and (14±0.4) meV/kbar,respectively, for the pressure co-efficients of E_{1l} and E_{1h}. Figure 1 shows the pressure dependence of E_{1l} and E_{1h} for two samples at 80K. The measured values of α are (13.1±0.2) and (13.6±0.3). For sample 2, the only contribution should be from the third term of Eq.2. The calculated values are 14.4±0.4 and 14.7±0.4 meV/kbar. The measured values were 14.5±0.2 and 14.6±0.3 meV/kbar. The estimated uncertainties in calculated values reflect those in the parameters.

The agreement between experiment and calculation for sample 2 is excellent. For sample 1, the measured value for E_{1l} is somewhat higher than predicted. More serious is the difference between the α's for E_{1l} and E_{1h} which is three times smaller than the predicted value. The parameters determining the splitting of E_{1l} and E_{1h} in Eq.(1b) are the deformation potential "b"(the value for GaSb is -2±0.2 eV) and the $S_{ij}(\sigma_{ij})$. Due to the pressure induced mixing of the light and heavy hole sub-bands, it is possible that tetragonal deformation for the sub-band states is substantially different from that of the bulk bands. An effective "b" of a third of its value in bulk GaSb will fit the data well.

Figure 2 shows the pressure dependence of the excitons from the higher sub-bands for sample1. It is clear that the α's decrease as the levels are higher in the wells. The horizontal axis is the sum of the electron and hole confinement energies of the

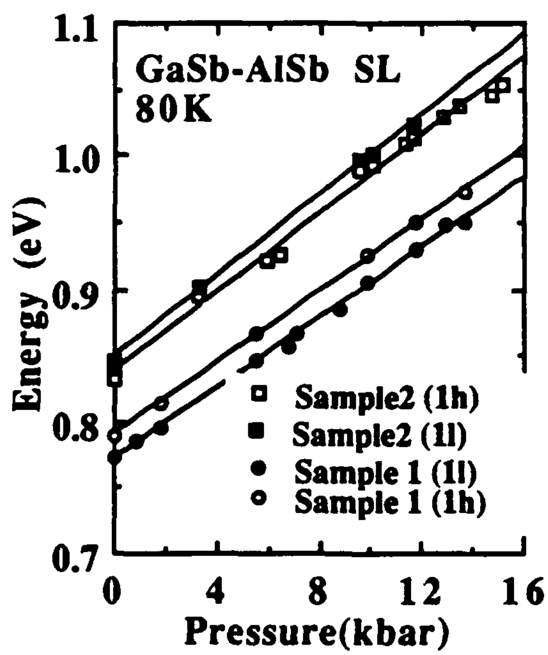

Fig.1 The pressure dependence of E_{1l} and E_{1h} for samples 1 and 2.

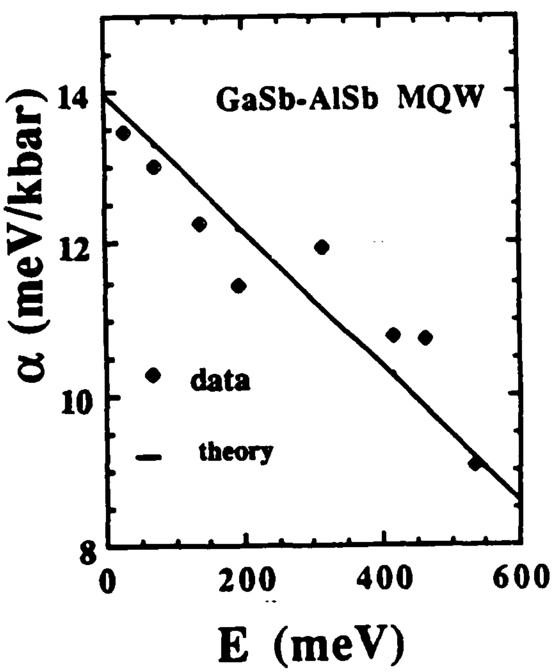

Fig2. Pressure co-efficients vs. sum of confinement energies for sample1.

corresponding transitions. The curve is calculated using the increase in effective masses with pressure(increase in band gap). The agreement is good for heavy holes. For light holes, however, data suggests a smaller rate of change in the light hole effective mass than predicted by **k.p** theory.

In conclusion, we have shown that the pressure coefficients of ground state(n=1) excitons in GaSb–AlSb MQW's grown on a GaAs substrate are lower (10-15%) than those grown on a GaSb substrate. This is due to the lower compressibility of GaAs than that of GaSb or AlSb. Additionally a uniaxial deformation alters the splitting of light and heavy hole sub-bands with pressure. The quantum confinement effects have an added contribution which is greater for narrow wells or higher sub-band states.

This work was supported by the Department of Energy, contract DE–FG02–89ER 45402 and the U.S. Army, contract No. DAAL 03–86–K–0083.

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4. The principal effect that alters confinement energies is the increase in the effective masses with the increase in band gaps due to pressure. We calculate the electron and light hole effective masses (units of free electron mass) in the z-direction(growth axis) to be 0.042 and 0.051 at 1bar and 0.054 and 0.082 at 20kbar, respectively. The heavy hole mass does not change. Other effects that alter confinement energies with presure are a) the changes in well depths due to different α's of well and barrier materials, b) possible changes in discontinuity ratio with pressure as postulated in Ref.2. Both effects will not alter the confinements significantly in our samples.

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PHYSICAL REVIEW B VOLUME 42, NUMB 0 15 AUGUST 1990

APPENDIX IV

Electronic transitions in CdT ider pressure

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We present a photoluminescence study of CdTe:Sb at 5 and K under hydrostatic pressures of 0 to 32 kbar. We determine the pressure coefficients of severa lectronic transitions: the neutral-acceptor-bound exciton A^0X, its phonon replica A^0X-LO, the ectron-to-acceptor transition e-A^0, its phonon replica (e-A^0)-LO, and four donor-acceptor peaks. A nonlinear pressure behavior is found for the main exciton peak. The linear term is 7.6±0.2 m V/kbar. We find that the binding energies of the A^0X and the bare acceptor change with pressure This change influences acceptor-bound magnetic polaron binding energies in the $Cd_{1-x}Mn_xTe$ alloys.

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INTRODUCTION

The growth of II-VI semiconductor heterostructures by molecular-beam epitaxy has produced unusual combinations of strained-layer superlattices that can be tailored to specific device applications. Among these are CdTe/ZnTe, CdTe/$Cd_{1-x}Mn_xTe$,[1] and CdTe/$Cd_{1-x}Zn_xTe$.[2] Due to lattice mismatch, the valence-band discontinuities depend on the interlayer strain as well as on the bulk energy gaps. The strain in the layers causes a splitting of the light- and heavy-hole bands, and the alternation of compressive and tensile stresses causes different well depths for light and heavy holes. It is therefore vitally important to know accurate hydrostatic and uniaxial deformation potentials of the bulk constituents in order to calculate strain-induced shifts in the valence bands.

In our present experiment, performed using photoluminescence (PL) at 5 and 15 K, we observe A^0X, its phonon replica (A^0X-LO), e-A^0, its LO-phonon replica [(e-A^0)-LO], and four deeper levels due to donor-acceptor (DA) recombination. We have obtained accurate linear and sublinear pressure coefficients for the appropriate transitions. Early measurements[3-5] of the pressure coefficient of CdTe were limited to the band gap, and were carried out at room temperature and 77 K with use of absorption and reflectivity. A recent work reports the pressure coefficients of the exciton and a DA peak at 2 K using PL.[6] The sample these authors used exhibited intense DA recombination, with the exciton appearing as a weak peak on the high-energy DA tail. This feature caused signal-to-noise problems, allowing them to obtain only a linear pressure coefficient. We will show that their inability to determine the second-order coefficient led to a linear term that is 15% smaller than our value, and consequently to errors of similar magnitude in their renormalization of previous uniaxial stress data. The errors are significant when these deformation potentials are used in calculations involving related strained-layer heterostructures.

Further impetus for studying bulk CdTe comes from recent interest in the diluted magnetic semiconductor (DMS) alloy $Cd_{1-x}Mn_xTe$. The DMS alloys display novel spin-dependent phenomena arising from the large *sp-d* exchange interaction. Among these novel phenomena are bound magnetic polarons (BMP), which are ferromagnetic spin clusters caused by the exchange interaction between the spin on the magnetic ion and a carrier spin localized at an impurity. The formation of BMP's gives rise to a magnetic binding energy (BE) in addition to the usual Coulombic term in acceptor-related transitions. In $Cd_{1-x}Mn_xTe$, BMP effects have been observed for both the neutron-acceptor-bound exciton,[7] A^0X, and the bare acceptor,[8] via the electron-to-acceptor transition e-A^0. Just as the Coulombic BE's for e-A^0 are larger than that of A^0X, the BMP BE's are larger, causing e-A^0 to shift rapidly away from A^0X with increasing Mn concentration up to $x \sim 0.25$.

We have recently investigated the tuning of the magnetic interactions in $Cd_{1-x}Mn_xTe$ with pressure.[9] We have found that the bare acceptor does not follow A^0X: the energy separation between e-A^0 and A^0X *decreases* with pressure for small Mn compositions ($x = 0.05$), while it *increases* with pressure for larger compositions ($x = 0.15$). Since the BE consists of Coulombic and magnetic terms, it is critical to disentangle the two. The pressure dependence of the Coulombic part is measured in the present experiment. We find that the Coulombic BE of A^0X increases faster with pressure than the BE of the bare acceptor, causing a net decrease in their separation. This allows us to determine the Coulombic "base line" and therefore the changes in the magnetic BE's in $Cd_{1-x}Mn_xTe$.

EXPERIMENTAL DETAILS

CdTe doped with $\sim 10^{17}$ Sb/cm^3 was grown using the vertical Bridgman technique. The sample was cleaved into a piece about $100 \times 100 \times 30$ (μm)^3 and loaded in a Merrill Bassett diamond-anvil cell. Argon, loaded cryogenically, was used as the pressure-transmitting medium. Fluorescence from the R_1-R_2 ruby lines was used to calibrate the pressure. A 0.85-m-focal-length double-grating monochromator or a 1-m focal-length single-grating monochromator with a GaAs photomultiplier and photon-counting electronics were used. Data were taken at 5 K (using a continuous-flow cryostat) or at 15 K (using a helium refrigerator). The pressure was measured accurate to ~0.25 kbar, and the pressure homogeneity, determined from the linewidth of the exciton, was better than ±0.5 kbar at the highest pressures. Data were obtained in the pressure range of 0–32 kbar, beyond which CdTe undergoes a phase transition to a metallic rocksalt phase and luminescence is quenched. The luminescence does not recover upon reducing the pressure: the ~20% decrease in volume[10] produces a large number of defects and microcrystallites that quench the radiative transitions.

RESULTS AND DISCUSSION

Photoluminescence (PL) spectra were excited with 0.5–2 mW of 5145-Å radiation from an argon-ion laser. The luminescence was intense. For example, the 1-bar spectrum shown in Fig. 1 was excited with 1 mW on a spot about 30 μm in diameter, and the intensity of the A^0X peak was 3×10^5 counts/sec at 15 K. The relative intensities of A^0X, e-A^0, and the DA peaks were found to vary with excitation intensity. We were therefore careful to choose a laser intensity that was convenient for the measurement and maintain it throughout the experiment.

As seen in Fig. 1, at 15 K we observe the A^0X, e-A^0, its LO-phonon replica (e-A^0)-LO, and deeper levels due to donor-acceptor (DA) recombination,[ ] labeled DA1 through DA4. The zero-phonon DA is observed as a weak shoulder at 5K. DA1 through DA4 are separated by LO-phonon energies, and are assigned to overtone LO-phonon replicas. Apart from A^0X-LO, which was seen only at 5 K, there were no significant differences between the 5- and 15-K data. The spectrum in the vicinity of the A^0X at 5 K and ambient pressure is shown in the inset of Fig. 1. In contrast to the spectra in Ref. 6, the intensity of the exciton peak remains high through the entire pressure range, allowing an accurate determination of the pressure coefficients.

The energies of the peaks as a function of pressure are plotted in Fig. 2. We fit the energies of all eight peaks to linear and nonlinear functions,

$$E(P)=E(0)+\alpha P\ , \tag{1}$$

and

$$E(P)=E(0)+\alpha P-\beta P^2\ , \tag{2}$$

where P is the pressure in kbar. We found that the residual sum of squares for A^0X, A^0X-LO, e-A^0, and (e-A^0)-LO transitions was 3–6 times lower when we used the nonlinear function, Eq. (2), than when we used the linear

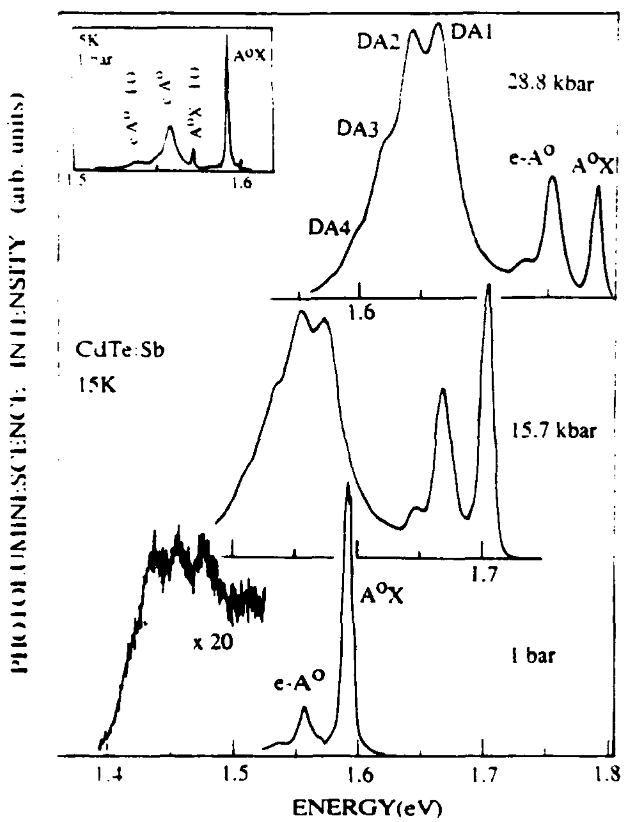

FIG. 1. PL spectra of CdTe:Sb at 15 K for several pressures. The A^0X, e-A^0, (e-A^0)-LO, and four DA transitions are observed. Inset is a 1-bar spectrum at 5 K, where A^0X-LO is seen.

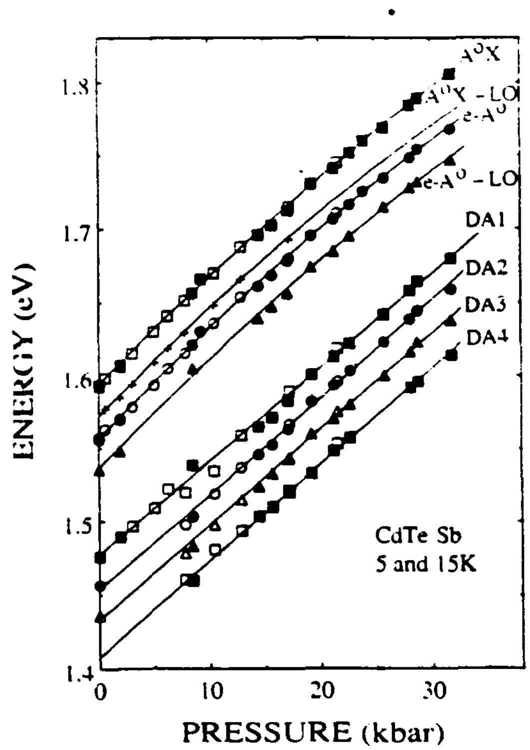

FIG. 2. Energies of the peaks observed in CdTe(Sb) as a function of hydrostatic pressure. The solid lines are least-squares fits to a nonlinear function [Eq. (2)] for A^0X, A^0X-LO, e-A^0, and (e-A^0)-LO, and to a linear function [Eq. (1)] for DA1 through DA4. The parameters obtained are listed in Table I. The open (solid) symbols are 5- (15)-K data. The fits are for the 15-K data except in the case of A^0X-LO.

TABLE I. Pressure coefficients of observed transitions.

Transition	$E(0)$ eV	α(meV/kbar)	β(meV/kbar^2)	Comments
Present work (CdTe, 15 K unless indicated otherwise)				
A^0X	1.594±0.002	7.59±0.19	−0.029±0.007	
A^0X-LO (5K)	1.572±0.002	7.74±0.20	−0.038±0.007	
e-A^0	1.556±0.002	7.91±0.18	−0.038±0.005	
(e-A^0)-LO	1.536±0.002	7.78±0.24	−0.034±0.007	
DA 1	1.477±0.002	6.39±0.09		
DA 2	1.452±0.002	6.60±0.08		
DA 3	1.432±0.002	6.52±0.07		
DA 4	1.407±0.002	6.57±0.06		
Previous works (CdTe)				
Band edge (Ref. 5)		8.0±0.2		77 K, absorption reflectivity
Band edge (Ref. 3)		7.9±0.2		300 K, reflectivity
Band edge (Ref. 4)	1.483	8.3	−0.004	300 K, absorption
Exciton (Ref. 6)		6.5±0.2		2 K, PL
Other related alloys				
A^0X (Ref. 9)	1.663±0.001	7.91±0.17	−0.036±0.005	15 K, $Cd_{0.95}Mn_{0.05}Te$
A^0X (Ref. 9)	1.826±0.001	7.66±0.2	−0.032±0.007	15 K, $Cd_{0.85}Mn_{0.15}Te$

function, Eq. (1). In contrast, the deeper levels did not show a significant nonlinearity when Eq. (2) was used, and the residual sum of squares did not differ much between Eq. (1) and Eq. (2). We therefore conclude that the shallow effective-mass-like states have nonlinear shifts with pressure, while the DA peaks shift linearly with pressure.

The pressure coefficients are listed in Table I. α and β are consistent with the values for A^0X that we have obtained for the $Cd_{1-x}Mn_xTe$ alloys.[9] Table I also lists pressure coefficients obtained from previous works. The 300- and 77-K measurements of the band edge give α's close to our α for A^0X (Refs. 3–5). In contrast, there is a large (15%) disagreement between our work and that of Dunstan *et al.*[6] who use PL at 2 K, and obtain a much smaller α. One would expect the pressure coefficients of Ref. 6 to be in much better agreement with our measurements, since both were performed at low temperatures. The discrepancy lies in the fact that Dunstan *et al.*[6] used a linear fit, and their lack of data at higher pressures prevented them from obtaining β. If we fit our A^0X energies to a linear function, Eq. (1), we obtain $\alpha = 6.62 \pm 0.11$ meV/kbar, close to the value of 6.5 meV/kbar obtained in Ref. 6. However, the residual sum of squares is 3 times larger than with a nonlinear fit. The linear and nonlinear fits to A^0X energies are shown in Fig. 3. The linear function misses the data points at both high and low pressures. The residuals (Fig. 3, inset) of the linear fit are large at both high and low pressures, and fall on a parabola (dashed curve), while those of the linear fit scatter more or less evenly about an almost flat line (solid curve). It is therefore clear that the nonlinear fit is superior. Since the nonlinear term β is fairly large,[12] forcing a straight line fit to the data can lead to a significantly smaller α.

The smaller-pressure coefficient of Ref. 6 is particularly

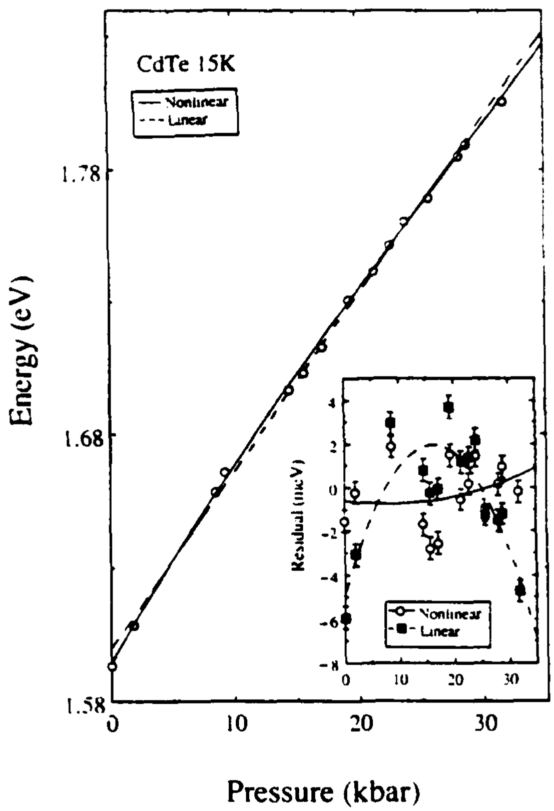

FIG. 3. A^0X energies as a function of pressure fit to linear (dashed line) and nonlinear (solid curve) functions with the parameters described in the text. Note that the linear function clearly misses data points at both high and low pressures. This is illustrated in the inset, where the residual of each fit is shown. The residuals of the linear fit fall on a parabola, with large residuals at low and high pressures (dashed curve), while the residuals of the linear fit scatter more or less evenly about an almost flat line (solid curve).

misleading in the low-pressure range, where the contribution of β is small and $\alpha=7.5$ should be used instead of 6.5 meV/kbar. Reference 6 used this smaller value to correct Thomas's shear deformation potentials,[13] where there were inconsistencies in the hydrostatic deformation potentials obtained from $\langle 100 \rangle$ and $\langle 111 \rangle$ uniaxial stress data. Corrected with our new α, the shear deformation potentials[14] are $b=1.4\pm0.4$ eV and $d=3.4\pm0.6$ eV. The error bars arise principally from the scatter in the uniaxial stress data.

Theoretical calculations of α's have ranged from 2.8 (empirical pseudopotential)[15] to 5.5 (linear muffin-tin orbitals)[16] and 8 meV/kbar (Phillips–van Vechten).[17] The last two values are in reasonable agreement with our results.

The effect of pressure on excitonic binding energies is fairly small, and is usually not noticed in PL experiments due to the large changes in the band gap with pressure. In the present experiment, however, we find that the energy separation between A^0X and e-A^0 changes with pressure, indicating that their Coulombic binding energies change. This energy separation, $\delta=E(A^0X)-E(e\text{-}A^0)$, is plotted as a function of pressure in Fig. 4. Despite the scatter, the trend toward a decreasing separation with pressure is clear, decreasing by $\sim$2.5 meV over 30 kbar. The changing separation is largely due to the fact that the A^0X BE, which involves the increasing electron effective mass, increases more rapidly than the BE of e-A^0, whose heavier hole mass barely changes.

A rough calculation can be made using a simple hydrogenic picture.[18] The effective rydberg for A^0X is

$$\mathcal{R}^*_{A^0X}=\frac{e^4\mu^*}{2\hbar^2\epsilon_0^2}, \quad (3)$$

where the reduced mass μ^* is given by

$$\frac{1}{\mu^*}=\frac{1}{m_e^*}+\frac{1}{m^*_{\mathrm{DOS}}}, \quad (4)$$

where $m^*_{\mathrm{DOS}\,h}$ is the density-of-states (DOS) effective mass for holes, $m^*_{\mathrm{DOS}\,h}=[(m^*_{\mathrm{lh}})^{3/2}+(m^*_{\mathrm{hh}})^{3/2}]^{2/3}$, m_e^*, m^*_{lh} and m^*_{hh} are the effective masses[19] for electrons ($0.096m_e$), light holes ($0.1\,m_e$), and heavy holes ($1.09m_e$), respectively, and ϵ_0 is the static dielectric constant. The effective rydberg for the bare acceptor, $\mathcal{R}^*_A$ is different from Eq. (3) only in that μ^* is replaced by $m^*_{\mathrm{DOS}\,h}$.

The effective masses and ϵ_0 are affected by pressure. We express the pressure dependence of the rydberg ($\mathcal{R}^*_{A^0X}$ or $\mathcal{R}^*_A$) as in Ref. 20,

$$\mathcal{R}^*(P)=\mathcal{R}^*(0)\exp(-2\kappa P)\frac{m(P)}{m(0)}, \quad (5)$$

where $\kappa=(1/\epsilon_0)(d\epsilon_0/dP)$, and $m(P)$ is the appropriate effective mass at a pressure P. The energy separation $\delta(P)$ then is

$$\delta(P)=\left[\mathcal{R}^*_{A^0X}\left[\frac{m^*_{\mathrm{DOS}\,h}(P)}{m^*_{\mathrm{DOS}\,h}(0)}-\frac{\mu^*(P)}{\mu^*(0)}\right]+\delta(0)\frac{m^*_{\mathrm{DOS}\,h}(P)}{m^*_{\mathrm{DOS}\,h}(0)}\right]\exp(-2\kappa P). \quad (6)$$

With the exception of κ, all the quantities in Eq. (6) are fairly well known. To our knowledge, there have been no experiments that measure ϵ_0 as a function of pressure in CdTe. The scatter in our data makes it difficult to use it to determine κ. We therefore use the following approach. We calculate the changes in the masses with pressure using the Kane three-band model[21] and use $\delta(0)=36.4$ meV, the zero-pressure energy separation between A^0X and e-A^0. Since ϵ_0 is expected to decrease with pressure,[22] we choose values of κ that give us values of $\mathcal{R}^*_{A^0X}$ that are typical for A^0X (25 ± 5 meV).[23] We fit our data to Eq. (6) using $\kappa=-10^{-4}$ to -5×10^{-4}, using $\mathcal{R}^*_{A^0X}$ as an adjustable parameter, and obtain $\mathcal{R}^*_{A^0X}$ to be 24 to 32 meV, respectively, which are reasonable values for the BE's. These fits (which are indistinguishable for the above-mentioned κ's) are shown in Fig. 4 as the solid line.

The κ's used above are consistent with what one expects. An order-of-magnitude estimate can be obtained from the Penn formula[24]

$$\epsilon_0\approx 1+(\hbar\omega_p/E_g)^2, \quad (7)$$

where $\hbar\omega_p$ is the plasma frequency, and E_g is the Penn gap. Since the Penn gap is close to the E_2 gap, corresponding to a maximum in the reflectivity,[25] it is reasonable to assume that pressure-induced changes in E_2 are followed by E_g. A theoretical calculation has obtained[26] $\alpha(E_2)=3$ meV/kbar. Using theoretical values at ambient pressure of $E_g=5.79$ and $\epsilon_0=10.3$ (Ref. 27), and assum-

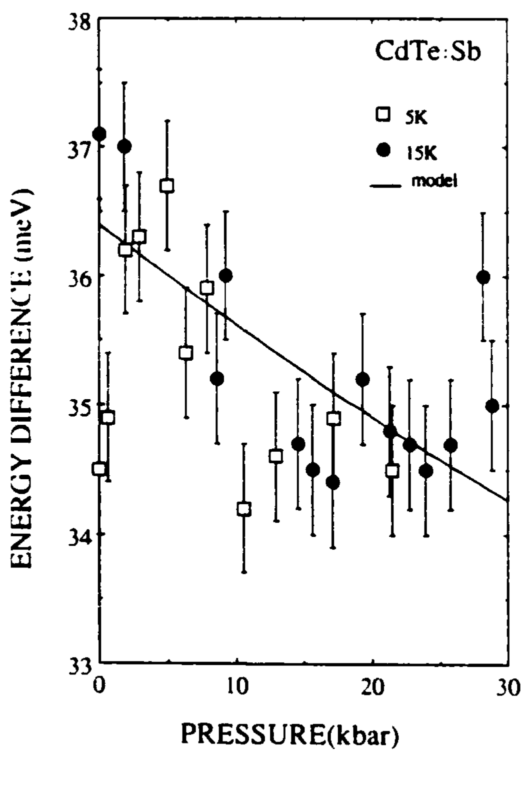

FIG. 4. The energy difference between A^0X and e-A^0 as a function of pressure. The solid line is a fit to Eq. (6), as described in the text.

ing that $\alpha(E_2)=\alpha(E_g)$, we calculate ϵ_0 at 30 kbar to be 10.0, giving $\kappa=-9\times10^{-4}$, close to the order of magnitude of κ that gives reasonable values for $\beta^*_{(A^0X)}$. Incidentally, holding $\kappa=0$ gives $\beta^*_{(A^0X)}=22$ meV, indicating that a large fraction of the changes in $\delta(P)$ arise from m_e^* (and therefore A^0X).

The above is an order-of-magnitude calculation that shows the origins of the trends in $\delta(P)$. A full calculation would require refinements in $\epsilon_0(P)$ and in calculating the effective masses, as well as a more sensitive measurement of $\beta^*_{(A^0X)}(P)$.

These measurements are of relevance in studies of $Cd_{1-x}Mn_xTe$, where the (A^0X)-(e-A^0) separation has both Coulombic and magnetic contributions. The pressure dependence of the Coulombic part is established in this experiment. The changes in the separation are about 3 times larger[9] in $Cd_{1-x}Mn_xTe$ than in CdTe, implying that the magnetic binding energies change more than the Coulombic part.

We have also observed systematic changes in the relative intensities of the A^0X, e-A^0, and DA peaks as a function of pressure. As mentioned before, the relative intensities are sensitive to the incident laser intensity and pressure. The spectra shown in Fig. 1 show how the DA intensity rises relative to A^0X at high pressures. All spectra were taken with a laser power of 1 mW. The pressure dependence suggests a resonance due to a higher band.

CONCLUSIONS

We have obtained accurate linear and sublinear pressure coefficients for the A^0X, A^0X-LO, e-A^0, and (e-A^0)-LO, and linear pressure coefficients for the four deeper levels due to donor acceptor (DA) recombination. We find that the A^0X and e-A^0 binding energies increase with pressure, causing a net decrease in the separation. This change is of importance in studies on the bound magnetic polaron in $Cd_{1-x}Mn_xTe$.

ACKNOWLEDGMENTS

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APPENDIX V To appear in *Proceedings of the 20th International Conference on the Physics of Semiconductors*, Thessaloniki, Greece, Aug. 1990.

THE BOUND MAGNETIC POLARON IN $Cd_{1-x}Mn_xTe$ UNDER PRESSURE

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ABSTRACT

We present a photoluminescence study of $Cd_{1-x}Mn_xTe$ (x = 0.0, 0.05, 0.15 and 0.20) under hydrostatic pressure at 15K. We find that the magnetic effects, measured via the acceptor bound magnetic polaron (BMP) binding energies, change with pressure. A phenomenological calculation of the BMP binding energies is presented, which leads us to conclude that the *sp-d* exchange integrals change with pressure. Surprisingly, the changes have opposite signs for the low and high x-values studied.

The diluted magnetic semiconductors (DMS) display novel spin dependent phenomena arising from the sizeable *sp-d* exchange interactions. Among these novel phenomena are bound magnetic polarons (BMP), which are ferromagnetic spin clusters caused by the exchange interaction between the spin on the magnetic ion and a carrier spin localized at an impurity[1]. The model Hamiltonian for the BMP is[2]

$$H = \frac{p^2}{2m^*} - \frac{e^2}{\varepsilon_0 r} - J \sum_j [\ (s.S_j)\, \delta(r - R_j)\ ] \qquad (1)$$

where m* is the effective mass, ε_0 is the static dielectric constant, s and S are the spins, and r and R are the position vectors of the carrier and the Mn^{2+} ions, respectively. The strength of the exchange interaction JN_0 is 880 meV for holes, allowing large acceptor BMP effects to be observed in the photoluminescence (PL) spectra. The formation of BMPs gives rise to a magnetic binding energy (BE) in the acceptor related transitions due to the third term in Eq. (1), in addition to the usual Coulombic BE.

The effects of x have been studied in $Cd_{1-x}Mn_xTe$ via the acceptor bound exciton[3], A^oX, and the electron to neutral acceptor, e-A^o transitions[4]. The e-A^o is somewhat simpler to interpret than the complicated three body A^oX problem. The BMP effects are also larger for e-A^o. Fig. 1 shows PL spectra under pressure for x = 0.05. The sharp peak at high energy is the A^oX, while the low energy peak is the e-A^o transition. With increasing Mn concentration x, the BMP BE increases faster for e-A^o than it does for A^oX, so that the separation between A^oX and e-A^o increases with x. The effective Rydbergs at 15K and 1 bar are shown in the inset of Fig. 1 for our four samples, which have x=0.0, 0.05, 0.15, and 0.20.

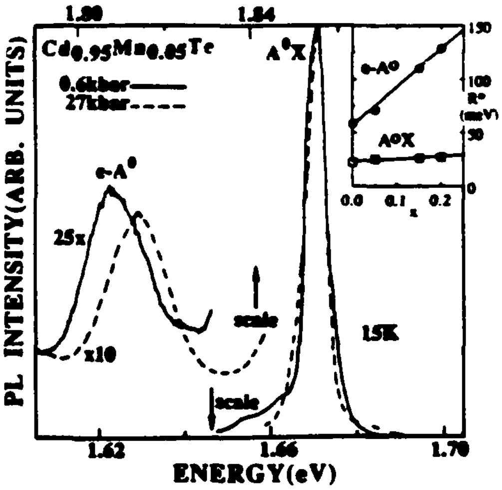

Fig. 1. PL spectra of $Cd_{0.95}Mn_{0.05}Te$ at 15K under pressure.

Our present experiments study the effect of hydrostatic pressure. $Cd_{1-x}Mn_xTe$ ($\sim 10^{17}$ cm^{-3} Sb) crystals were grown using the vertical Bridgman technique. PL was excited using 0.2 to 10 mW of 5145Å radiation from an Ar^+ laser. Measurements were conducted at 15K in a diamond anvil cell, with argon as the pressure transmitting medium. Our low temperature measurements have allowed us to study both the magnetic and bandgap effects.

In this paper we concentrate on the changes in the magnetic effects under pressure. It is evident from Fig. 1 that the separation between A^oX and e-A^o for x = 0.05 decreases with increasing pressure, indicating changing BE's. We measure the transition energies under pressure, and thence obtain the energy separation $\delta(P) = E(A^oX) - E(e\text{-}A^o)$ for all samples[5]. Looking at the separations directly is more accurate than looking at differences in the pressure coefficients, which are affected by statistical errors over the whole pressure range. In the four panels of Fig. 2 we display $\delta(P)$ for the four samples, with approximately the same energy scale. Using $\delta(P)$ we obtain the total Rydberg (Coulombic + BMP) for the bare acceptor, $R^*_A(P)$, which is the sum of the A^oX BE, $R_{A^oX}(P)$ and $\delta(P)$:

$$R^*_{A,\,Coul+BMP}(P,\, x\neq 0) = R^*_{A^oX,\,Coul+BMP}(P,\, x) + \delta(P,x)$$

$$\approx R^*_{A^oX,\,Coul}(P,\, x=0) + R^*_{A^oX,\,BMP}(P=0,\, x\neq 0) + \delta(P,x) \quad (2)$$

Here the first term is the Coulombic contribution to A^oX, which is independent of x, and therefore taken to be the x = 0 value at each P. The second term is the BMP contibution[3] to A^oX at 15K, which varies with x, and is taken to be 3, 4.5, and 5 meV for the three x's. In comparison to the much larger BMP term for e-A^o, it is assumed to be independent of P. The third term $\delta(P)$ we obtain from our measurements (Fig. 2).

In order to obtain the pressure dependence of the Coulombic BE, the first term in Eq. (2), we study changes in the BE's due to the Coulomb interaction in the non-magnetic sample, CdTe, where the magnetic terms in Eq.(2) are absent. The effect of pressure on excitonic binding energies is fairly small, and is usually not noticed in PL experiments due to the large changes in the band gap with pressure. It can, however be noticed when we compare two transitions in the same sample. In Fig. 2(a), despite the scatter, the trend toward a decreasing separation with pressure is clear, decreasing by ~2.5 meV over 30 kbar. The changes in $\delta(P)$ are largely because the A^oX BE, which involves the increasing electron effective mass, increases more rapidly than the BE of e-A^o, whose heavier hole mass barely changes. A rough calculation is made using a simple hydrogenic picture[6], shown by the dashed line in Fig. 2(a). We assume that ε_0 is a constant and the effective masses change according to the three band **k.p** model. For x=0, the effective Rydberg of the bare acceptor, $R^*_{A,\,Coul}(P)$, is found to increase slightly with pressure from 58.6 to 58.8 meV over a pressure range of 0–32 kbar, while that of A^oX, $R^*_{A^oX,\,Coul}$, increases from 22.2 to 24.7 meV, changing $\delta(P)$ from 36.4 to 34.1 meV.

When this change in the Coulombic BE's is compensated for in the other samples, we obtain the changes in $\delta(P)$ due to BMP effects, indicated by the dashed lines in Fig. 2 (b)-(d). It is interesting to note in Fig. 2 that $\delta(P)$ for x = 0.05 decreases by more than the decrease in $\delta(P)$ for x = 0, implying that the BMP BE decreases with pressure. In contrast, the BMP BE *increases* with pressure for the higher x's.

A phenomenological calculation of the total BE of the acceptor, $R^*_{A,\,Coul+BMP}(P)$

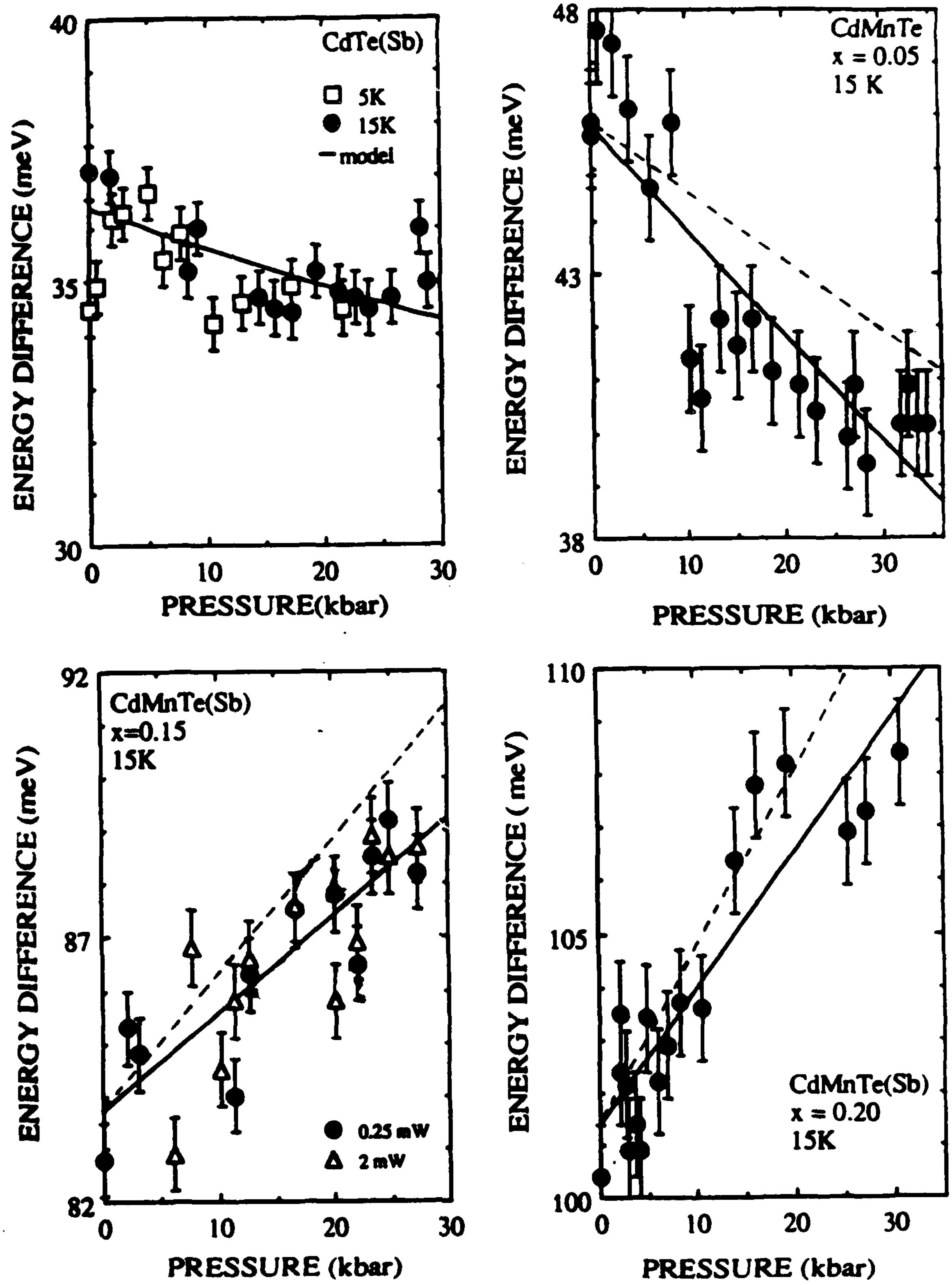

Fig. 2. The energy separations between A^0X and e-A^0, δ(P), for the four samples at 15K. The ordinates in all four panels is approximately the same. The dashed lines for x>0 represent the magnetic part of δ(P), obtained by subtracting the Coulombic contribution to δ(P) from the x=0 panel.

is performed for $x > 0$ following the technique in Ref. 2. The acceptor hole is treated in a one-band model with a hole mass of 0.4 m_0, $\varepsilon_0 = 10.76$, and T = 15K. The Mn concentration x at each pressure P is increased to account for the volume change under pressure. In the presence of Mn, the exchange potential (Eqs. (15) and (42) in Ref. 2) is a highly nonlinear equation. A numerical calculation is made, with a hydrogenic wavefunction as the starting point. An iterative process is used to in a two parameter space to obtain the binding energy and while ensuring wavefunction normalization. $R^*_{A,\,Coul}(P)$ at x=0 at each pressure, as obtained above, was used as the input, while adjusing $JN_0\bar{x}$ to obtain the experimental bare acceptor BE, relative to the band edge,

We find that the change in the volume alone under pressure does not account for changes in the acceptor BE, and that the exchange energy $JN_0\bar{x}$ has to change with pressure. Removing the volume dependence, the relative change in the exchange integral with pressure,

$$\frac{J\,(P)}{J\,(0)} = \frac{JN_0\bar{x}(P)}{JN_0\bar{x}(0)}\,\frac{x(0)}{x(P)} \qquad (3)$$

for the three samples is shown in Fig. 3. The change in J has opposite signs in the paramagnetic (x<0.1) and spin glass (x>0.1) regimes. This is an interesting conclusion, particularly since exchange integrals are usually regarded as a constant for a given family of materials. First principles calculations are under way to explain the effect.

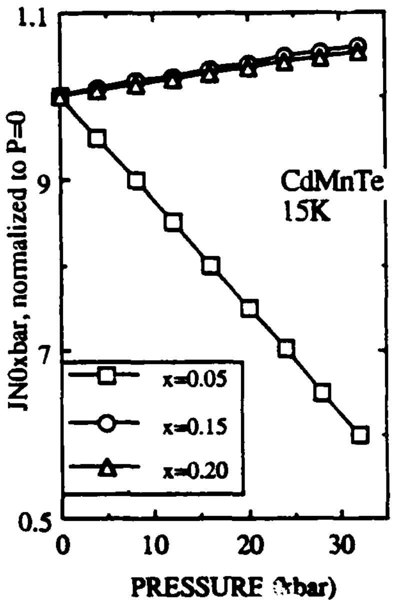

Fig. 3. The change in the exchange integral with pressure.

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