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Oscillatory behavior of the continuum states in $In_xGa_{1-x}As/GaAs$ quantum wells due to capping-barrier layers of finite size

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Photoreflectance spectra of $In_xGa_{1-x}As/GaAs$ single quantum wells have shown above-barrier oscillations, of amplitude comparable to those of transitions involving only bound states. The spacing between the oscillation extrema increases with energy according to the relation $E_n = E_0 + an^2$ for the nth extremum. These results demonstrate experimentally that the continuum states are influenced by the finite extent of the barrier on the side of the well which terminates the device (the cap layer). The high potential at the surface of the cap and the finite size of the cap layer produce quantum interference in the continuum state wave functions which leads to oscillations in the probabilities of finding the carriers in the various regions of the structure. The modulation is expected to be determined mainly by $\sin^2(k_b t)$, where t is the thickness of the cap layer and k_b is the wave vector in the barrier, and includes the carrier effective mass. Depending on the value of t, these cap-related oscillations are observed for the various types of carriers in photoreflectance experiments; their visibility depends on the well width.

Semiconductor devices of reduced dimensionality (quantum wells, superlattices, etc.) owe their interesting properties to quantum phenomena related to the physical size of the active layers. It is also known that, depending on the probing technique, the cladding layers surrounding the active quantum-well region may contribute to the phenomena observed,[1-4] but little research has been made on the influence of their spatial extent. If the carriers diffuse coherently throughout the device, remote interfaces can become an important part of the potential configuration. In the ideal model commonly used in calculations, a quantum well is considered to be surrounded by barriers of finite height but infinite extent on each side. In most cases, the barrier on the side of the buffer layer extends over a large distance (of the order of 1 μm). However, the cap layer on the other side of the well is generally much thinner (see Fig. 1), and the energy distribution of the carriers near the well may be modified by the presence of the external surface, which represents a high potential for these carriers within the semiconductor. The influence of the surface potential will be more important for continuum states than for bound states because their wave functions are not restricted to the well region.

Even in the absence of a nearby high potential, simple calculations show the presence of resonant states in the continuum for energies above the quantum well. They are believed to play an important role in the capture of the carriers by the well,[5,6] even though there is little experimental evidence to that effect and the results are sometimes contradictory.[7] In any case, the continuum states play an important role because they are the states to which the carriers are first excited when energies larger than the barrier are used.

In this paper we present preliminary experimental evidence for the effects of the high potential at the device surface on the continuum states in simple structures. These consist of single quantum wells (SQW) with thin ($t < 100$ nm) cap layers. Detailed experimental[8] and theoretical[9] accounts, including the influence of an applied electric field, will be presented in subsequent papers. Here, we will describe photoreflectance (PR) results; PR experiments were chosen for simplicity, to minimize electric field effects as much as possible. The spectra show strong oscillations at energies above that of the barrier. These oscillations are very different from the Franz-Keldysh (FK) oscillations observed in bulk materials, or

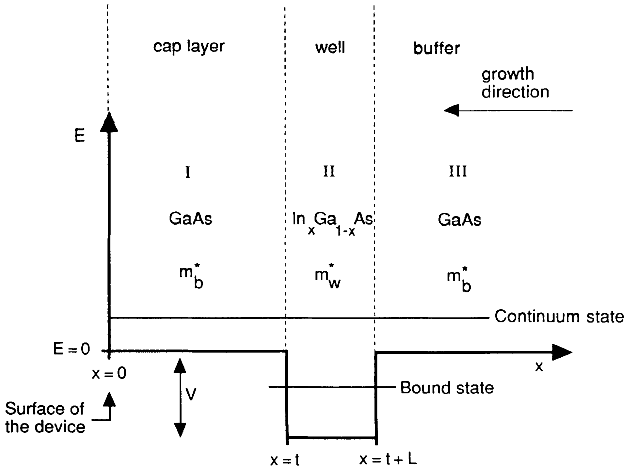

FIG. 1. Band diagram of a single quantum well with a thick buffer layer, a well width L, a capping barrier layer of finite size (cap width t), and a high potential at the surface at $x = 0$.

from the Wannier-Stark ladders created by an external electric field in superlattices.[10] For the effect discussed here, the extrema of oscillations scale as $E_n = E_0 + an^2$, whereas FK oscillations follow the relation $E_n = E_0 + a(n - \frac{1}{2})^{2/3}$. The quadratic relationship is a consequence of the boundary condition imposed on the cap layer wave function at the surface: $\Phi_{\rm cap}(x=0)=0$. Hence for the continuum states, $\Phi_{\rm cap} \alpha \sin(k_b x)$ where $k_b = (2m_b^* E/\hbar^2)^{1/2}$ is the wave vector in the cap layer, m_b^* is the effective mass, and x is the position; $x=0$ is at the surface, and the well starts at $x=t$, as shown in Fig. 1. The wave functions in the well and buffer regions are found by standard methods, and after some elementary algebra and integration of the probability density for the various regions, it follows that for above-barrier energies, the probabilities of finding the carriers in the various regions (the probability of finding carriers in the well region is often called the "well occupancy") will exhibit oscillations in energy, which are determined mainly by $\sin^2(k_b t)$, t being the cap layer thickness. Since the extrema of $\sin^2(k_b t)$ are given by

$$E_n = E_0 + \frac{\pi^2 \hbar^2}{8 t^2 m_b^*} n^2 , \tag{1}$$

the slope of the plot of the experimental extrema versus n^2 provides a measurement of the actual value of the cap thickness t. It is also expected that for a given t, the spacing between adjacent extrema will depend on the value of m_b^*. For example, for large enough t, the oscillations due to the heavy holes which have a large effective mass will be very dense and therefore difficult to detect experimentally, while the electrons will still give observable oscillations because of their smaller effective mass. Hence, the type of carriers causing detectable oscillations is expected to change from the heavy holes to the electrons as t is increased.

The samples studied here [grown by the metalorganic vapor-phase epitaxy technique on a Si-doped (100) GaAs substrate] were $\rm In_{0.16}Ga_{0.84}As$ SQW grown on a thick (1.0 μm) GaAs buffer layer, and terminated by a much thinner GaAs cap layer. The epitaxial material was undoped (so the band curvature at the surface should be minimal), with typical residual n-doping concentration in the range of 10^{14} cm^{-3}. In this paper, results are presented for cap thicknesses of 50 and 67 nm, and a fixed (3.5 nm) well width. The band diagram shown in Fig. 1 describes the situation for either the electrons or the heavy holes; the light holes are of type II,[11] and will not be discussed here. The potential at the surface of the sample is of the order of several electron volts (the work function of the semiconductor), whereas the depth (V) of the well is in the range of 100 meV.

Figure 2, curve a shows a 77-K PR spectrum for the SQW with a 50-nm cap layer. The low-intensity (about 1 mW/cm^2) light source used to modulate the PR was either a second monochromator at a fixed wavelength or an attenuated laser beam. The energy of the modulating light was larger than the energy gap of the barrier (GaAs), and larger than the energy of the probing beam as well. Within the above conditions, the oscillations were not affected by the choice of the energy of the modulating light. Two structures dominate the spectra at energies lower than the GaAs band gap, the $11H$ transition between the electrons and heavy holes on their first confined level, and a transition at an energy which would correspond to the energy difference between the GaAs valence-band edge to the first confined electron level. For energies above the GaAs gap (above the barrier), a series of oscillations appears. If one uses the model of a barrier of infinite spatial extent on each side of the SQW, the only quantum-well–related peak which could occur at above-gap energies (in the absence of an electric field[12]) would in this case correspond to a transition from the resonant continuum state of the heavy holes to the GaAs electron-band edge at about 30 meV above the GaAs gap. Another above-gap phenomenon which is commonly observed with semiconductors in modulation spectroscopy is the FK effect. But if one numbers the extrema consecutively as it is usually done for the FK effect, instead of an $E_n = E_0 + a(n - \frac{1}{2})^{2/3}$ dependence, one obtains a fit of the form $E_n = E_0 + an^2$; see Fig. 3, curve a. If the heavy holes are mainly responsible for the oscillations, the slope obtained from this graph would correspond to a cap-layer thickness of $t = 44$ nm according to Eq. (1). It is interesting to compare the results to a $\sin^2(k_b t)$ plot, for $t = 44$ nm, and where the heavy-hole effective mass of GaAs enters in k_b; see curve c of Fig. 2, and compare with curve a. Considering the simple assumptions used in the calculations, the model reproduces quite remarkably the positions of the minima and maxima of the experimental PR spectrum throughout the range of oscillation. Near the GaAs gap, the oscillations of curve c are very dense, and therefore may not have been resolved experimentally, or may be convoluted with weak FK oscillations resulting from a small residual electric field, or even slightly modified by this small field. Furthermore, the apparently irregular variations of the peak amplitude of the first few oscillations may be partly due to modulation of the electron con-

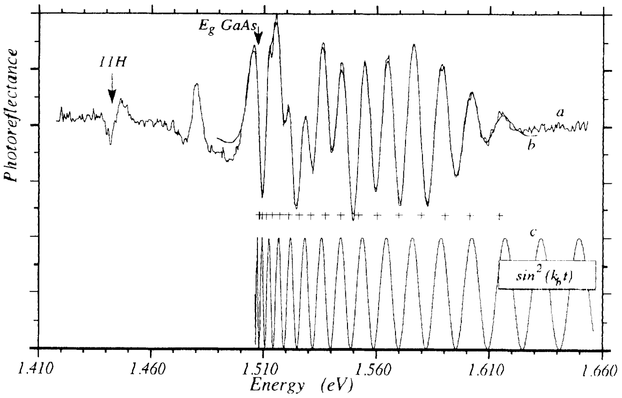

FIG. 2. Curve a: PR spectrum at $T = 77$ K showing above-barrier oscillations for an $\rm In_{0.16}Ga_{0.84}As/GaAs$ SQW with a well width of 3.5 nm, a cap-layer width of 50 nm, and a buffer of 1 μm. Curve b: Fit of the above-gap PR oscillations using Eq. (2) with the calculated transition energies marked by the crosses. Curve c: $\sin^2(k_b t)$ for $t = 44$ nm and using the effective mass of the heavy hole ($m_b^* = m_{\rm hh}^* = 0.37 m_0$); $k_b = [2m_b^*(E - E_g^{\rm GaAs})/\hbar^2]^{1/2}$.

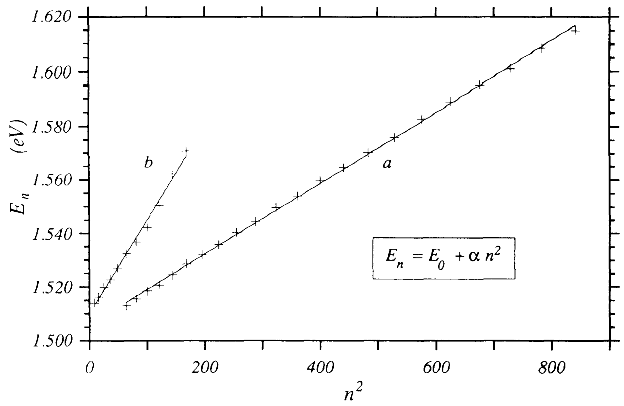

FIG. 3. Quadratic relationship between the energy positions (E_n) of the extrema and their index number (n) when the minimum and maximum are numbered in a Franz-Keldysh fashion. Curve a is for the oscillations of Fig. 2, curve b is for those of Fig. 4.

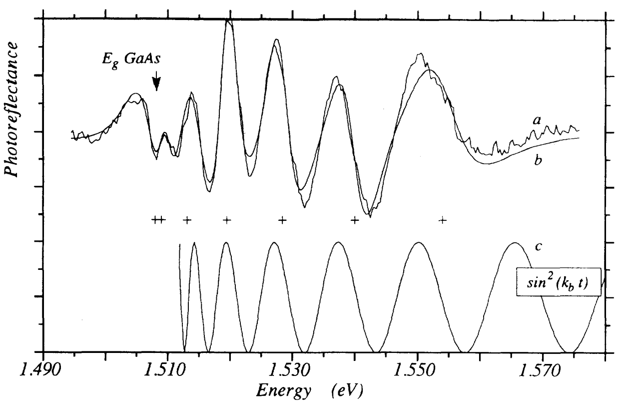

FIG. 4. Same as Fig. 2 but for a cap layer of thickness of 67 nm; in curve c, $t=67$ nm is used together with the electron effective mass ($m_b^* = 0.0665 m_0$).

tinuum states and to the usual resonant continuum state. The $\sin^2(k_b t)$ factor modulates the probabilities, and thus it is expected to yield the positions of the extrema; the amplitude of the oscillations in the probabilities can be shown to decrease as the energy over the well increases. However, the oscillations in the PR spectra seem to vanish more rapidly than predicted by the calculations. This may be partly related to the penetration depth of the probing light which varies rapidly in this spectral range. The cap-layer thickness found by this method is slightly different from the nominal value [which was verified with secondary-ion-mass spectroscopy (SIMS) measurements]; this is likely a consequence of neglecting the actual line shapes in the PR spectrum when numbering the extrema. The exact positions of the peaks of the well occupancy calculated for the heavy holes with $t=50$ nm are shown by the crosses in Fig. 2. The transitions at above-barrier energies are from the peak of the oscillations of the well occupancy of the heavy-hole continuum to the band edge of the electron continuum (or to the single electron bound state; but this would also result in oscillations at energies below the gap, which have not been observed). Using these values of energies (E_j), the PR line shape was fitted with third derivatives of three-dimensional critical points of the form[13]

$$S(E) = \mathrm{Re}\left[\sum c_j e^{i\theta_j}(E - E_j + i\Gamma_j)^{-m_j}\right] . \qquad (2)$$

To fit the data, the energies (E_j) and the order of the derivative ($m_j = 2.5$) were fixed, and the amplitudes (c_j), broadenings (Γ_j), and phases (θ_j) of the transitions were left as fitting parameters. The fit obtained with the E_j calculated for a value of $t=50$ nm, shown in curve b of Fig. 2, is in excellent general agreement with the experimental spectrum.

As explained above, for larger t, it is expected that the contribution to the oscillatory spectrum would eventually change from the heavy hole to the electron continuum. In the second example, a cap layer width of 67 nm was chosen, the well width being kept the same. The below-gap results (not shown) were comparable to those obtained in Fig. 2, curve a, as expected for bound-state-related transitions. Figure 4, curve a displays the above-barrier PR results for this SQW sample. As in Fig. 2, the crosses in Fig. 4 show the theoretical positions of the transitions, calculated for the electrons with $t=67$ nm in this case, which were used in Eq. (2) to fit the line shapes of the PR spectrum (see curve b). The quadratic fit for this sample (Fig. 3, curve b) gives a slope which corresponds to a 67-nm cap layer if one uses the electron effective mass in Eq. (1). Curve c of Fig. 4 showing a $\sin^2(k_b t)$ plot with k_b containing the electron effective mass, and $t=67$ nm, also can be compared to the experimental results of Fig. 4, curve a. The agreement with the actual thickness confirms that for larger t, the type of carriers responsible for the observable oscillations has changed from heavy holes to electrons.

For barrier-terminated samples (as for the $\mathrm{In}_x\mathrm{Ga}_{1-x}$-As/GaAs system), calculations show that the contrast in the cap-related quantum interference will be more pronounced for thin wells (like the ones used here), or in the case of multiple quantum wells. The reason the oscillations shown here are so strong (their amplitudes are even larger than the amplitude of the transitions involving bound states) is therefore the result of a favorable combination of cap and well thicknesses, as well as the low intensity of the modulating light. Spectra obtained with samples having larger well widths also showed oscillations related to their respective cap-layer thicknesses, but their amplitudes were much smaller than the amplitude of the transitions involving bound states. The literature contains several examples[11,14,15] of results which show above-barrier spectral structures. If thin cap layers were used, it is possible that some of these results may incorporate cap-layer effects as discussed here. This may help to interpret the results of Ref. 15, which describes quadratic above-gap oscillations.

In conclusion, one cannot assume the barrier to be infinite in extent in many actual quantum-well systems, and the cap-layer thickness (and its nature: barrier-terminated samples like the $\mathrm{In}_x\mathrm{Ga}_{1-x}\mathrm{As}$/GaAs system, or well-terminated samples like it are often the case with the $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$/GaAs system[3]) must be considered in the design of the samples, since it may significantly influence the properties of the system. In particular, experimental evidence is presented here which clearly shows that the continuum states over a SQW are very much influenced by the finite size of the cap layer. Instead of observing only the resonant continuum states, predicted by the usual model in which a SQW is surrounded by barriers of finite height but infinite extent, intense above-barrier oscillations related to the oscillations in the probabilities of finding the carriers in the various regions induced by finite cap layers were observed in PR. The energy spacing between the oscillation extrema increases as the energy increases, in contrast with the Franz-Keldysh case for which the spacing decreases as the energy increases. Under favorable conditions, this phenomenon can dominate the spectra, and the different type of carriers can be responsible for the effect, depending on the cap-layer thickness.

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