Conduction-Valence Landau Level Mixing Effect

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The electronic Landau level structures of the symmetric Alsb-Al_xGa_{1-x}Sb-InAs-Al_xGa_{1-x}Sb-AlSb quantum wells are investigated within a six-band $\mathbf{k}\cdot\mathbf{p}$ finite difference method. We demonstrated that the conduction-valence Landau level mixing can yield a significant spin splitting for the InAs conduction-band electrons and therefore produce a prominent electron double-line structure with a nearly field-independent energy separation in the cyclotron-resonance spectra. This mixing effect can also yield strong oscillations in the electron cyclotron-resonance mass, amplitude, and linewidth. [S0031-9007(96)01082-4]

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Cyclotron resonance (CR) in quasi-two-dimensional systems has been studied extensively for the last two decades. High-mobility two-dimensional (2D) systems with InAs single quantum wells (QW's) have become available in recent years, and several groups have studied the CR of these systems [1–4]. Heitman *et al.* [3] observed strong oscillations in CR linewidth and amplitude for electrons in semimetallic GaSb-InAs-GaSb QW's; linewidth maxima and amplitude minima were observed at even filling factors (ν's). Recently, Kono *et al.* [2] observed not only strong oscillations in CR linewidth and amplitude for electrons but also a strong CR mass oscillation in the semimetallic Al_xGa_{1-x}Sb-InAs-Al_xGa_{1-x}Sb QW's with $x < 0.3$; linewidth maxima, amplitude minima, and abnormal mass jumps occur near even filling factors. Clearly, the nonparabolicity of InAs conduction band is not the cause of the oscillations [4,5]. Most surprisingly, as reported by Cheng *et al.* [1], the far-infrared (FIR) magnetospectroscopy on semimetallic Al_xGa_{1-x}Sb-InAs-Al_xGa_{1-x}Sb QW structures has revealed not only an electron CR line (*e*-CR line), but also two new transition lines (*e*-*X* and *h*-*X* lines), when sufficient holes (in Al_xGa_{1-x}Sb) coexist with electrons (in InAs) and the magnetic field (B) is high enough. In this Letter, we shall demonstrate that the phenomena described above are caused by the conduction-valence Landau level mixing (CV LLM) effect, i.e., the conduction-valence state mixing effect in "nonzero" magnetic fields. The conduction-valence state mixing effect, which will be studied in this Letter, generally appears in the type-II broken-gap QW's such as the semimetallic GaSb-InAs-GaSb QW, in which the conduction-band minimum of InAs is lower than the valence-band maximum of GaSb. The type-II QW system studied here is the symmetric AlSb-Al_xGa_{1-x}Sb-InAs-Al_xGa_{1-x}Sb-AlSb QW's (see inset in Fig. 1), in which the thickness of the two Al_xGa_{1-x}Sb layers are the same. It may be worth pointing out that the CV LLM effects have been observed experimentally, but thus far in the 2D electron-hole systems [1–3]. This can be understood by the fact that the CV LLM takes place near the Fermi energy (E_F) when holes coexist with electrons.

To study the conduction-valence state mixing effect, we calculate the electronic Landau level structures ($B \neq 0$) and electronic band structures ($B = 0$) for the symmetric AlSb-Al_xGa_{1-x}Sb-InAs-Al_xGa_{1-x}Sb-AlSb QW's, within a six-band $\mathbf{k}\cdot\mathbf{p}$ finite difference method. The six-band $\mathbf{k}\cdot\mathbf{p}$ finite difference method is basically an effective nearest layer-orbital method [6]; however, it can reproduce a fairly accurate lowest conduction band near $k_\parallel = 0$ [6], rather than $k = 0$ as reported in Refs. [7] and [8]. To illustrate the physical origin for the appearance of a prominent "double-line" (*e*-CR and *e*-*X* lines) [1] structure in the CR spectra, the calculation is given for the electronic Landau level structures for a type-II broken-gap InAs-$Al_{0.1}Ga_{0.9}$Sb superlattice at $k_z = 0$. In these calculations, the band bending effect is not taken into account, the InAs conduction-band minimum is used as the reference energy, and the band discontinuity ΔE (valence-band

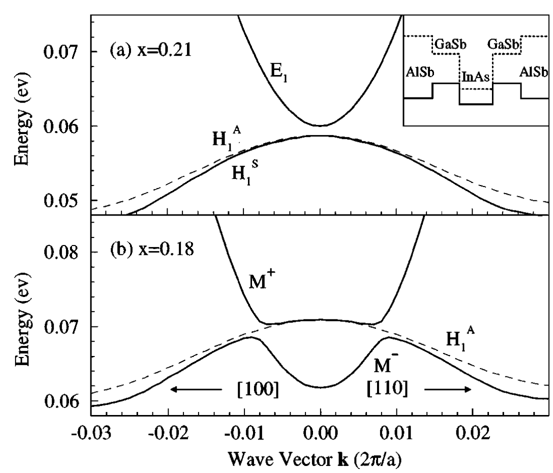

FIG. 1. The electronic band structures for the symmetric (a) AlSb-$Al_{0.21}Ga_{0.79}$Sb-InAs-$Al_{0.21}Ga_{0.79}$Sb-AlSb and (b) AlSb-$Al_{0.18}Ga_{0.82}$Sb-InAs-$Al_{0.18}Ga_{0.82}$Sb-AlSb QW's with a 159 Å thick InAs layer and 73 Å thick Al_xGa_{1-x}Sb layers.

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maximum of $Al_xGa_{1-x}Sb$ minus conduction-band minimum of InAs) is taken to be (0.4x-0.15)eV.

The 6×6 $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian matrix at zero magnetic field $H_0(\mathbf{k})$ (in the basis $u_1 = |s\uparrow\rangle$, $u_2 = |s\downarrow\rangle$, $u_3 = |\frac{3}{2}, \frac{3}{2}\rangle$, $u_4 = |\frac{3}{2}, \frac{1}{2}\rangle$, $u_5 = |\frac{3}{2}, -\frac{1}{2}\rangle$, and $u_6 = |\frac{3}{2}, -\frac{3}{2}\rangle$ is given in the upper left 6×6 block of the Eq. 13 in Ref. [7]. The Hamiltonian in a magnetic field along the z direction is [9,10]

$$H = H_0(\mathbf{K}) + \frac{\hbar e B}{m_0 c}(\kappa J_z + g_c S_z), \qquad (1)$$

where $\mathbf{K} = \mathbf{k} + (e/\hbar c)\mathbf{A}$, J_z and S_z are the z component of the hole and electron spin, respectively, κ is a Kohn-Luttinger parameter, g_c is the g factor for conduction-band electrons, and m_0 is the free electron mass. The values for κ and g_c are taken from Ref. [11]. At $B = 0$, because $\mathbf{k}_\parallel$ is a good quantum number, the envelop function associated with u_α state (F_z^α) is a function of $\mathbf{k}_\parallel$ [i.e., $F_z^\alpha = F_z^\alpha(\mathbf{k}_\parallel)$]. At $B \neq 0$, $F_z = F_z(n) = (c_1\varphi_n, c_2\varphi_{n+1}, c_3\varphi_{n-1}, c_4\varphi_n, c_5\varphi_{n+1}, c_6\varphi_{n+2})$ [9], with $n = -2, -1, 0, \dots$ and vanishing coefficients for $n < 1$ for components with negative oscillator index. Here F_z denotes the six-dimensional column vector whose components are F_z^α, and φ_n denotes the nth harmonic oscillator eigenfunction.

Figure 1 shows the electronic band structures of the symmetric (a) AlSb-$Al_{0.21}Ga_{0.79}$Sb-InAs-$Al_{0.21}Ga_{0.79}$Sb-AlSb and (b) AlSb-$Al_{0.18}Ga_{0.82}$Sb-InAs-$Al_{0.18}Ga_{0.82}$Sb-AlSb QW's. Recall that there are two $Al_xGa_{1-x}Sb$ regions, each containing a single state for the first heavy hole H_1 band. Since the QW is symmetric, by taking linear combinations of the H_1 states in the two $Al_xGa_{1-x}Sb$ regions, we can obtain a pair of symmetric (labeled H_1^S) and antisymmetric (labeled H_1^A) states. Normally these two states are nearly degenerate around $k_\parallel = 0$ as a result of the weak heavy-light hole band mixing [see Fig. 1(a)]. However, as shown in Fig. 1(b), when the conduction E_1 band minimum is lower than the H_1 band maximum, the E_1 band interacts with the H_1^S band to form a pair of H_1-E_1 mixed bands (labeled M^+ and M^-). Because of the conduction-valence band mixing, an anticrossing between the H_1^S and E_1 bands will take place and lead to a small energy gap between the M^+ and M^- bands. In Fig. 1, it is clear that for an intrinsic QW, the band structure exhibits a semimetal behavior for $x = 0.18$, but a semiconductor behavior for $x = 0.21$. This indicates that the semiconductor-semimetal transition, which occurs when the Al composition x reaches a critical value x_c, exists in the "intrinsic" AlSb-Al_xGa_{1-x}Sb-InAs-Al_xGa_{1-x}Sb-AlSb QW system. Apparently this is also true for the symmetric Al_xGa_{1-x}Sb-InAs-Al_xGa_{1-x}Sb QW system in which the two hole-confined layers are formed due to the band bending effect. Note that for an intrinsic InAs-GaSb superlattice, no semimetallic band structure can be obtained even though the E_1 band minimum is lower than the H_1 band maximum [12].

In Fig. 2, it is found that the M^+ band is identical to the E_1 band at high energies. However, as the energy decreases, the M^+ band becomes "flatter" than the E_1 band due to the conduction-valence band mixing effect. This means that the M^+ band exhibits a "type-II" nonparabolic behavior. Recall that the conduction band for bulk InAs, which becomes flatter as the electron energy increases, exhibits a type-I nonparabolic behavior. Because of the type-II nonparabolic effect, a heavier electron CR mass can be observed at low magnetic fields in the CR spectrum if the Fermi energy becomes lower. As reported in Ref. [2], at low magnetic fields the electron CR masses after LED illumination are heavier than those before LED illumination for the semimetallic Al_xGa_{1-x}Sb-InAs-Al_xGa_{1-x}Sb QW's with $x = 0.1$ and 0.2 (samples 1 and 2). This clearly results from the type-II nonparabolic effect, since the Fermi energy is lowered after LED illumination.

It is known that the type-I band nonparabolicity can yield CR mass oscillation with negative mass jumps (mass decreasing rapidly) occurring near the odd ν's [4,5]. Similarly, the type-II band nonparabolicity can also yield CR mass oscillation but with positive mass jumps (mass increasing rapidly). Indeed, this phenomenon has been observed in Figs. 2 and 3 of Ref. [2]. However, the positive mass jumps occur near (at) the even ν's instead of the odd ν's. We attribute this to the CV LLM effect, which will be studied in the rest of this Letter. Before studying the CV LLM effect, for convenience, we denote the $E_1(n, S_z)$ ($S = \frac{1}{2}$ or $-\frac{1}{2}$) as the nth Landau level for the E_1 band with electron spin of S_z, and the $H_1(m, J_z)$ ($J_z = \frac{3}{2}$ or $-\frac{3}{2}$) as the mth Landau level for the H_1 band with hole spin of J_z.

In Fig. 3, qualitatively we present a two-band model system, in which the Hamiltonian for negative spin (H) has been given in Eq. (1) of Ref. [9] and the Hamiltonian for

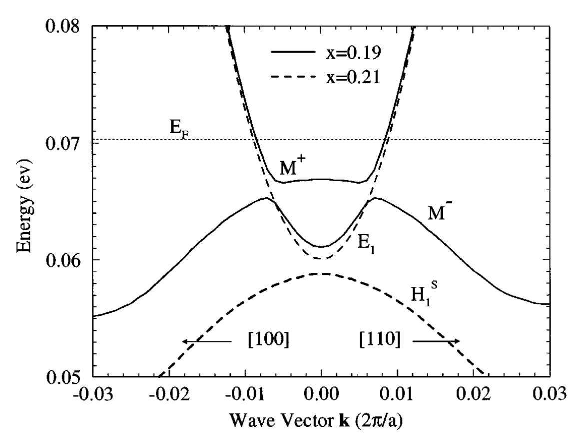

FIG. 2. The solid lines show the M^+ and M^- bands of the symmetric AlSb-$Al_{0.19}Ga_{0.81}$Sb-InAs-$Al_{0.19}Ga_{0.81}$Sb-AlSb QW, and the dashed lines represent the E_1 and H_1^S bands of the symmetric AlSb-$Al_{0.21}Ga_{0.79}$Sb-InAs-$Al_{0.21}Ga_{0.79}$Sb-AlSb QW. The thicknesses for the InAs and Al_xGa_{1-x}Sb layers are 159 and 73 Å, respectively.

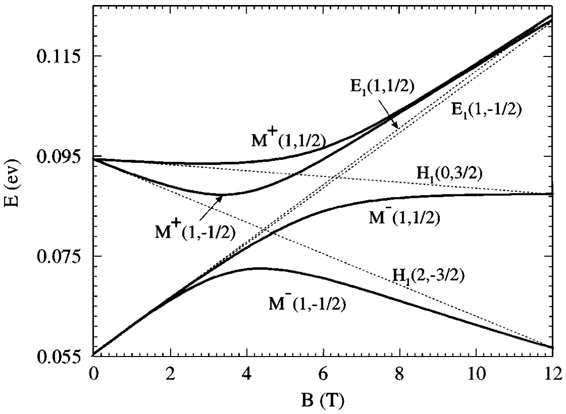

FIG. 3. Mixed Landau level structures $M^+(1, \pm\frac{1}{2})$ and $M^-(1, \pm\frac{1}{2})$ (solid lines) for an InAs-$Al_{0.1}Ga_{0.9}Sb$ superlattice with 159 Å thick InAs layers and 61 Å thick $Al_{0.1}Ga_{0.9}Sb$ layers at $k_z = 0$. Before mixing, they were $E_1(1, \pm\frac{1}{2})$, $H_1 = (2, -\frac{3}{2})$, and $H_1(0, \frac{3}{2})$ (dotted lines).

positive spin (H^*) is simply the complex conjugate of H. It is seen that the $E_1(n, S_z)$ is only coupled with the $H_1(n - 1, \frac{3}{2})$ for $S_z = \frac{1}{2}$ but with the $H_1(n + 1, -\frac{3}{2})$ for $S_z = -\frac{1}{2}$ (e.g., $n = 1$ in Fig. 3). A pair of the mixed Landau levels, in which one is electronlike, while another is holelike at a fixed B, is thus formed for each n and S_z. In this Letter, we refer to this phenomenon as the CV LLM effect. In each pair, for convenience, we denote the $M^+(n, S_z)$ and $M^-(n, S_z)$ as the mixed Landau levels with the higher and lower energies, respectively. It should be noted that, due to the CV LLM effect, the $M^+(n, \frac{1}{2})$ [$M^-(n, \frac{1}{2})$] becomes electronlike when the energy of the $E_1(n, \frac{1}{2})$ is higher [lower] than that of the $H_1(n - 1, \frac{3}{2})$, and $M^+(n, -\frac{1}{2})$ [$M^-(n, -\frac{1}{2})$] becomes electronlike when the energy of the $E_1(n, -\frac{1}{2})$ is higher [lower] than that of the $H_1(n + 1, -\frac{3}{2})$. By examining the $n = 1$ case in Fig. 3, it is found that the two electronlike Landau levels are the $M^+(1, -\frac{1}{2})$ and $M^-(1, \frac{1}{2})$ at $B \approx 4.5$–6.5 T, the $M^+(1, \pm\frac{1}{2})$ at about $B > 6.5$ T, and the $M^-(1, \pm\frac{1}{2})$ at about $B < 4.5$ T. This clearly results from the fact that the energies of the $E_1(1, \pm\frac{1}{2})$, which are nearly degenerate, equal that of the $H_1(0, \frac{3}{2})$ at about 6.5 T, but equal that of the $H_1(2, -\frac{3}{2})$ at about 4.5 T. Moreover, the energy separation between the two electronlike Landau levels is about 10 meV at $B \approx 4.5$–6.5 T, but it is smaller than 3 meV elsewhere and is about zero at high and low fields. This is mainly because the two electronlike Landau levels shift to the opposite energy sides [$M^+(1, -\frac{1}{2})$ to higher energy, $M^-(1, \frac{1}{2})$ to lower energy] at $B \approx 4.5$–6.5 T, but shift to the same energy side at other magnetic fields, compared to the energies of the $E_1(1, \pm\frac{1}{2})$. Certainly, at high and low fields, the CV LLM effect is insignificant; thus, the two electronlike Landau levels become nearly degenerate [i.e., the $M^+(1, \pm\frac{1}{2})$ ($M^-(1, \pm\frac{1}{2})$) become identical to the $E_1(1, \pm\frac{1}{2})$ at high (low) fields]. From the above discussions, we conclude that for each electron Landau level index n, due to the CV LLM effect, the energy splitting between the two electronlike Landau levels may become significant and vary slightly in a certain magnetic field range (e.g., $B \approx 4.5$–6.5 T in Fig. 3). We refer to this phenomenon as the electronlike Landau level splitting effect.

In Fig. 4(a), it is seen that the energy separation between two electronlike Landau levels at $B \approx 4$–7 T [transitions (5) and (6)] is about the same as that at $B > 10$ T [transitions (1) and (2)]. This indicates that the electronlike Landau level splitting effect is nearly field independent. Because of the electronlike Landau level splitting, as shown in Fig. 4, a prominent "double-line" structure with 3–5 meV energy separation can be observed in a fairly long magnetic field range in the CR spectrum. This novel phenomenon indeed has been observed in the experiments (see Fig. 2 of Ref. [1] and the Fig. 4.20 of Ref. [13]). Note that the authors of Ref. [1] explain this novel phenomenon due to internal excitonic transitions. However, the strongest argument against this interpretation is the fact that, as mentioned in Ref. [1], the magnetic field increases the exciton binding energy drastically [14], and therefore the energy

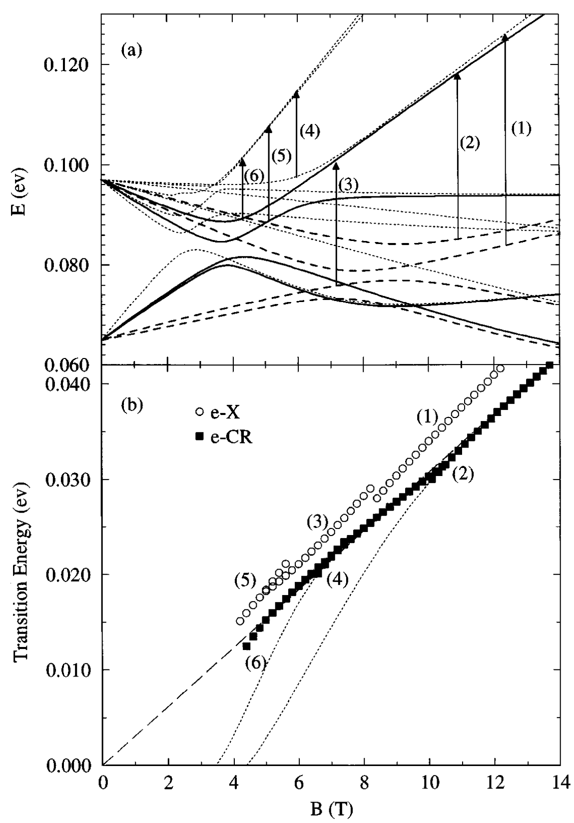

FIG. 4. (a) Electronic Landau level structures and (b) some electronlike-to-electronlike (open circles and solid squares) and holelike-to-electronlike (dotted lines) transition energies as a function of magnetic field, for a symmetric AlSb-$Al_{0.1}Ga_{0.9}$Sb-InAs-$Al_{0.1}Ga_{0.9}$Sb-AlSb QW with a 159 Å thick InAs layer and 67 Å thick $Al_{0.1}Ga_{0.9}Sb$ layers.

separation between the two lines should increase with increasing magnetic field. In this Letter we mainly emphasize the most-observable electronlike-to-electronlike transition. However, at some magnetic fields we may also observe the holelike-to-electronlike [e.g., near the end point on the right-hand side of the dotted line in Fig. 4(b)], electronlike-to-holelike, and holelike-to-holelike transitions. This means that an "electron" or a "hole" multiple-line structure is also expected to be seen at some magnetic fields in the CR spectra [13]. In each electron double-line structure, we denote the *e*-CR line and the *e*-*X* line as the lines with the lower and higher energies, respectively. The same notations have been used in Ref. [1]. As for a two-band model system presented in Fig. 3, the *e*-CR lines and the *e*-*X* lines are caused by the $M^+ \rightarrow M^+$ transitions $[M^+(N, S_z) \rightarrow M^+(N+1, S_z), M^+(N-1, S_z) \rightarrow M^+(M, S_z)]$ and the $M^- \rightarrow M^+$ transitions $[M^-(N, S_z) \rightarrow M^+(N+1, S_z), M^-(N-1, S_z) \rightarrow M^+(N, S_z)]$, respectively, where N is the last occupied electron Landau level index.

It is clear that when the magnetic field is strong enough not only the type-I but also the type-II band nonparabolicity can yield oscillations in the CR mass, amplitude, and linewidth of the *e*-CR line; the mass jumps, linewidth maxima, and amplitude minima occur near the odd ν's. As pointed out in Ref. [5], this is because the mass jumps, linewidth maxima, and amplitude minima appear in the CR spectrum at the positions of the "double resonances," which are close to the odd ν's. [Recall that at double resonance, the transitions $M^+(N, S_z) \rightarrow M^+(N+1, S_z)$ and $M^+(N-1, S_z) \rightarrow M^+(N, S_z)$ contribute equally to the energy absorption.] However, when the CV LLM effect is also taken into account, the intensity of the transition $M^+(N-1, S_z) \rightarrow M^+(N, S_z)$ may become much weaker than that of the transition $M^+(N, S_z) \rightarrow M^+(N+1, S_z)$ at the odd filling factor $\nu = 2N+1$ due to the holelike behavior for the $M^+(N-1, S_z)$. Thus the position of the double resonances must be shifted away from the vicinity of the odd filling factor $\nu = 2N+1$. It may be shifted to the vicinity of the even filling factor $\nu = 2N$ if the intensity of the transition $M^+(N-1, S_z) \rightarrow M^+(N, S_z)$ becomes observable but still fairly weak at $\nu = 2N$. From this we conclude that the mass jumps, linewidth maxima, and amplitude minima can occur near (or at) the even ν's, due to the CV LLM effect (see Figs. 2 and 3 in Ref. [2]). Moreover, the CV LLM effect can significantly reduce the intensity of the *e*-CR line at even ν's and therefore lead to a strong oscillation in the amplitude. For the type-II broken-gap QW's, the type-II nonparabolicity of the M^+ band, which can yield strong oscillations in the CR mass and linewidth, is indeed caused by the CV LLM (or conduction-valence band mixing) effect. This means that, for the type-II broken-gap QW's, the CV LLM effect can yield strong oscillations not only in the amplitude but also in the CR mass and linewidth (see Fig. 2 in Ref. [2]). It is worth noting that for a fixed N at certain magnetic fields, the energy separation between the two electronlike Landau levels [e.g., $M^+(N, \pm\frac{1}{2})$] may not be large enough to produce two absorption lines in the CR spectrum. In this case, we may see an extra linewidth maximum or a significantly enhanced linewidth maximum [see Fig. 2(c) in Ref. [2]]. The electron-hole recombination may slow down the change of CR mass and decrease the intensity of the *e*-CR line from its maximum value (see Fig. 2 in Ref. [2]].

In conclusion, we have developed a six-band $\mathbf{k} \cdot \mathbf{p}$ finite difference method to investigate the electronic band structures and electronic Landau level structures of the symmetric AlSb-Al_xGa_{1-x}Sb-InAs-Al_xGa_{1-x}Sb-AlSb QW's, in which the semimetallic band structure exists for an intrinsic QW with $x < 0.3$. We have demonstrated that the CV LLM can yield a significant spin-splitting for the InAs conduction-band electrons and therefore produce a prominent electron double-line structure with a nearly field-independent energy separation in the CR spectra. The CV LLM can also yield strong oscillations in the electron CR mass, amplitude, and linewidth; the mass jumps, amplitude minima, and linewidth maxima may occur near the even filling factors. It may be worth pointing out that in this Letter a two-band model is presented in Fig. 3 to illustrate the physical origin of the above phenomena. This implies that the CV LLM effect presented in this Letter, which may not be observed when the influence of the light-hole band becomes significant, qualitatively can be regarded as the conduction and heavy-hole Landau level mixing effect. Our results are in very good agreement with the experiment [1–3,13].

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[1] J.-P. Cheng, J. Kono, B.D. McCombe, I. Lo, W.C. Mitchel, and C.E. Stutz, Phys. Rev. Lett. **74**, 450 (1995).
[2] J. Kono, B.D. McCombe, J.-P. Cheng, I. Lo, W.C. Mitchel, and C.E. Stutz, Phys. Rev. B **50**, 12 242 (1994).
[3] D. Heitmann *et al.*, Phys. Rev. B **34**, 7463 (1986).
[4] M.J. Yang *et al.*, Phys. Rev. B **47**, 6807 (1993).
[5] E.B. Hansen and O.P. Hansen, Solid State Commun. **66**, 1181 (1988).
[6] Shiow-Fon Tsay, Z.M. Chau, Ikai Lo, and Jih-Chen Chiang (unpublished).
[7] Yia-Chung Chang, Phys. Rev. B **37**, 8215 (1988).
[8] Jih-Chen Chiang, Appl. Phys. Lett. **64**, 1956 (1994).
[9] A. Fasolino and M. Altarelli, Surf. Sci. **142**, 322 (1984).
[10] G.Y. Wu, T.C. McGill, C. Mailhiot, and D.L. Smith, Phys. Rev. B **39**, 6060 (1989).
[11] P. Lawaetz, Phys. Rev. B **4**, 3460 (1971).
[12] M. Altarelli, Phys. Rev. B **28**, 842 (1983).
[13] J. Kono, Ph.D. thesis, State University of New York at Buffalo, New York (1995).
[14] X. Xia *et al.*, Phys. Rev. B **46**, 7212 (1992).