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Theoretical and experimental investigation of doped-channel p-type quantum wells

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The influence of ionized impurity scattering on the hole mobility in δ-doped-channel AlGaAs-InGaAs quantum wells is investigated. Improvements by a factor of 2.5 were observed experimentally when moving a δ-doped impurity plane across the quantum well towards an interface, highlighting the scope of selective doping and wave-function engineering techniques to enhance the transport mobility of such devices. Theoretical hole mobility calculations were performed and reveal an overestimation of the transport mobility, common to the random-phase approximation (RPA), that is much stronger for p-type structures than for n-type structures. This effect is partially attributed to an underestimation of the screening charge distribution width. Using a lower limit for this distribution of around 50 Å, it is shown that the RPA can provide accurate predictions between samples with different impurity distributions and densities.

I. INTRODUCTION

Heterojunction field effect transistor (FET) designs based on the modulation-doped high electron mobility transistor (HEMT) approach have been widely used to produce devices with high operating speed. However, as the sheet carrier density in these modulation-doped devices is limited by the band offset, there is a considerable interest in doped-channel devices for high power applications. These give an increased carrier density and current capability, but at the expense of a degraded mobility.1,2

When designing such channel-doped structures, one would obviously like to minimize the effect of ionized impurity scattering on the device performance. Selective doping (using, for example, δ doping) or wave-function engineering techniques can be used to tailor the position of the carrier distribution and achieve a maximum separation with respect to the impurities. The work by Masselink3 showed that moving the impurity plane towards the quantum-well interface in an n-type channel-δ-doped quantum well (QW), thereby reducing the wave-function overlap, can result in a considerable improvement in the low-temperature mobility. Our group recently reported on a series of n-type device structures which demonstrated the possibility of obtaining doped channel structures with a high channel density (≈5×10¹² carriers/cm²) combined with a high mobility and saturation drift velocity comparable to existing devices.4 This was achieved by using a combination of edge-δ-doping and grading the InₓGa₁₋ₓAs quantum well, thus achieving a separation between the carriers and the impurity plane.

This paper specifically concerns the investigation of p-type channel-doped AlGaAs-InGaAs structures. Experimental results for the hole transport mobility in a set of channel-δ-doped AlGaAs-InGaAs QW’s are compared with the results of a theoretical model of carrier transport based on the random-phase approximation (RPA) formalism.5–7 This work thus provides insight in the scope of selective doping to optimize high-density hole gas structures for device applications, as well as information about the accuracy of the RPA model when applied to hole structures.

II. EXPERIMENTAL

Two sets of p-type 60 Å InGaAs-AlGaAs QW’s were grown by molecular-beam epitaxy (MBE), all consisting of a 1000 Å Al₀.₃₃Ga₀.₆₇As buffer layer grown at 580 °C, followed by 2000 Å Al₀.₃₃Ga₀.₆₇As over which the temperature was gradually lowered to 510 °C, a 60 Å In₀.₁₅Ga₀.₸₅As QW, 2000 Å Al₀.₃₃Ga₀.₆₇As over which the temperature was increased to 580 °C, capped by 100 Å GaAs. This first set (A) contains six samples, δ doped at either 2.0×10¹² cm⁻² or 3.5×10¹² cm⁻² at the center of the QW, at 15 Å from the top QW interface, or at 5 Å from the top QW interface. From now on, the latter three doping positions will be referred to as center, 1/2, and edge doped. The structures of the second set (B) contain four δ-doped planes. Two of the δ-doped planes were placed in the well at 5 Å from the top and bottom interfaces, the first sample doped at 1.2 and the second at 1.7×10¹² cm⁻². The two other δ-doped planes were placed in the barriers at 30 Å from the top and bottom interfaces, respectively, doped at 0.65 and 0.80×10¹² cm⁻², providing an additional 10¹² carriers cm⁻² to the QW (the rest of the carriers are expected to be lost to the surface and substrate). The structures were set up such to exhibit a symmetrical confinement potential to avoid the lifting of Kramer’s degeneracy that can become significant in unsymmetrical structures at such high densities. X-ray diffraction revealed a slightly lower indium composition than specified in set B of
about 13%. Note that special attention was paid in the design of all structures to ensure that only one subband was populated.

The structures were analyzed by Hall and resistivity measurements, both at room temperature and at 77 K. It proved impossible to determine the quantum mobilities because of the low mobilities of such p-type channel-doped devices.

III. THEORETICAL MODEL

The theoretical model consists of two separate parts. First, to obtain the carrier density, envelope functions, subband occupancies, and band structure, a self-consistent Poisson-Schrödinger (SCPS) solver is used (Sec. III A). The obtained quantities are then translated to experimentally verifiable quantities like the Hall mobility and Hall density via an ionized impurity scattering model (Sec. III B).

A. SCPS calculations

The self-consistent Poisson-Schrödinger solver used in this work has previously been successfully applied to the investigation of n-type δ-doped QWs. However, the valence-band dispersion relations are now calculated using a six-band effective-mass model which has been reduced to two \(3 \times 3\) Hamiltonians using a unitary transformation. Because of the added complexity of the unitary transformation, inner products between wave functions are evaluated within a simpler four-band approach as the spin-orbit component only accounts for a very small fraction (of the order of a few percent) of the total wave function. The four-band approximation is thus not expected to significantly affect the wave-function overlap.

The valence-band lineup was determined by taking the valence band of GaAs as a reference level and using the band offset ratios given by Refs. 10 and 11. All other material parameters were taken from Ref. 12. It is assumed that the substrate is in charge equilibrium and that the Fermi level at the top air-GaAs interface is pinned at 0.4 eV above the valence band. The latter value, which is not critical for the wide barriers as used in this work, is in qualitative agreement with Ref. 13.

B. Impurity scattering in heterostructures

The presence of an ionized impurity in an otherwise perfect crystal introduces a potential fluctuation that can cause the electrons to scatter. This potential fluctuation \(\phi(r)\) is equal to the Coulomb potential of the impurity itself \(\phi^{\text{ext}}(r)\) plus the accompanying screening potential, which can be seen as a response of the system to the introduction of the charged impurity. Various methods to obtain the exact total potential fluctuation have been proposed but there is a much more convenient implementation of the effects of screening, as it follows from Fermi’s golden rule that only the projection of this total potential on the initial and final wave functions involved in the scattering process \(\psi_n\) and \(\psi_n'\) are required, \(\phi_{nm'}(r) = \langle \psi_n'(r) | \phi(r) | \psi_n(r) \rangle\). As a result, the screening effects can conveniently be accommodated by introducing a dielectric response matrix \(\varepsilon_{nm,mm'}\). In this paper the screening of the Coulomb scattering potential is taken into account within the random-phase approximation (RPA) which has proved to be very successful. Despite its apparent complexity, this approach reduces to the much simpler Thomas-Fermi approximation (TFA) in the long-wavelength limit. We will not give the explicit form for the RPA dielectric response matrix as it has previously been presented in the literature.

Using the dielectric response matrix to describe the scattering potential, it follows directly from Fermi’s golden rule that the scattering rate per unit angle for a transition \(|n,k\) \(\rightarrow |n',k'\) in a δ-doped system is given by

\[
\Gamma_{nn'}(\theta) = \frac{m^* e^4 N_D}{8 \pi \hbar^3 (\varepsilon_0 \varepsilon_r q)^2} \sum_{m,m'} \varepsilon_{nn',mm'}^{-1}(q) \times \int dz f_{n,k}(z) f_{n',k'}(z) \exp(-q|z-z_0|)^2,
\]

where \(m,m'\) run over all subbands, \(N_D\) is the impurity density of the δ-doped plane located at \(z_0\), \(f_{n,k}\) is the envelope-function vector to \(|n,k\). All other variables have their usual meaning. The total transport scattering rate \((\tau_{\text{tr}})^{-1}\) for a given transition is then obtained by including the form factor \([1 - \cos(\theta)]\) and integrating over all angles. The above model reduces to that of Masselink and Thobel when modeling a single conduction-band level. In this case, the carrier mobility is directly given by \(\mu = e \tau_1^\text{tr}/m^*\) and the dielectric response matrix takes the form \(\varepsilon(q) = [1 + 1/2a_0^2 q]\), where \(a_0^2\) is the effective Bohr radius. Note that all effective masses should be taken as \(m^*(E) = \hbar^2 k(\partial E/\partial k)^{-1}\) as this is the relevant definition of effective mass when modeling an ensemble of carriers.

The situation is slightly more complicated in the valence-band case. To comply with the previous literature, we now write \(f_{n,k}(z) f_{n',k'}(z) = g_{n,k}(z) g_{n',k'}(z) G_{n,n',k,k'}\). Here \(g_{n,k} = \int f_{n,k}(z)\) such that \(g_{n,k}\) denotes the probability distribution perpendicular to the direction of the quantum well. Ehrenreich’s overlap function \(G_{n,n',k,k'}\) (Ref. 20) originates from the fact that the hole wave function at finite \(k\) is no longer described by a single envelope function. Rather, it is now given by \(\psi = \sum_i f_i u_{i0}\), where \(u_{i0}\) are the zone-center solutions and the summation over \(i\) runs over all bands explicitly used in the effective-mass expansion. The overlap function thus contains all the effects imposed by band mixing. Analytic expressions for \(G_{n,n',k,k'}\) for bulk material have been presented by Wiley and show that the overlap function deviates significantly from unity. Figure 1 shows the results obtained for various two-dimensional QW structures. As expected, quantum confinement and strain reduce the band mixing and push the overlap function for low in-plane momentum to unity. However, it is clear that the overlap factor has to be taken into account at higher densities.

Temperature effects are neglected in the evaluation as the thermal broadening at 77 K is smaller than the energy scale at which an appreciable change of the effective mass occurs. As the contribution of phonon scattering is negligible for such heavily doped structures at this temperature, the experimental results are directly comparable to the theoretical calculations which are effectively performed at the absolute zero.
ratio of 1.72 between the conductivity with and without tor. Lyo23 performed a similar calculation for two-interaction for an ionized impurity limited bulk semiconductor with a much lower electron density than featured in this work. Thus, transport mobility can be obtained by adopting an empirical scaling factor of about 2.

The origin of such a scaling factor is thought to be caused by the presence of electron-electron (e-e) scattering. One has to note that e-e scattering is momentum conserving, so that the process itself does not affect the mobility. However, it can negatively affect the mobility by scattering carriers to parts of the Brillouin zone that are stronger affected by the other available scattering mechanisms. Its action is thus not described by Matthiessen’s rule, but rather by a scaling factor such as introduced earlier. To illustrate, Appel22 obtained a factor of 1.72 between the conductivity with and without e-e interaction for an ionized impurity limited bulk semiconductor. Lyo23 performed a similar calculation for two-dimensional heterostructures and obtained a limiting scaling factor of 2 when the e-e scattering rate is much larger than the ionized impurity scattering. Hu24 finds a scaling factor that depends on the position of the impurity plane for a system with a much lower electron density than featured in this work of $1.5 \times 10^{11} \text{cm}^{-2}$. This factor takes the value of about 1.67 when the e-e interaction becomes dominant. All of this supports the view that electron-electron interaction is the main cause for the observed deviation between experimental and theoretical ionized impurity limited mobility in n-type structures.

Turning to the p-type structures of this work, it is found that the discrepancy between the theoretical and experimental transport mobility is substantially larger. Not only do the theoretical results now overestimate the mobility by a substantially higher factor of approximately 8, but the prediction for the trend of set B is also inaccurate (Fig. 2). Obviously, insight of the cause of the discrepancies is required to be able to successfully use the RPA to model hole devices. Although hole-hole interaction effects are expected to add to the scaling factor, it seems unlikely that such an indirect mechanism would solely account for the observed deviation. Thus, as scattering is well understood, it follows that the most likely cause for the deviation is an overestimation of the screening effects.

The TFA and RPA predict that the screening charge around an impurity is located within a distance of the order of the effective Bohr radius. Incoming holes with a wavelength much longer than this radius will not scatter as they will not be able to resolve the separation between impurity and screening charge, and effectively see zero charge. In contrast, holes with a wavelength shorter than this radius would be able to see the individual components and thus scatter.

Since we are essentially modeling the Fermi contour, we have so far been using a screening charge distribution width related to the Bohr radius of that of the carriers at the Fermi energy. However, this results in an overestimation of the screening as the carriers nearer the band edge simply cannot produce such a narrow distribution due to the nonparabolic dispersion and lower mass. Furthermore, we find that the Bohr radius becomes comparable to the two-dimensional (2D) Wigner-Seitz radius ($r_s$) for effective masses around $m^* = 0.12m_0$ at $10^{12} \text{cm}^{-2}$ or $m^* = 0.21m_0$ at $3 \times 10^{12} \text{cm}^{-2}$, compared to a typical value of $m^* = 0.3m_0$ for the structures presented in this work. As a result, we indeed expect the RPA to break down when modeling highly doped p-type structures as the screening charge distribution such as predicted by RPA is too narrow to be sustained by the available hole system.

One possible method to obtain a realistic screening charge distribution width is by imposing a maximum limit to the screening mass in the dielectric response matrix. It is important to note that changing this mass only affects the distribution and not the amount of the screening charge. Fixing the screening mass would result in a mass dependency of the hole mobility at low temperature of $\mu \propto (m^*)^{-2}$. Such a mass dependency was actually observed by Fritz25 in a set of $\text{In}_{0.3}\text{Ga}_{0.7}\text{As-GaAs QW's}$ for hole masses above $m^* = 0.14m_0$. The latter corresponds to a Bohr radius of about 50 Å, and provides confirmation that a lower limit to the distribution width is a reasonable assumption.

Figure 3 shows a comparison between calculated and experimental hole mobilities. The theoretical mobilities were scaled by a factor 8.
matrix only. All other parameters were unchanged. Slightly better overall agreement between theory and experiment is obtained. This is especially visible in the trend in the structures of set B where now correctly a decreasing mobility with increasing density is predicted as the mass dependency in the screening has been eliminated. The scaling factor has also been reduced to 4.5, which is in better agreement with that found in electron mobility calculations and the corresponding explanation in terms of hole-hole interaction. The fact that the high-density edge-doped structure of set A has a slightly higher experimental mobility than that predicted theoretically can be explained by segregation effects. A simple way to simulate this is to reevaluate the mobility for the transport mobility in two-dimensional heterostructures calculated within the RPA is substantially larger then that found in the electron case. It was postulated that the larger hole mobility scaling factor is at least partially caused by an underestimation of the screening charge distribution width in such a nonparabolic system.

A first attempt to account for the latter was done by adjusting the effective mass in the dielectric response matrix. An upper limit of this effective mass of \( m^* = 0.14m_0 \), corresponding to a lower limit of about 50 Å for the screening charge distribution width, was deduced from literature results. Despite the relative simplicity of the approach, it was shown that the predictive power of the RPA scattering model is increased and can now provide reasonable accurate qualitative predictions for the transport mobility in \( p \)-type two-dimensional hole gases. Unlike the conduction-band case, there is no theoretical work available that describes the contribution of hole-hole scattering to the scaling factor in two-dimensional hole gases.

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