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Effects of an electric field on the continuum energy levels in $In_xGa_{1-x}As/GaAs$ quantum wells terminated with thin cap layers

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Electroreflectance was used to study the influence of an electric field on the bound and the continuum states of $In_xGa_{1-x}As/GaAs$ quantum-well structures of various well widths, terminated by thin cap layers. Optical transitions involving only bound states were not significantly affected for the cap-layer thicknesses studied, and are Stark shifted as expected by the electric field. However, strong oscillations are observed in the spectra at energies larger than the barrier band gap, and are due to quantum interference in the continuum state wave functions which is related to the finite size of the cap layer. These oscillations, which do not follow a Franz-Keldysh relation, shift linearly with the electric field.

I. INTRODUCTION

The quantum-mechanical physics involved in semiconductor heterostructures of reduced dimensionality (quantum wells, superlattices, etc.) is generally well understood,[1–3] and is the basis of the interesting properties of these systems. However, it has been shown recently[4,5] that the ideal quantum-well (QW) potential in which one considers a quantum-well system to be terminated on either side by barriers of finite height, but infinite in extent, needs to be modified to take into account the finite size of the thin cap layers often used in actual devices. The bound states of such devices are shifted to higher energy for cap layers thinner than about 10 nm, and the continuum states exhibit oscillations, for example, in the well occupancy, for cap layers as large as 100 nm. The oscillations discussed here, which are observed at above-barrier energies, are very different from the often observed Franz-Keldysh (FK) oscillations,[6] and also different from the above-barrier oscillations predicted recently[7] for a quantum-well structure surrounded with infinite (or very large) barriers in an applied electric field: The spacing between the extrema of these oscillations decreases as the energy increases, similar to the FK oscillations, whereas the spacing between the extrema of the cap-related oscillations discussed in the present paper increases with energy. In order to better understand the optical and electrical properties of such quantum-well systems terminated with thin cap layers, it is necessary to study quantum-well structures in the vicinity of a high potential, which in the present case is provided by the external surface of the cap layer. Photoreflectance (PR) results obtained on samples having cap layers of 50 and 67 nm demonstrate the influence of a finite-size cap layer in the flat-band condition.[4] Since many experiments or devices involve electrical properties, it is also of prime interest to study the behavior of such a system under an applied electric field. This paper presents electroreflectance (ER) results displaying the influence of an electric field on the continuum states for QW structures having cap layers between 50 and 100 nm. ER experiments permit a good control of the applied electric field, and are thus particularly useful to verify the selection rules and to observe the Stark shifts of the bound states. The same type of experiments dramatically illustrate the influence of the finite size of the cap layer on the continuum states in quantum-well structures having thin cap layers. The results presented here on the $In_xGa_{1-x}As/GaAs$ system would also be valid for other similar systems terminated with thin-barrier cap layers. We first show the influence of the cap-layer thickness as obtained with detailed ER experiments performed on three equivalent single quantum wells (SQW's) having different cap-layer thicknesses. We then present results obtained with samples having different well widths. Finally, to verify the influence of the additional wells on the cap-related continuum states oscillations, we briefly discuss the ER results obtained on a multiple quantum well (MQW) having the same characteristics as one of the SQW samples.

II. EXPERIMENT

The electron and the heavy-hole bound states of the $In_{0.165}Ga_{0.835}As/GaAs$ samples studied here have been calculated and are reported in Fig. 1, together with the structural parameters of the samples. The light holes are not confined[8] in SQW's for this system, and will not be discussed here. The readers are referred to a previous paper[4] for the growth and experimental details. The bound energy levels are not affected by the cap-layer thicknesses, because the smallest cap layer studied here was 50 nm thick and changes induced by the size of the cap layer are only expected for a cap thinner than about 10 nm.[5] For the continuum states, a model considering a thin cap layer, as in the band diagram depicted in Fig. 2, must be used since the continuum states of a SQW are

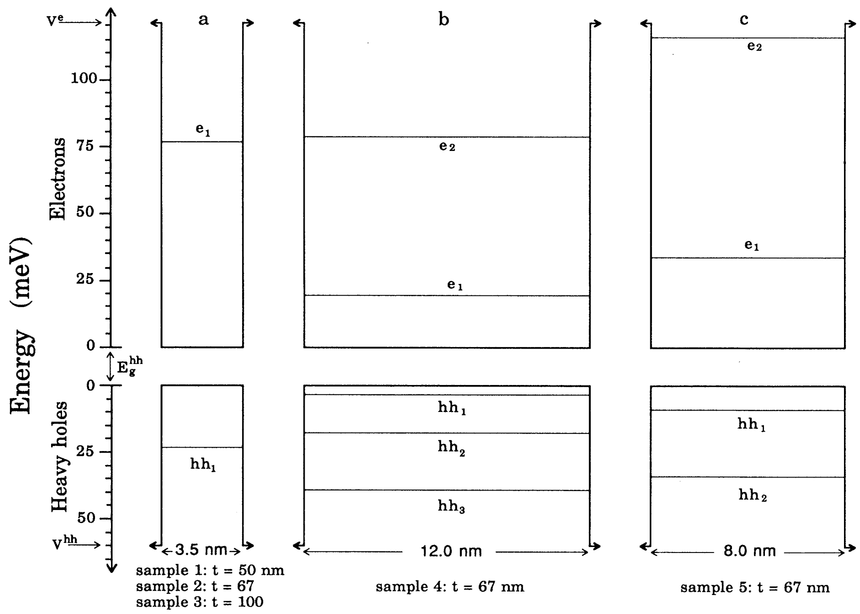

FIG. 1. Calculated bound states for the various $In_{0.165}Ga_{0.835}As/GaAs$ SQW's studied, for the electrons (top) and for the heavy holes (bottom). e_i and hh_i are the ith electron and heavy-hole levels, respectively, separated by the heavy-hole band gap E_g^{hh}. (a) is for samples 1, 2, and 3, (b) for sample 4, and (c) for sample 5. The buffer layer was 1.0 μm thick for all the samples, and t is the cap-layer thickness.

significantly affected by the finite size of the cap, and thus by the vicinity of the high potential at the surface. Figure 2 depicts the quantum-well structure in a uniform linear potential; for simplicity, band curvatures and potential nonuniformities will not be considered in the calculations, even though they would improve the accuracy of the theoretical predictions; the trends of the behaviors in the electric fields are well described using the uniform potential.

A. SQW's, influence of the cap-layer thickness

Figure 3 shows 77-K spectra of sample 1, which has one electron and one heavy-hole bound state, as illustrated in Fig. 1(a), for different electric-field values. For positive biases, the sample approaches the flat-band condition, since the built-in field caused by the semitransparent gold Schottky barrier evaporated on the surface is canceled by the applied voltage. The near-flat-band condition [as encountered previously in PR (Ref. 4)] occurs between curves v and vi of Fig. 3, at a bias voltage of about +0.5 V. The spectra display features associated with the $11H$ peak, some intermediate transitions labeled A and B, the GaAs gap, and most of all, the cap-related above-barrier oscillations. As the field is increased, the $11H$ peak is Stark shifted. The Stark shift for this sample is small, as expected for a narrow well. It is not clear why the amplitude of the $11H$ peak evolves from a maximum at both extremities of applied voltages to a minimum for an applied voltage near 0 V, but it may be partially explained by the leakage of the carriers from the well into the adjacent layers as the electric field tilts the bands.

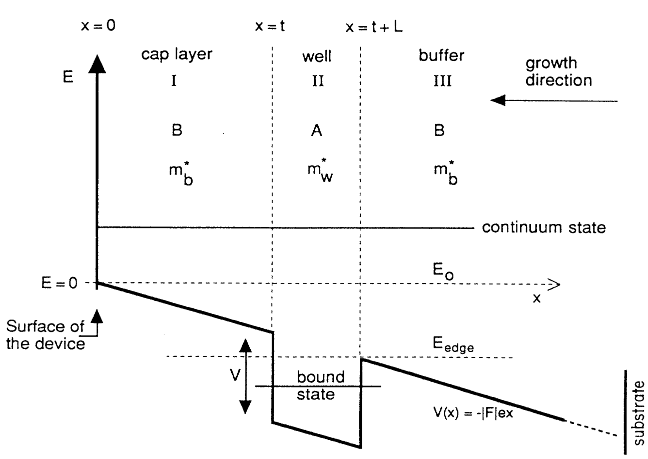

FIG. 2. The band diagram of a SQW, width L, with a capping barrier layer of finite size (t), and a thick buffer layer, when an applied electric field ($|F|$) lowers the potential away from the surface. E_{edge} is the edge of the energy continuum.

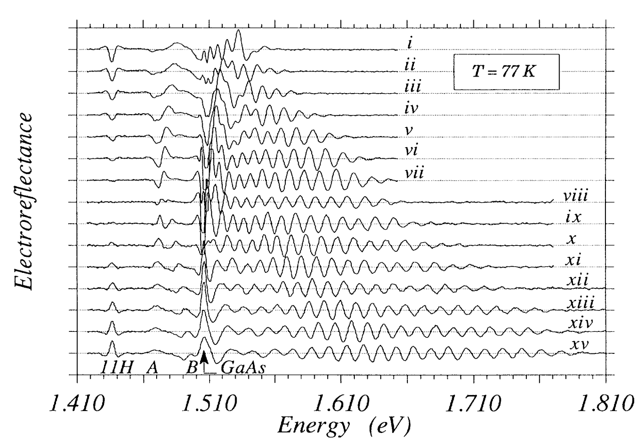

FIG. 3. ER spectra of sample 1 (L = 3.5 nm, t = 50.0 nm), at T = 77 K, for bias voltages between 1.4 (curve i) and −1.4 V (curve xv) by increments of 0.2 V.

"A" is associated with the real-space indirect, bound-unbound $11L$ transition, and "B", which is shifting toward higher energies as the field is increased, is associated with the $e1$-cH transition (where cH means the continuum of the heavy holes). The extrema of the cap-related above-barrier oscillations in Fig. 3 are displaced toward higher energies with increasing electric field, and, also, the spectral energy range for which the experimental oscillations are visible increases with the electric field. This can be related directly to the electric-field dependence of the cap-related oscillations of the well occupancy, as discussed in Ref. 5. The experimental value of the shift of the extrema of oscillations of Fig. 3 is ~ 4.3 meV/kV/cm. This is larger than the calculated shift of the well occupancy, which was found to be $+2.9$ meV/kV/cm for $t = 50.0$ nm for the heavy holes. The difference arises probably because the actual potential configuration is not exactly that shown in Fig. 2.

For the same sample, the theoretical prediction of the variation of the well occupancy (P_w) as a function of the applied electric field for a fixed energy above the well can be compared with the corresponding experimental results. Figure 4(a) shows the calculated P_w as a function of the electric field for four different energies: 8, 9, 10, and 11 meV above the center of the well. This is compared to the experimental ER signal obtained at a fixed wavelength (a fixed energy above the well) as the bias voltage is varied [Fig. 4(b)]. A quantitative comparison is difficult because the actual values of electric field are not known, since the built-in field cannot be evaluated precisely for this sample; nevertheless, qualitatively the experimental results vary as theoretically predicted.

Since the above-barrier oscillations are related to weakly temperature-dependent parameters such as the size of the cap layer, they should not be strongly influenced (i.e., shifted in position relative to the other spectral features) by the temperature. Figure 5 shows the ER results of sample 1 obtained at various temperatures, for a bias voltage of -1.0 V; the horizontal axis represents the energy measured from the $11H$ peak. The $11H$ peak itself is shifting as expected with temperature, but the relative positions of the cap-related peaks are not substantially affected.

The corresponding ER results obtained with sample 2 are shown in Fig. 6. As expected, for energies smaller than the gap, the spectra are similar to those of Fig. 3 for sample 1 which had the same well width. However, the above-barrier oscillations are very different from those of the previous sample, which has a different cap-layer thickness (50 nm vs 67 nm). A PR spectrum obtained with sample 2 (see Fig. 4 of Ref. 4) demonstrated that, because of the effective-mass dependence of the oscillations [see Eq. (1) of Ref. 4], the carriers contributing to the observable oscillations changed from the heavy holes to the electrons for larger cap-layer thicknesses. The near-flat-band condition (as encountered previously in PR) occurs here at a bias of about $+600$ mV, and corresponds to spectral oscillations related to electrons for a cap thickness of 65 nm. Furthermore, for this sample the calculated displacement of the extrema of oscillations is 4 meV/kV/cm, and from Fig. 6, the measured displacement is ~ 6 meV/kV/cm. Here again the observed displacement is slightly larger than predicted, the discrepancy being likely attributable to band bending.

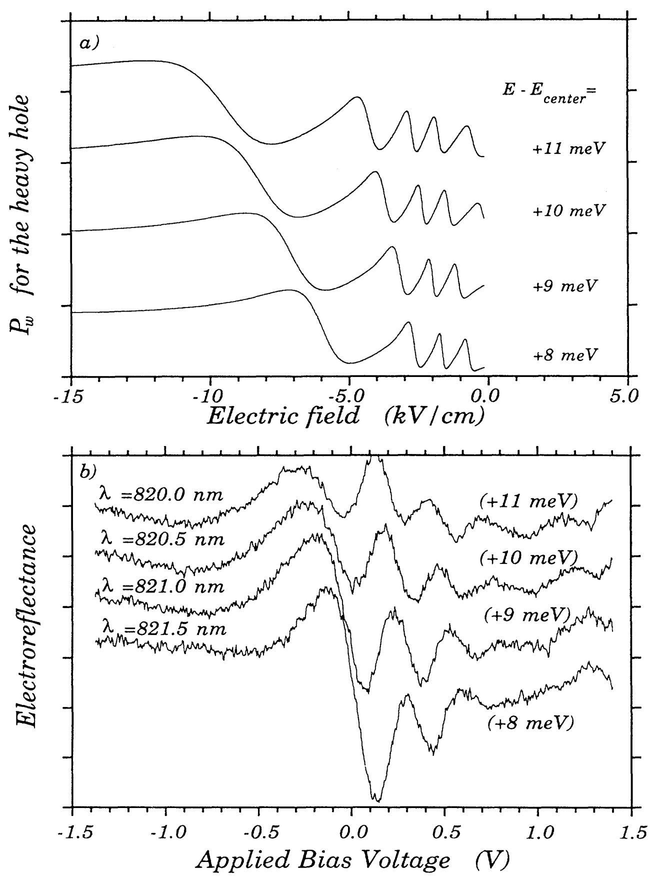

FIG. 4. (a) The calculated electric-field dependence of the well occupancy (P_w) for fixed energies above the center of the well. (b) ER measured at the corresponding fixed wavelengths as a function of the applied voltage for sample 1.

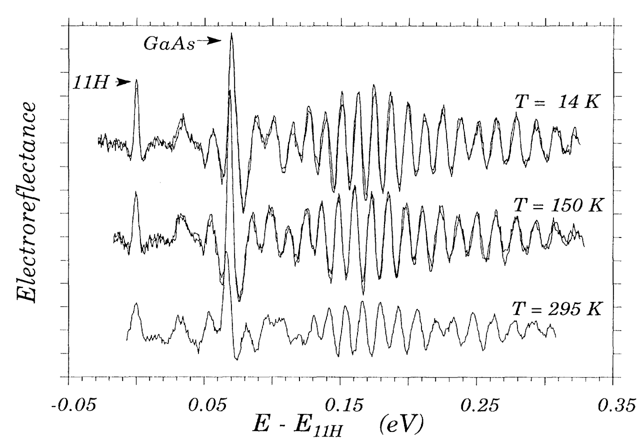

FIG. 5. ER spectra of sample 1 compared at various temperatures. The horizontal axis is the energy measured relative to the $11H$ peak. The spectra were all obtained at a bias voltage of -1.0 V.

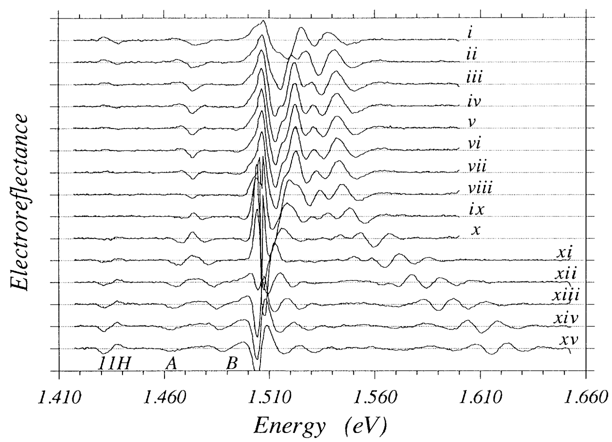

FIG. 6. ER spectra of sample 2 ($L = 3.5$ nm, $t = 67.0$ nm), at $T = 77$ K, for bias voltages between 1.4 (curve *i*) and -1.4 V (curve *xv*) by increments of 0.2 V.

Sample 3 further verifies that the oscillations of the continuum states are strongly dependent on the cap-layer thickness t. Figure 7 shows ER spectra of sample 3 for different electric-field values. Once again, the below-barrier results are similar to those obtained with the other two samples having well widths of 3.5 nm. For above-barrier energies, the ER spectra obtained near the flat-band condition give oscillations which correspond to the electrons for a cap-layer thickness of 100 nm, as determined by plotting (not shown) the positions of the extrema of oscillations as a function of the square of their indices (the E_n vs n^2 plot as in Fig. 3 of Ref. 4). However, for this sample, the displacement of the extrema of oscillations with the electric field is surprisingly small, probably because the cap is thicker and the well is farther from the surface (where the band bending is different). The extrema of the ER spectra are displaced by ~ 3.5 meV/kV/cm, whereas the calculated displacement is 6 meV/kV/cm. At large positive biases, the spectra display a different structure at about 25 meV above the barrier (marked by an arrow where $k_w L = \pi$), which could be associated with the usual resonant continuum states of the heavy holes. This indicates that for large enough cap-layer thicknesses, the usual resonant continuum states become more significant, whereas for thinner cap layers, quantum interference effects dominate the spectra under certain conditions.

B. SQW's, influence of the well width

The first three samples, which had a well width of 3.5 nm, gave strong cap-related above-barrier oscillations as expected for narrow wells.[5] In contrast, the next two samples, having larger well widths, give above-barrier oscillations which are weaker relative to the other spectral features. Sample 4 has a nominal well width of 12.0 nm and a cap-layer width of 67 nm. This sample has two bound electron levels and three bound heavy-hole levels, as illustrated in Fig. 1(b). As seen in Fig. 8, which shows the ER results obtained with sample 4, the spectra display only very weak cap-related above-barrier oscillations, not visible at first observation; however, it will be shown below (in Fig. 12) that these oscillations are actually present. For energies above the GaAs gap, the spectra of both samples 4 and 5 are dominated by FK oscillations, especially for the negative biases. From an E_n vs $(n - \frac{1}{2})^{2/3}$ plot obtained with the FK oscillations, one can calculate the electric field for the different bias and use these values to calibrate the field; for example, curve *xiv* in Fig. 8 at -1400 mV corresponds to an electric field of 20.7 kV/cm. Furthermore, the dependence of the electric field on the applied voltage gives a direct measurement of the thickness of the undoped regions across which the voltage is applied, and of the built-in electric field. From Fig. 8, it can be found that the electric field varies linearly with the applied voltage correspondingly to a 0.8-μm undoped region (the difference from the thickness of 1.08 μm expected from the growth parameters is probably due to the nonuniformity in the applied field); the built-in electric field is 3.0 kV/cm, which

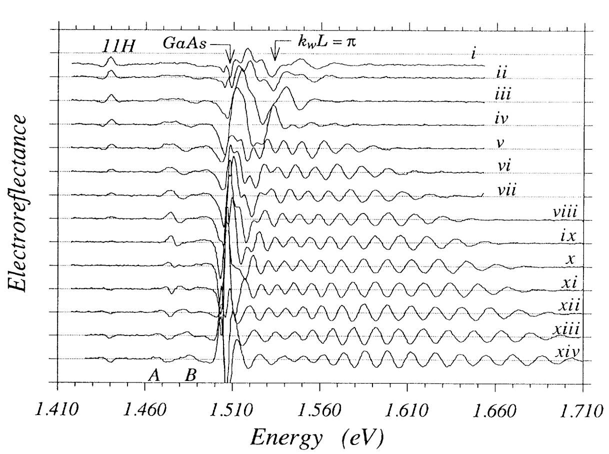

FIG. 7. ER spectra of sample 3 ($L = 3.5$ nm, $t = 100.0$ nm), at $T = 77$ K, for bias voltages between 1.2 (curve *i*) and -1.4 (curve *xiv*) by increments of 0.2 V.

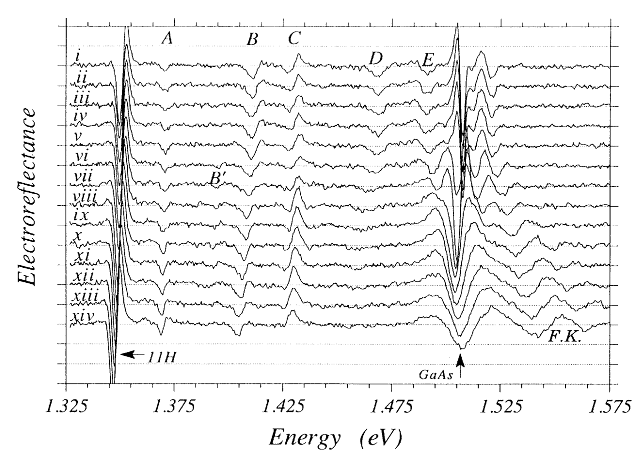

FIG. 8. ER spectra of sample 4 ($L = 12.0$ nm, $t = 67.0$ nm), at $T = 77$ K, for bias voltages between 1.2 (curve *i*) and -1.4 (curve *xiv*) by increments of 0.2 V.

means that the electric field should be zero at ~240 mV, i.e., between curves *vi* and *v*.

In Fig. 8, several features are observed between the $11H$ peak and the GaAs gap. From standard calculations, the labeled peaks could be assigned to A: $12H$; B': $13H$; B: $11L$ and/or $21H$; C: $22H$; D: $21L$ and/or $23H$; and E: ec-$3H$, where ec denotes the electron continuum. One may also note that the various peaks are Stark shifted as the electric field is changed. For example, Fig. 9 displays the shift of the $11H$ peak position [found from a line-shape analysis using Eq. (2) of Ref. 4] as a function of the applied voltage. For the range of electric fields studied here, the total shift in energy of the $11H$ peak is 3.5 meV, and behaves as expected in a quadratic fashion,[3] as shown by the solid line in Fig. 9. The energy variations of the other peaks of Fig. 8 are less pronounced, except "E", which shifts in a peculiar way: it is strongly displaced toward higher energies as the magnitude of the electric field is increased. The behavior of this feature will be discussed further in connection with similar peaks observed with the next sample. The amplitude of some features changes with the applied electric field: for example, "A", which is associated with a transition forbidden in the absence of field, strengthens as the magnitude of the field is increased (i.e., toward negative applied voltages); and peak B', which is allowed in zero field, is weak, and almost only observable for an applied voltage close to the zero-field situation. All these amplitude variations related to the parity of the transitions are predicted by symmetry consideration of the wave functions of the carriers.[1]

Sample 5 has a nominal well width of 8.0 nm, and a cap-layer thickness of 67 nm (the same as samples 4 and 2). This sample has two electron and two heavy-hole bound states, as illustrated in Fig. 1(c). The ER results for this sample are shown in Fig. 10. The spectra are similar to those of the previous example except that fewer transitions are observed in the energy range between the $11H$ peak and the GaAs gap, as expected since this sample has two instead of three confined heavy-hole levels.

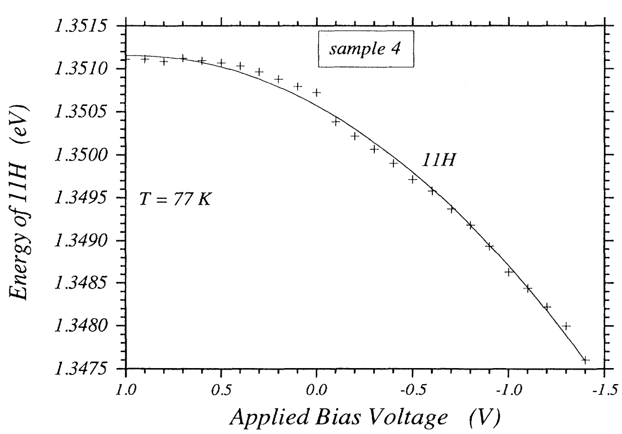

FIG. 9. The Stark shift of the $11H$ transition of sample 4. The crosses are the values obtained from a line-shape analysis of the ER spectra of Fig. 8, and the solid line shows the quadratic relationship.

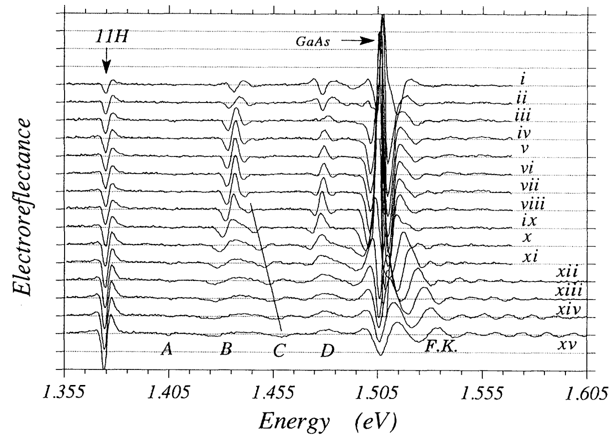

FIG. 10. ER spectra of sample 5 ($L = 8.0$ nm, $t = 67.0$ nm), at $T = 77$ K, for bias voltages between 1.4 (curve *i*) and -1.4 V (curve *xv*) by increments of 0.2 V.

Here again the spectra are dominated by the FK oscillations at above-gap energies, especially for negative biases, but it will be shown below (Fig. 12) that this sample also exhibits some weak cap-related above-barrier oscillations. As with the previous sample, the FK oscillations were used to calculate the electric-field values for the different applied voltages, and the dependence of the electric field on the applied voltage gives an undoped region of 1.2 μm (again, compare with the nominal value of 1.07 μm), and a net built-in electric field of 1.0 kV/cm. Thus the electric field is 12.5 kV/cm for curve *xv* at -1400 mV, and zero at $V_a \sim 120$ mV (i.e., between curves *vii* and *viii*). The below-gap assignment for the features at energies above the $11H$ peak is as follows: A: $12H$; B: $11L$; C: $21H$ and/or ec-$1H$; and D: $22H$. As before, the amplitudes change with the electric field, and the peaks are shifted in energy. The shifts of the $11H$, B, and C peaks with the electric field are plotted in Fig. 11. The total shift (1.0 meV) of the $11H$ peak is not as large as the one obtained with sample 4, because of the smaller range of electric field covered, and because of the different well width, but the functional relationship seems to be quadratic here again. Peak B is also shifting toward smaller energies, and its small displacement could be accounted for by a Stark shift. The peculiar shift of peak C is opposite to that of A and B, and is similar to the one observed with the previous sample (peak E, Fig. 8). When compared to the usual Stark shifts, it shows a much stronger displacement (here 21 meV) toward *increasing* energies, and it is *linear* with a slope of 1.5 meV/kV/cm. It could be argued that peak B and the shifting peak C are just a single transition which broadens with the electric field, but this is unlikely because the broadening would be asymmetric, and exaggeratedly large (no such broadening has been observed with other transitions). It could also be argued that the shift is in reality an exchange of amplitude between two transitions as the electric field is varied, but the continuity of the gradual displacement between consecutive spectra and the quality of the line-shape fit that can be obtained with a single transition favor the assignment of "C" to a single transition with a strong positive shift. Moreover, the transitions which give rise to peaks C of Fig. 10, E of Fig. 8, and B of Figs. 3, 6, and 7 all involve continuum states: the electron continuum states for peak E (sample 4) and for peak C (sample 5), and the heavy-holes continuum states ($e1$-cH) for peak B (samples 1–3). These large positive shifts may be understood by recalling that the continuum states are strongly affected by the finite size of the cap layer and the high potential at the surface. The carriers excited in the continuum states should relax to the lowest maximum of the well occupancy before they relax into the bound states; because this peak is shifting toward higher energies as the field is increased, the transitions involving such continuum states would be displaced accordingly. The lowest peak of the well occupancy is calculated to be displaced by ~ 1 meV/kV/cm, and by 1.4 meV/kV/cm for electron continuum states for a cap layer thickness $t = 65$ nm and well widths of 12.0 and of 8.0 nm, respectively. The value of the shift obtained experimentally with sample 5 (1.5 meV/kV/cm) compares particularly well with the calculated value of 1.4 meV/kV/cm.

Samples 4 and 5 have larger well widths, and a cap-layer thickness of 67 nm and therefore did not show strong cap-related above-barrier oscillations. However, repeated slow scans, at higher sensitivity, of the positively biased ER spectra reveal these oscillations. For comparison, Fig. 12 displays the results (obtained with samples 4 and 5, together with spectra v) of Fig. 6 for sample 2. It is clear from Fig. 12 that all samples having a cap-layer thickness of 67 nm (samples 2, 4, and 5) produced oscillations with extrema at similar energies; only the amplitude of the oscillations of the samples having wider wells is smaller.

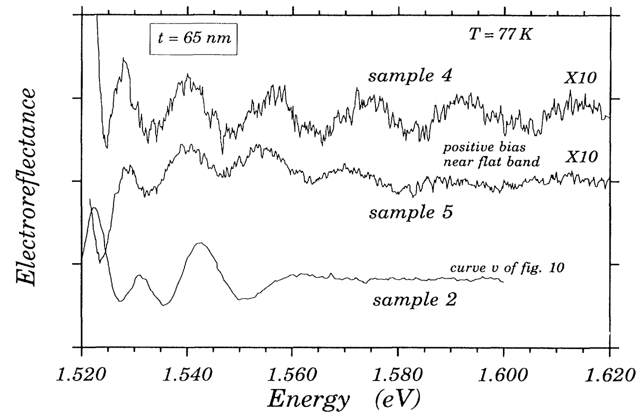

FIG. 12. The ER at higher sensitivity for samples 4 and 5 (compared with the spectrum of sample 2, which has the same cap-layer thickness), showing the above-barrier cap-related oscillations.

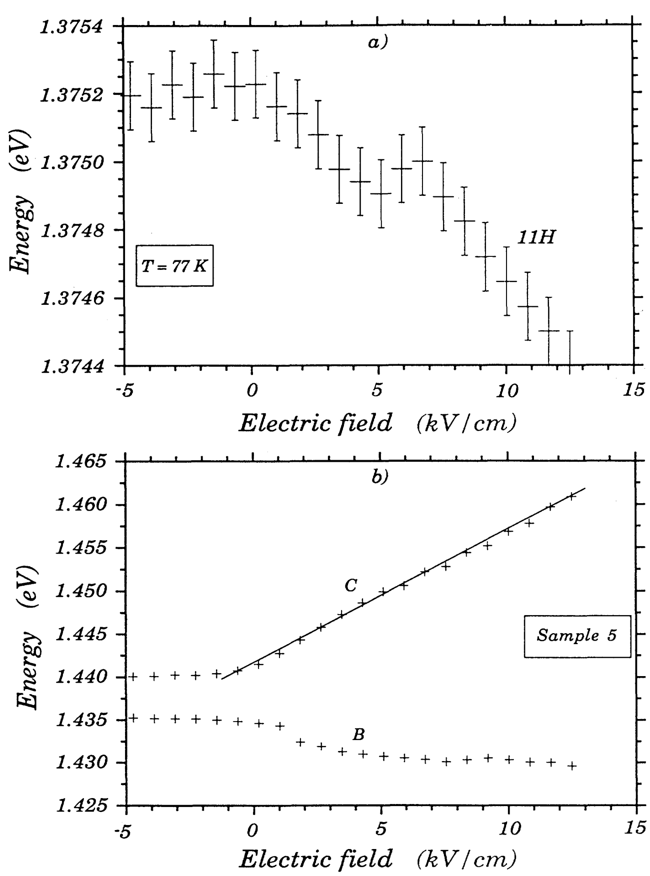

FIG. 11. (a) The Stark shift of the $11H$ transition, and (b) the shift in energy of the intermediate transitions, labeled B and C in Fig. 10 for sample 5 at $T = 77$ K.

It is interesting to consider the amplitude of the $11H$ peak, relative to the other spectral features, for all five samples (see Figs. 3, 6, 7, 8, and 10). The $11H$ increases as the well width is increased: the first three samples with narrow (3.5-nm) wells all display weak $11H$ peaks, while sample 5, where $L = 8.0$ nm, has a stronger $11H$ peak than the first three samples, but not one as large as sample 4, where $L = 12.0$ nm. Indeed, for an equal well depth, the capture efficiency of the well should improve if the wells are wider. This indicates that there is a well-width-dependent tradeoff between the continuum states and the bound states: narrow wells display strong continuum-state features and weaker bound-state-related transitions, whereas the opposite is true for wider wells.

C. MQW

In this section, we present ER results obtained with a MQW sample with five wells having the same well width, alloy composition, and cap-layer thickness as the SQW sample 5; the wells are separated with barriers 10 nm thick, so that the overlap of the wave function provides an energy spread for the electron ground states of only 2 meV. It is thus possible to compare directly the experimental results obtained with the MQW with those of the SQW in Fig. 10. Such a comparison will highlight the changes induced by the presence of additional wells on the cap-related quantum interference in the continuum states.

Figure 13 shows the ER spectra obtained with the MQW sample for various electric fields. At below-gap energies, the spectra are compared to those of Fig. 10 (the

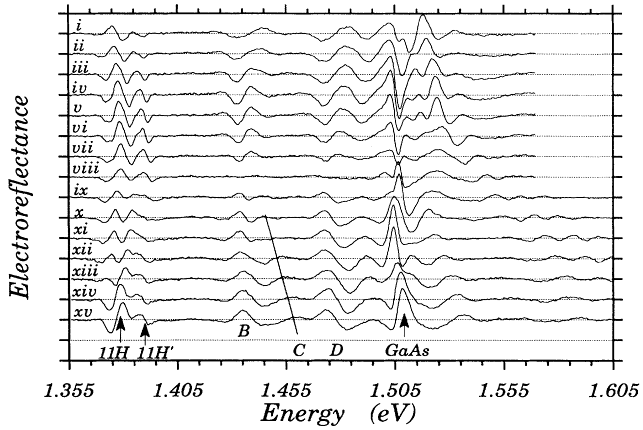

FIG. 13. ER spectra of the MQW at $T = 77$ K (five wells, $L = 8.0$ nm, barriers $d = 10.0$ nm, $t = 67$ nm), for bias voltages between 1.4 (curve *i*) and -1.4 V (curve *xv*) by increments of 0.2 V.

labels have the same meaning), except for the $11H'$ peak, which could occur because one of the five wells has a slightly different alloy composition or well width. The $11H'$ transition was also observed in photoluminescence and photovoltage spectra. The feature labeled *C*, associated with the continuum states (explained in the previous section), is shifting as in Fig. 10 for the SQW. For above-gap energies, the cap-related oscillations are much more pronounced than those seen in the spectra of the SQW in Fig. 10, as expected from theoretical calculations which predict an enhancement of the contrast in the oscillations of the probabilities of finding the carriers in the various regions in the case of a MQW structure.[5] The above-barrier oscillations of Fig. 13 are comparable to the oscillations observed in the ER spectra of sample 2 (Fig. 6), which has the same cap-layer thickness but a narrower well width. At positive biases, the spectra display the cap-related oscillations for the corresponding cap thickness of the electrons. As the negative bias increases the electric field, the extrema of the oscillations are shifted toward higher energies, as observed with the SQW's.

III. CONCLUSIONS

$In_xGa_{1-x}As/GaAs$ quantum-well structures having thin cap layers have been studied in the flat-band condition, and as a function of the applied electric field by PR and ER. As expected from theoretical considerations, transitions involving only bound states did not show any cap-related effects for the thicknesses studied (the smallest cap thickness was $t = 50$ nm), but the ER spectra have been used to verify that those transitions follow the expected selection rules and are Stark shifted. Systems with thinner cap layers have been investigated by Moison *et al.*[9] in order to study the effect of the cap layer on the bound energy levels in $Al_xGa_{1-x}As/GaAs$ quantum wells. The expected blueshift in transitions involving bound states for a thin cap layer was not observed due to surface states. Also, superlattices terminated with a higher barrier have been studied by Ohno *et al.*[10] They demonstrated that bound states of the well adjacent to that high barrier are modified by this different electronic environment. However, in either case, luminescence techniques were used, and the important effects of the cap-layer thickness on the continuum states were not verified. These continuum states can play a crucial role in some devices.[11] In the present study, the influence of the cap size on these continuum states was clearly demonstrated experimentally: strong cap-related energy-dependent oscillations are observed in PR and ER spectra for above-barrier energies. In the absence of electric field, the extrema of the oscillations follow a $\sin^2(k_b t)$ relationship, where t is the cap-layer thickness (i.e., the distance from the high potential to the well), and $k_b(E)$ contains m_b^*, the semiconductor effective mass in the cap layer, and E the energy above the barrier. In the case of the samples studied here, for a cap layer of 50 nm, the heavy holes make the dominant contribution, whereas for thicker cap layers the oscillations are due to the electrons. The extrema of these oscillations are expected to shift (linearly) in energy as an electric field is applied to the QW structure with a thin cap layer. The shifts observed experimentally follow qualitatively the predictions, but do not always correspond to the exact values expected for a uniform electric field, especially for thicker cap layers, suggesting that the potential depicted in Fig. 2 does not perfectly model the band diagram, most likely due to band bending. Thin wells showed more pronounced cap-related oscillations, and, also, as the cap-layer thickness increases, the spectral contribution of the usual resonant states increases, and the spectra tend to those expected where there are barriers of infinite extent on each side. The literature contains several examples[8,12,13] of spectra displaying above-barrier spectral structures observed in modulation spectroscopy of MQW samples. If thin cap layers were used, it is possible that some of these results may incorporate cap-layer effects such as those discussed here, since the contrast in cap-related quantum interference of the continuum states is enhanced by the presence of additional wells in the case of the MQW's, as was shown in Sec. II C.

ACKNOWLEDGMENTS

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