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Tunneling through indirect-gap semiconductor barriers

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Tunneling-current measurements in $Ga_{1-x}Al_xAs$-GaAs-$Ga_{1-x}Al_xAs$ heterostructures under hydrostatic pressure show that nonresonant tunneling occurs preferentially through the lowest potential barrier, while resonant tunneling is determined solely by a Γ-point profile. For fixed voltages, the low-temperature current through a 100 Å–40 Å–100 Å structure with $Ga_{0.60}Al_{0.40}As$ barriers increased with pressure, up to 11 kbar. The rate of increase showed an abrupt rise at ~4 kbar, which is attributed to tunneling through a Γ-X barrier. This interpretation is consistent with a rapid increase of the tunneling current in AlAs-GaAs-AlAs, even at low pressures. On the other hand, a negative-resistance feature associated with resonant tunneling via quantum-well states, shifted smoothly to lower voltages with pressure, indicating that the energy of the confined states is established by a pressure-dependent Γ-point profile.

In a semiconductor heterostructure composed of a thin dielectric layer A between slabs of a n^+-doped material B, an electron with energy in the forbidden gap of the film has a finite probability of tunneling through it. If the fundamental gaps of both A and B are at the same point of the Brillouin zone, e.g., Γ, the potential barrier for tunneling is the energy difference $E(\Gamma_A)-E(\Gamma_B)$. We examine here the question of which potential barrier controls the tunneling of electrons through an indirect-gap semiconductor, in which $E(\Gamma_A)-E(\Gamma_B)$ is no longer the minimum barrier.[1]

We have chosen the $Ga_{1-x}Al_xAs$ system, whose band structure can be drastically changed with variations in x or by the application of hydrostatic pressure. At atmospheric pressure, the minimum band gap of $Ga_{1-x}Al_xAs$ is direct for $0 \leq x < 0.45$, and located at the Γ point. For $x > 0.45$, the conduction band at X is lower in energy than at Γ, making the system indirect. Thus, the minimum potential barrier for an electron to tunnel through a thin $Ga_{1-x}Al_xAs$ film between two n^+-type GaAs electrodes is determined by the energy difference $E(\Gamma_{Ga_{1-x}Al_xAs})-E(\Gamma_{GaAs})$ if $x \leq 0.45$, and $E(X_{Ga_{1-x}Al_xAs})-E(\Gamma_{GaAs})$ if $x > 0.45$. A third barrier of comparable height arises from the $L_{Ga_{1-x}Al_xAs}-\Gamma_{GaAs}$ discontinuity.[2]

So far, the few studies reported reach conclusions that, at first sight, seem contradictory. Resonant tunneling experiments in double-barrier AlAs heterostructures are consistent with a potential configuration defined exclusively by the Γ point.[3,4] However, tunneling measurements through AlAs single layers have been explained by a Γ_{GaAs}-X_{AlAs} barrier,[5] and experiments on $Ga_{0.54}Al_{0.46}As$ also favor a substantial contribution of the X point.[6]

A closer look to the various tunneling processes may explain this paradox. We can consider two kinds of processes regarding the conservation of momentum perpendicular to the tunneling direction, assumed to be the [100] direction: direct and indirect tunneling.[7] The former occurs between the same extrema of the projected Brillouin zones of GaAs and $Ga_{1-x}Al_xAs$. An example of this is a Γ-point process, with a Γ-Γ barrier. Indirect tunneling, in which perpendicular momentum is not conserved, requires inelastic scattering with impurities, phonons, etc. This is the case of tunneling via the four L-point valleys (Γ-L barrier), and via two of the three X-point valleys [010] and [001], with a Γ-X barrier. Tunneling involving the X minimum at [100] can occur as a direct process.

The relative contribution of the various mechanisms is determined by the tunneling probabilities, which depend on the barrier height and effective mass of each path, and by the rate of electron transfer between Γ and the other zone extrema. Since m^Γ is the lightest, for $x < 0.4$, tunneling $Ga_{1-x}Al_xAs$ is expected to be direct and to proceed almost exclusively through the Γ-Γ barrier.[8] The mass along [100] of the L ellipsoids $m^L_{[100]}$, is about twice as large as m^Γ, so that when the L point becomes lower in energy than the Γ point ($x > 0.5$), tunneling through Γ-L may become significant.[9] Similarly, $m^X_{[100]}$ for the [010] and [001] X ellipsoids is about three times m^Γ, and therefore indirect Γ-X tunneling could be important beyond $x = 0.45$, when the Γ-X barrier is the lowest. The extreme case corresponds to AlAs, in which $E(\Gamma_{AlAs})-E(\Gamma_{GaAs})=1.05$ eV, $E(L_{AlAs})-E(\Gamma_{GaAs})=0.39$ eV, and $E(X_{AlAs})-E(\Gamma_{GaAs})=0.16$ eV. The small Γ-X barrier can therefore explain the single-barrier tunneling measurements of Bonnefoi, Chow, McGill, and Burnham[5] and of Hase, Kawai, Kaneko, and Watanabe.[6]

On the other hand, resonant tunneling is a direct process, sensitive to the Γ-Γ barrier. Consequently, the confined quantum states in the potential between two barriers are determined by a Γ-Γ profile, as shown by the results of Bonnefoi *et al.*[3] and Tsuchiya, Sakaki, and Yoshino[4] on AlAs-GaAs-AlAs. (There is also a direct-tunneling channel through the [100] X ellipsoid that leads to confined states in $Ga_{1-x}Al_xAs$ via a Γ-X profile, as recently demonstrated.[10])

The experiments reported here confirm the validity of these concepts based on the effective-mass approximation. We have relied on the fact that under hydrostatic pressure the Γ- and L-point energies of GaAs increase (relative to the top of the valence band) at a rate of 10.5 and 5.5 meV/kbar^{-1}, respectively, while the X point goes down by 1.5 meV kbar^{-1}. The pressure coefficients of $Ga_{1-x}Al_xAs$ are similar to those of GaAs (Ref. 11). Thus, in the direct-gap regime ($x \leq 0.45$) $Ga_{1-x}Al_xAs$ undergoes a transition to indirect-gap material at a critical pressure that decreases linearly with increasing x, from $\sim$40 to 0 kbar. The valence-band discontinuity between GaAs and $Ga_{1-x}Al_xAs$ is taken to be independent of pressure, which, as explained below, is a good assumption.

Resonant and nonresonant tunneling was observed in undoped double-barrier heterostructures AlAs-GaAs-AlAs and $Ga_{0.60}Al_{0.40}As$-GaAs-$Ga_{0.60}Al_{0.40}As$, sandwiched between n^+-type GaAs electrodes (Si doped to 10^{18} cm^{-3}). The thickness of each layer in the former structures was 50 Å. In the latter, the barrier widths were 100 Å and the well thickness was either 40 or 60 Å. In all cases, the heterolayers were grown by molecular-beam epitaxy on (100)-oriented n^+-type GaAs substrates.

The samples (mesa-eteched circles, 250 μm in diameter) were enclosed in a Be-Cu cell, together with a calibrated InSb pressure gauge. Hydrostatic pressure was applied at room temperature by compressing the liquid (kerosene) in which they were immersed, and the cell was subsequently cooled to 77 K. The hydrostatic nature of the pressure was confirmed by resonant tunneling measurements, up to 11 kbar, in AlAs-GaAs-AlAs heterostructures clad by p^+-type GaAs contacts. The negative-resistance features associated with resonant tunneling through heavy- and light-hole states[12] remained unchanged up to the highest pressure. This shows the absence of uniaxial-pressure components, which would have produced a change in the relative position of the heavy- and light-hole resonances,[13] and the independence with pressure of the valence-band discontinuity.

The current-voltage (I-V) characteristics of the 40-Å-well heterostructure are shown in Fig. 1(a) for representative pressures. The low-voltage current, followed by a negative conductance region starting at $\sim$0.25 V, corresponds to resonant tunneling of electrons through the only confined state in the well. The onset of a positive conductance at $\sim$0.5 V represents tunneling through one of the $Ga_{0.60}Al_{0.40}As$ barriers, as the other one has effectively disappeared under the high bias.

The off-resonance current increases with increasing pressure p reducing the peak-to-valley ratio of the resonant component, and at high p dominates the tunneling process, even at low bias. A similar behavior is found for the 60-Å-well sample, in which two resonant tunneling structures[10] at 0.11 and 0.45 V disappear in a background of pressure-induced nonresonant current. The effect is even more dramatic in the AlAs-GaAs-AlAs heterostructure [see Fig. 1(b)], where the disappearance takes place at much lower pressures.

The increase of current with pressure, at constant voltage, is shown in Fig. 2 for the $Ga_{0.60}Al_{0.40}As$ barrier. At 0.55 V, a critical pressure $p_c \sim 4$ kbar separates two re-

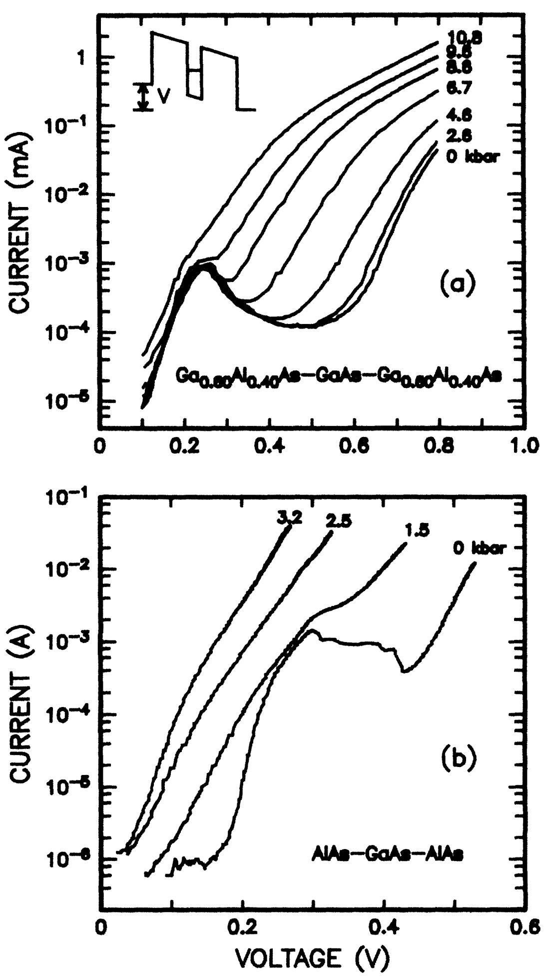

FIG. 1. Current-voltage characteristics at 77 K, for representative pressures, of (a) $Ga_{0.60}Al_{0.40}As$-GaAs-$Ga_{0.60}Al_{0.40}As$ and (b) AlAs-GaAs-AlAs, double-barrier heterostructures. (See sketch in the inset.) In the former, the thickness of the barriers is 100 Å, and that of the well is 40 Å. For the latter, the thickness of each layer is 50 Å. In (a) an apparent flat conductance at high bias and high pressure is a consequence of large series resistance. A similar effect, also present in AlAs-GaAs-AlAs, has been corrected in (b).

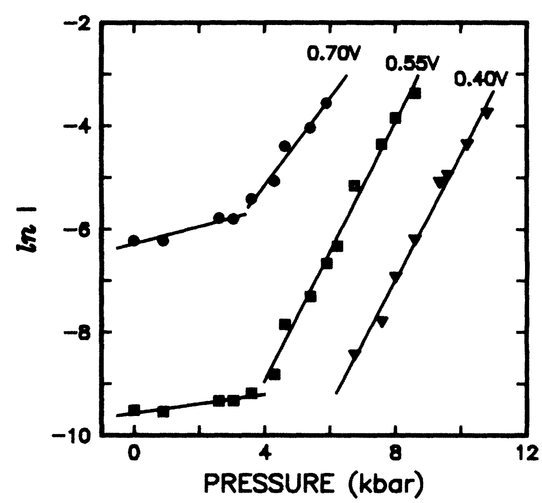

FIG. 2. Tunneling current, in logarithmic scale, vs hydrostatic pressure, at constant bias, for the sample of Fig. 1(a). The voltages shown correspond to total biases applied to the samples. The actual voltage drop in the double-barrier heterostructure may be smaller, especially for the highest bias at high pressure. For $V \leq 0.4$ V, the current is dominated at low pressures by resonant tunneling, and its value does not change appreciably with pressure.

gions of very different slopes: 0.092 and 1.26 kbar^{-1}. At higher bias, e.g., 0.70 V, the behavior is similar, although the slope at high pressures is affected by series resistance [see Fig. 1(a)]. At lower bias, e.g., 0.40 V, the rapid current increase is also observable at high pressure.

Since at high bias the electron energy is above the top of the barrier near the collector, the current change can be analyzed in terms of variations of the electron effective mass and of the height of a single potential barrier. At 0.55 V, tunneling occurs in the Fowler-Nordheim regime, and

$$\frac{d(\ln I)}{dp} = -0.685\frac{m^{1/2}V_B^{3/2}w}{V}\left[\frac{1}{2}\frac{d(\ln m)}{dp}+\frac{3}{2}\frac{d(\ln V_B)}{dp}\right], \tag{1}$$

where the effective mass m is in units of the free-electron mass, the height of the barrier V_B is in eV, its width w is in angstroms, and the voltage drop across it V is in volts.

As pressure enhances the effective mass, any increase in tunneling current is due to a reduction of the barrier height. Using Γ-point parameters, $m=0.101$, $V_B=0.28$, $w=100$, $V=0.23$, and $d(\ln m)/dp=0.005$, we get $dV_B/dp=-1.7$ meV kbar^{-1} for $p<p_c$, and -17 meV kbar^{-1} for $p>p_c$. The small decrease of the barrier height at low pressure is consistent with electrons tunneling through a Γ-Γ barrier. In addition, it shows that the pressure coefficients of the fundamental energy gaps of GaAs and $\mathrm{Ga_{0.60}Al_{0.40}As}$, although similar, are slightly different, in agreement with previous suggestions that the latter is smaller than the former.[14,15] However, the abrupt decrease of V_B above p_c is incompatible with tunneling exclusively via Γ-Γ.

We attribute the discontinuity of dV_B/dp to indirect tunneling through the Γ-X barrier. The critical pressure of ~ 4 kbar agrees well with the estimated value of the direct-indirect transition in $\mathrm{Ga_{0.60}Al_{0.40}As}$, and, above p_c, dV_B/dp is comparable to the rate of decrease of the X point, relative to the Γ point of GaAs. Further support to this interpretation is provided by tunneling measurements in AlAs-GaAs-AlAs heterostructures.

The tunneling current through AlAs barriers increases rapidly with pressure, as seen in Fig. 1(b), at a rate $d(\ln I)/dp=2.09$ kbar^{-1} for a total bias of 0.20 V. An analysis similar to the one leading to Eq. (1), for a Γ-Γ discontinuity of 1.05 eV, in the rectangular-barrier limit, yields $dV_B/dp>0.2$ eV kbar^{-1}, which is unrealistic. As in $\mathrm{Ga_{0.60}Al_{0.40}As}$, the current increase is attributed to tunneling through the very low Γ-X barrier.

For the proposed Γ-X tunneling channel to be comparable to the Γ-Γ path, m^X should not be very heavy, relative to m^Γ. Its value can be estimated from our result of $d(\ln I)/dp$, if we take dV_B/dp to be the difference between the pressure coefficients of the Γ and X points -12 meV kbar^{-1}. For the $\mathrm{Ga_{0.60}Al_{0.40}As}$ barrier we get $m^X=0.18$, and for AlAs, $m^X=0.26$. These values correspond to the mass along the [100] direction, that is the transverse mass of the [010] and [001] X ellipsoids. The good agreement with the values available in the literature,[9] ranging from 0.19 to 0.27, has to be taken cautiously, however.

The above analysis has several limitations. First, precise values for the band parameters used are unknown. Second, we have used the formalism of the WKB approximation for a single barrier, ignoring quantum reflections, as well as charge accumulation in the barriers and any voltage drop in the electrodes. These simplifications introduce uncertainties in our estimations, although probably not large for $\mathrm{Ga_{0.60}Al_{0.40}As}$ barriers. In AlAs, the value for the effective mass is more questionable, since we have used an expression corresponding to the Fowler-Nordheim regime, which is outside the voltage range of the measurements. A more realistic estimation, using a trapezoidal potential, would increase somewhat the effective mass.

In addition to decreasing Γ-X, pressure lowers the Γ-L barrier, and since $m^L_{[100]}$ is ~ 0.11 (Ref. 16), a substantial amount of current may tunnel through the latter at high pressure. This path should be more important in $\mathrm{Ga_{0.60}Al_{0.40}As}$ than in AlAs, since for the latter the Γ-L barrier is more than twice the height of $\Gamma-X$. The relative contribution of the inelastic channels, however, depends not only on individual tunneling probabilities but also on the unknown rates of electron transfer from the Γ to the X and L points.

The effect of pressure on the Γ-Γ barrier can be derived directly from resonant tunneling. Although not apparent in Fig. 1(a), a careful analysis of the conductance versus bias shows that the negative-resistance structure of $\mathrm{Ga_{0.60}Al_{0.40}As}$-GaAs-$\mathrm{Ga_{0.60}Al_{0.40}As}$ shifts to lower voltages with increasing p. Figure 3 illustrates this dependence for the voltage of minimum conductance, which is directly related to the energy E_0 of the confined state in the quantum well. The $p=0$ value is in reasonable agreement with the calculated confinement energy in the presence of an electric field. A Γ-Γ profile also explains the negative-resistance voltage in AlAs-GaAs-AlAs, in agreement with previous works.[3,4]

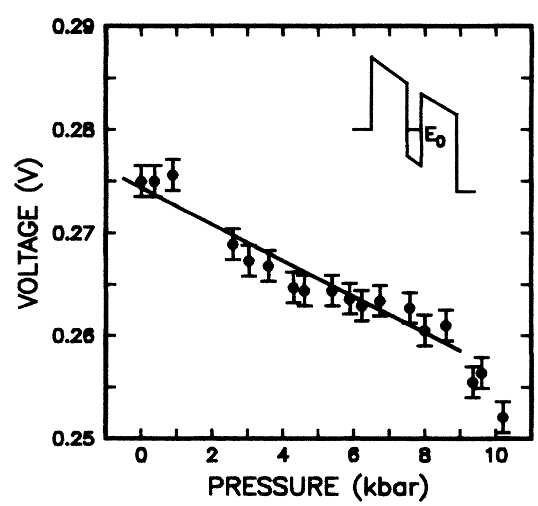

FIG. 3. Voltage of minimum conductance vs pressure, for the sample of Fig. 1(a). The energy of the quantum state in the GaAs well is approximately half this voltage. A least-squares fit to the data (●) up to 8.5 kbar gives a slope of -1.76 mV kbar^{-1}. A larger decrease above 9 kbar results from the dominant presence of nonresonant current. The inset sketches the potential profile that leads to negative resistance.

Assuming that the voltage drop outside the double barrier is independent of pressure (which is invalid at very high bias, as seen in Fig. 1), the observed shifts must arise from the pressure-induced increase of the effective mass and possibly from a reduction of the barrier height. The smooth decrease of the resonant voltage with increasing p, well beyond p_c, confirms that only the Γ-Γ barrier is involved in resonant tunneling. An apparently larger shift at very high p (>9 kbar), results from the large nonresonant background that shifts the voltage of minimum conductance to lower values. The observed rate of decrease of the quantum state, $dE_0/dp=-0.88$ meV kbar^{-1}, can be accounted for by a barrier decrease of 3 meV kbar^{-1} together with a mass enhancement, which alone would produce a downshift of 0.3 meV kbar^{-1}.

The reasonable agreement between this estimation and dV_B/dp derived from nonresonant tunneling supports the interpretation that for $p<p_c$ indirect tunneling through the Γ-L barrier does not contribute significantly. Furthermore, it indicates that the pressure coefficients of GaAs and $Ga_{0.60}Al_{0.40}As$ for the Γ point are slightly different. An analogous difference for the X and L points would change the quantities deduced here; however, the main conclusions, that the X point contributes significantly to indirect tunneling beyond the direct-indirect transition, and that resonant tunneling is determined by direct tunneling, should remain valid. In cases in which the transfer rate from Γ to other points would strongly favor the Γ-Γ path over others (e.g., Γ-X), the former could dominate for very thin barriers, even when Γ-Γ is significantly higher than Γ-X.

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[1]This work has been presented in part at the American Physical Society Meeting, Las Vegas, 1986: E. Calleja, E. E. Mendez, and W. I. Wang, Bull. Am. Phys. Soc. **31**, 394 (1986).

[2]We have used the following band discontinuities (in eV):

$E(\Gamma_{Ga_{1-x}Al_xAs})-E(\Gamma_{GaAs})$	$0.70x$	$0\le x\le 0.45$
	$0.70x+1.15(x-0.45)^2$	$0.45<x\le 1$
$E(L_{Ga_{1-x}Al_xAs})-E(\Gamma_{GaAs})$	$0.30+0.092x$	$0\le x\le 1$
$E(X_{Ga_{1-x}Al_xAs})-E(\Gamma_{GaAs})$	$0.44-0.42x+0.14x^2$	$0\le x\le 1$

These expressions have been determined using the data of H. C. Casey, Jr. and M. B. Panish, *Heterostructure Lasers* (Academic, New York, 1978), Pt. B, p. 17, for the various energy gaps; and the results of J. Batey and S. L. Wright, J. Appl. Phys. **59**, 200 (1986), for the valence-band discontinuities. The Γ-L and Γ-X energies for GaAs at low temperatures have been taken from D. E. Aspnes, C. G. Olson, and D. W. Lynch, Phys. Rev. Lett. **37**, 766 (1976), and U. Venkateswaran, M. Chandrasekhar, H. R. Chandrasekhar, T. Wolfram, R. Fischer, W. T. Masselink, and H. Morkoç, Phys. Rev. B **31**, 4106 (1985), respectively.

[3]A. R. Bonnefoi, R. T. Collins, T. C. McGill, R. D. Burnham, and F. A. Ponce, Appl. Phys. Lett. **46**, 285 (1985).

[4]M. Tsuchiya, H. Sakaki, and J. Yoshino, Jpn. J. Appl. Phys. **24**, L466 (1985); M. Tsuchiya and H. Sakaki, *ibid.* **25**, L185 (1986).

[5]A. R. Bonnefoi, D. H. Chow, T. C. McGill, and R. D. Burnham, Bull. Am. Phys. Soc. **31**, 395 (1986).

[6]I. Hase, H. Kawai, K. Kaneko, and N. Watanabe, J. Appl. Phys. **59**, 3792 (1986).

[7]E. O. Kane, J. Appl. Phys. **32**, 83 (1961).

[8]D. C. Taylor, P. S. S. Guimaraes, B. R. Snell, L. Eaves, F. W. Sheard, G. A. Toombs, J. C. Portal, L. Dmowski, K. E. Singer, G. Hill, and M. A. Pate, in *Proceedings of the Second International Conference on Modulated Semiconductor Structures, Kyoto, 1985* [Surf. Sci. (to be published)].

[9]The effective mass of $Ga_{1-x}Al_xAs$ at the Γ point has been taken as $0.066+0.088x$ [H. J. Lee, L. Y. Juravel, J. C. Woolley, and A. J. Spring-Thorpe, Phys. Rev. B **21**, 659 (1980)]. Since for the L and X points, when $x>0$, only the density-of-states mass is known, we have used in the full range of compositions the mass-tensor components of GaAs. [See, e.g., J. S. Blakemore, J. Appl. Phys. **53**, R123 (1982).] For the pressure dependence, we have assumed that $d(\ln m)/dp=d(\ln E_G)/dp$, where E_G is the appropriate energy gap.

[10]E. E. Mendez, E. Calleja, C. E. T. Gonçalves da Silva, L. L. Chang, and W. I. Wang, Phys. Rev. B **33**, 7368 (1986).

[11]As the pressure coefficients of the L and X points for $Ga_{1-x}Al_xAs$ ($x>0$) are not well known, we have used the values for GaAs, given by J. S. Blakemore, J. Appl. Phys. **53**, R123 (1982). The pressure coefficient of Γ for GaAs has been taken from the low-temperature measurements of D. J. Wolford and J. A. Bradley, Bull. Am. Phys. Soc. **29**, 291 (1984), which agrees with the value reported by U. Venkateswaran, M. Chandrasekhar, H. R. Chandrasekhar, B. A. Vojak, F. A. Chambers, and J. M. Meese, Phys. Rev. B **33**, 8416 (1986).

[12]E. E. Mendez, W. I. Wang, B. Ricco, and L. Esaki, Appl. Phys. Lett. **47**, 415 (1985).

[13]A. Pinczuk, D. Heiman, R. Sooryakumar, A. C. Gossard, and W. Wiegmann, Surf. Sci. **170**, 573 (1986).

[14]N. Lifshitz, A. Jayaraman, R. A. Logan, and R. G. Maines, Phys. Rev. B **20**, 2398 (1979).

[15]U. Venkateswaran *et al.*, Ref. 11.

[16]D. E. Aspnes, Phys. Rev. B **14**, 5331 (1976).