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Pressure dependence of the bandgap energy and the conduction-band mass for an n-type InGaAs/GaAs strained single-quantum well

E. D. Jones^a, S. T. Tozer^b, and T. Schmiedel^b

a) Sandia National Laboratories, Albuquerque, NM

b) National High Magnetic Field Laboratory, Tallahassee, FL

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We report the measurement of the pressure dependence for the bandgap energy E_g and conduction-band mass m_c for an 80Å-wide n-type $\text{In}_{0.20}\text{Ga}_{0.80}\text{As}/\text{GaAs}$ single-strained-quantum well at 4.2K for pressures between 0 and 35 kbar and fields up to 30 tesla. The bandgap energy E_g , at each pressure, was determined by extrapolating the magnetoluminescence "fan-diagram" to zero magnetic field. The pressure dependence of the bandgap energy was found to be quadratic with a linear term of about 10.3 meV/kbar and a small, -2×10^{-2} meV/kbar², quadratic contribution. Analyses of the pressure dependent 4.2-K magnetoluminescence data yield a conduction-band mass logarithmic pressure derivative $\partial \log(m_c)/\partial P = 0.56\% \text{ kbar}^{-1}$.

Keywords: photoluminescence, pressure, quantum well, strain

Eric D. Jones, MS 0601
Sandia National Laboratories
P. O. Box 5800
Albuquerque, NM 87185-0601
voice: (505) 844-8752
fax: (505) 844-3211
internet: edjones@sandia.gov

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A knowledge of the band-structure parameters is necessary for analyses of important semiconductor properties. One parameter important to semiconductor devices such as field effect transistors and lasers is the carrier mass. As is well known, the carrier mobility is strongly dependent upon the effective mass. There have been many [1] different experimental measurements for the effective mass and they include the temperature dependence of the amplitude of the Shubnikov - deHaas oscillation, magnetophonon and cyclotron resonances, interband magneto-optic effects and interband magnetoluminescence. The band-structure parameters are dependent on external perturbations such as temperature and pressure. In particular, the bandgap energy and effective masses are strongly dependent on pressure. The pressure dependence of the bandgap energy has been studied by many authors [1], however, the pressure dependence of carrier masses have not been as well studied. Of interest to this paper, are magnetophonon measurements [2] of the logarithmic pressure derivatives $\partial \log(m_c)/\partial P$ of the conduction-band masses of 0.62 and 0.70% kbar⁻¹ for bulk InP and GaAs, respectively.

Photoluminescence (PL) characterization of semiconductor structures has been a valuable diagnostic measurement for a number of years. The effects of external magnetic field perturbations on the PL spectrum have been utilized to determine the bandgap energy and conduction and valence-band masses [3]. In this paper, we combine low-temperatures, magnetic fields, and hydrostatic pressure to measure the pressure dependence of both the bandgap energy E_g and conduction-band mass m_c for an 80-Å-wide n-type In_{0.20}GaAs_{0.80}/GaAs strained-single-quantum-well (SSQW). These results are compared to previously reported [1] bandgap energy pressure coefficients for InGaAs/GaAs SSQW's and to a simple $k \cdot p$ calculation for the pressure dependence of the conduction-band mass.

The InGaAs/GaAs SSQW structure was prepared using molecular beam epitaxy. The SSQW structure (#BC042) consisted of a single 8-nm-wide $\text{In}_{0.20}\text{Ga}_{0.80}\text{As}$ strained quantum-well and unstrained GaAs barriers. The quantum well barrier material was silicon-doped, with a spacing of about 8 nm between the 3-nm-wide silicon-modulation layer and the quantum well. The 4-K 2D-carrier concentration N_{2d} and mobility μ are respectively $5 \times 10^{11} \text{ cm}^{-2}$ and $1.2 \times 10^4 \text{ cm}^2/\text{Vsec}$. The magnetoluminescence measurements were made at 4.2K, and the magnetic fields varied between 0 and 30 tesla. The luminescence measurements were made with an Argon-ion laser operating at 514.5 nm and an IEEE-488-based data acquisition system. The direction of the applied magnetic field is parallel to the growth direction, i.e., the resulting Landau orbits are in the plane of the quantum well. With this geometry, all measurements concerning the conduction and/or valence-band masses refer to their *in-plane* values. The laser excitation and sample signal were respectively brought in and carried out along the same 600 μm 0.37 N.A. optical fiber. The laser power at the tip of the fiber was 10 mW or 2.7 W/cm^{-2} for the tip power-density.

A small BeCu piston-cylinder diamond anvil cell, 8.75-mm-diameter and 11-mm-height, was used to generate the pressures [4]. Initially, a solution of methanol:ethanol:water in the ratio of 16:3:1 [5] was used as a pressure medium. Later work, which included the highest pressures, was performed with helium loaded as a superfluid because the alcohol medium has been known to introduce strain in samples at low temperatures [6]. In our data reported here, there were no observable changes noted with these two pressure media. The pressure was generated at room temperature and the cell was allowed to settle mechanically before inserting into low temperature liquid. The pressures noted in the data are those taken at the experimental temperatures using the ruby PL as a pressure manometer [7]. The optical fiber was positioned directly on top of the 1.7-mm-thick diamond. Because of the distance between the fiber tip and the sample, the power den-

sity at the sample is difficult to determine. However, based spectra obtained from our previous magnetoluminescence measurements [3], where the fiber is placed directly on the sample, the lasers power density at the sample is estimated to be less than 1 W/cm^2 .

Figure 1 shows a typical 4.2-K magnetoluminescence spectrum at a pressure of 8.5 kbar. The large PL peak is the *allowed* A00 transition between the between $n_c = 0$ to the $n_v = 0$ Landau levels. The smaller intensity peaks on the high energy side (right) of the allowed A00 peak are the zeroth-order forbidden transitions [8] F10, F20, ... between the $n_c = 1, 2, \dots$ and the $n_v = 0$ Landau levels. The low intensity PL peak on the low energy side (left) of the principal A00 peak is the LO-phonon sideband from the zeroth-order forbidden F20 transition [9]. Phonon sidebands, their origins, etc., will not be discussed here. The energy of each PL peak, i.e., A00, F10, F20,... can be expressed in terms of only the Landau index n_c when the temperature kT is much less than $\hbar\omega_v$, the valence-band cyclotron resonance energy. Because of the large (60 meV) strain induced splitting between the heavy and light-hole valence-bands the ground-state in-plane valence-band masses found [3] in InGaAs/GaAs SSQW's are "light" with an average mass of $m_v \approx 0.15$. Therefore the condition $kT \ll \hbar\omega_v$ is satisfied for all 4.2-K data presented here. The energy $E(n_c)$ of each peak is thus given by (cgs units)

$$E(n_c) = E_g + \left(n_c + \frac{1}{2} \right) \left(\frac{e\hbar B}{m_c c} \right) + \frac{1}{2} \left(\frac{e\hbar B}{m_v c} \right), \quad (1)$$

where m_c and m_v are the conduction and valence-band masses, and B is the applied magnetic field. By measuring the PL peak energy for the allowed and zeroth-order transitions and extrapolating the data to zero field, the bandgap energy E_g can unambiguously be determined. Figure 2

shows the result of this exercise giving $E_g = 1414.2$ meV from the 4.2K, 8.5 kbar magnetoluminescence data.

As can be seen from Eq. (1) and Fig. 1, the energy difference δE between each of the A00, F10, F20, ... peaks yields information [3] about the conduction-band mass m_c , i.e., calculating the $\delta E(1) = (F10 - A00)$, $\delta E(2) = (F20 - F10)$, etc., energy difference, $\delta E(n_c)$ is given by

$$\delta E(n_c) \equiv E(n_c) - E(n_c - 1) = \left(\frac{e\hbar B}{m_c c} \right), \quad (2)$$

where $\delta E(n_c)$ is the difference between the $E(n_c)$ and $E(n_c - 1)$ transition energies. Thus by plotting $\delta E(n_c)$ as a function of magnetic field B , the conduction-band mass m_c at each pressure can uniquely be determined. Figure 3 is a plot of $\delta E(n_c)$ for the data shown in Fig. 2, i.e., 4.2K and 8.5 kbar. The slope of a straight line best-fit to the data shown in Fig. 3 yields $m_c = 0.082$ for a pressure of 8.5 kbar. All masses are expressed in units of the free electron mass m_0 .

Thus at each pressure, graphs similar to that shown in Figs. [2] and [3] were used to determine bandgap energy E_g and conduction-band mass m_c . Figure 4 shows all the pressure dependent information for the bandgap energy E_g and the conduction-band mass m_c between ambient and 36 kbar. The left axis is for the bandgap energy E_g and the right axis is for the conduction-band mass m_c . A quadratic functional form $E(P) = E_g + aP + bP^2$ is used to fit the bandgap energy data and a best fit occurs with $E_g = (1329 \pm 1)$ meV, $a = (10.3 \pm 0.2)$ meV/kbar, $b = (-2.2 \pm 0.5) \times 10^{-2}$ meV/kbar². For the pressure dependent conduction-band mass data (right axis), a linear best-fit yields an ambient-pressure intercept of $m_c = 0.076$ and a slope $\partial m_c / \partial P = 0.0044$ kbar⁻¹. Because of the scatter to the mass data, no quadratic functions were used to fit the data.

The ambient-pressure bandgap energy $E_g = 1329$ meV is in excellent agreement with the data reported in the literature [3] for these samples. However, the intercept value for the conduction-band mass is somewhat larger than the previously reported $m_c = 0.067$ [3]. Because the mass determination relies on the numerical difference between two experimental transition energies, the data reported in [3] had many spectra taken at different magnetic fields in order to achieve higher accuracy. However, the slope $\partial m_c / \partial P$ and not the intercept value for m_c is of interest here. Using the Fig. 4 derived values for $m_c(P=0)$ and $\partial m_c / \partial P$, the logarithmic pressure derivative is $\partial \log(m_c) / \partial P = (0.56 \pm 0.07)\% \text{ kbar}^{-1}$. An estimate for $\partial \log(m_c) / \partial P$ based on $k \cdot p$ theory can be made as follows. Herman and Weisbuch [10] have performed a five-level $k \cdot p$ calculation and using their results, the conduction-band mass can be calculated from

$$\frac{1}{m_c} - 1 = \frac{2}{3} \frac{M^2}{E_g} + \frac{M^2}{E_g + \Delta}, \quad (3)$$

where M is the momentum matrix element connecting the p-like valence band with the s-like conduction band, and Δ is the split-off valence-band energy resulting from a finite spin-orbit interaction. All contributions from higher lying conduction-band states treated by [5] are ignored here. For simplicity, we will also ignore the contribution from split-off valence-band, e.g., $\Delta = 0$. Then, from Eq. (3),

$$\frac{\partial \log(m_c)}{\partial P} = \frac{(1 - m_c)}{E_g} \frac{\partial E}{\partial P}. \quad (4)$$

Using $E_g = 1329$ meV, $\partial E / \partial P = 10.3$ meV/kbar and $m_c = 0.076$, Eq. (4) predicts a logarithmic pressure derivative $\partial \log(m_c) / \partial P = 0.72\% \text{ kbar}^{-1}$, which for the assumptions made, is in good

agreement with our experimental value. There are several contributions to Eq. (4) that need to be taken into account before serious quantitative comparisons can be made, and a few are (1) the effect nonparabolic conduction-bands, (2) contributions to Eq. (3) from the higher energy conduction-band states, and (3) the correction due to the split-off valence-band. For the InGaAs/GaAs sample reported here, the nonparabolic conduction-band mass has been studied in detail with the result that from $k = 0$ (zone-center) to the 2D-conduction-band Fermi energy of about 40 meV, the mass m_c varied between 0.065 to 0.067. Thus, for the InGaAs/GaAs SSQW reported here, the effects of nonparabolic conduction bands can be ignored. However, for quantum well systems such as InGaAs/InAlAs on InP, the nonparabolic effects may be large because the conduction-band mass varies [11] from 0.041 to 0.066. The other simplifying assumptions, i.e., ignoring contributions to Eq. (4) from the excited conduction-band states and the split-off valence-band state (with the appropriate pressure coefficients) must be investigated further.

In conclusion, we have shown the utility of performing low-temperature, high-pressure magnetoluminescence measurements which have the unique ability to make not only accurate band-gap energy determinations, but also the capability to obtain information concerning the pressure coefficients for band-masses.

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References

- [1] See for example, *Physical Properties of III-V Semiconductor Compounds* by S. Adachi, (Wiley, NY 1992).
- [2] G. D. Pitt, J. Lees, R. A. Hoult, and R. A. Strandling, *J. Phys. C* **6** (1973) 3282.
- [3] See for example, E. D. Jones, *Twenty-Sixth State-of-the-Art Program on Compound Semiconductors (SOTAPOCS XXVI)*, Edited by D. N. Buckley, S. N. G. Chu, H. Q. Hou, R. E. Sah, J. P. Vilcot, and M. J. Deen, page 127 (Electrochemical Society, Pennington, NJ 1997), and references therein.
- [4] S.W. Tozer (unpublished)
- [5] G.J. Piermarini, S. Block, and J.D. Barnett, *J. Appl. Phys* **44** (1973) 5377.
- [6] D.J. Welford and J.A. Bradley, *Solid State Communications*. **53** (1985) 1069.
- [7] R.A. Forman, G.J. Piermarini, J.D. Barnett, and S. Block, *Science* **176** (1972) 284.
- [8] S. K. Lyo, E. D. Jones, and J. F. Klem, *Phys. Rev. Lett.* **61** (1988) 2265.
- [9] S. K. Lyo, E. D. Jones, and J. F. Klem, *J. Phys. Condens. Matter*. **8** (1996) L363.
- [10] C. Hermann and C. Weisbuch, *Phys. Rev. B* **15** (1977) 823.
- [11] N. Kotera, Y. Shimamoto, T. Mishima, and N. Miura, *Physica B* **227** (1996) 349.

Figure Captions

Figure 1. Magnetoluminescence spectrum at 4.2K and 8.5 kbar. The large peak near 1420 meV is the "allowed" $n_c = 0$ to $n_v = 0$ interband Landau level transition.

Figure 2. Fan-diagram for the allowed A00 and zeroth-order forbidden transitions F10, F20, etc., at 4.2K and 8.5 kbar. The zero-field bandgap energy is 1329 meV.

Figure 3. Energy difference (Eq. 3) for the 8.5 kbar fan-diagram data shown in Fig. 2. The slope of a linear best-fit line yields an ambient pressure conduction band mass of $m_c = 0.082$.

Figure 4. Pressure dependence of the bandgap energy E_g (left axis) and conduction-band mass m_c (right axis). The slopes of the two best-fit lines are respectively 10.3 meV/kbar and 0.0044 kbar^{-1} .