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11. Quantum transport: Silicon inversion layers and InAlAs-InGaAs heterostructures.
Quantum transport: Silicon inversion layers and InAlAs–InGaAs heterostructures

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I. INTRODUCTION

Electron transport properties of quasi-two-dimensional (Q2D) systems have been studied quite extensively, experimentally as well as theoretically. The inversion layer at a silicon interface represents the most widely employed physical realization of the Q2D concepts and the electron mobility of the inversion layer electrons is one of the most important parameters for device characterization. It has been confirmed experimentally that for substrates with low doping densities, the electron mobility follows a universal curve when plotted as a function of the effective electric field. However, pushing the devices towards scaling limits necessarily leads to thinner oxide films (<10 nm) and higher substrate dopings (>10$^{17}$ cm$^{-3}$). For these devices, it was recently demonstrated that experimental mobilities significantly deviate from the universal curves near the threshold voltage as a consequence of significant depletion charge scattering.

Since the invention of the modulation doping technique, transport properties of two-dimensional electron gases in high-mobility modulation doped AlGaAs–GaAs heterojunctions (MDHs) have also been a subject of great interest from both the technological and fundamental point of view. The enhanced mobilities in these structures are attributed to the spatial separation of the electrons from their parent donors, which significantly reduces the scattering rate from the remote impurities. This has stimulated much research toward their application in low-power, high-speed devices. Recently, there has been an increased interest devoted to the growth of InAlAs–InGaAs lattice matched heterojunctions which have better carrier confinement due to a larger conduction-band discontinuity and a lighter conduction-band effective mass (compared to AlGaAs–GaAs). However, since the electron gas in the InAlAs–InGaAs MDH is mostly localized within a ternary random alloy (InGaAs), alloy scattering is much more effective so that it is hard to imagine that the low-temperature mobility of InGaAs based modulation doped heterostructures may exceed the very high mobilities already reported in AlGaAs–GaAs heterostructures.

The theoretical model for the calculation of the subband structure and the electron mobilities of the Q2D electron gas, taking into consideration all major scattering mechanisms and both intrasubband and intersubband scattering, is briefly described in Sec. II. In Sec. III, devoted to transport in silicon inversion layers, we describe the influence of depletion charge scattering on the mobility results near the threshold gate voltage. We also show how the weighting coefficients for the inversion and depletion charge densities, which appear in the definition of the average electric field, vary with doping density. Low-temperature transport properties of the modulation doped In0.4Al0.6As-In0.4Ga0.6As heterostructures are discussed in Sec. IV. Some concluding comments related to the present work are given in Sec. V.

II. THEORETICAL MODEL

The subband structure is obtained from a self-consistent solution of the Schrödinger and Poisson equations, coupled with the Dyson equation for the retarded Green’s function. Exchange-correlation corrections to the chemical potential are calculated within the local density approximation. The self-energy contributions from the various scattering mechanisms are evaluated by employing the self-consistent Born approximation. Screening is treated within the random phase approximation. In the calculation of the conductivity, we have taken account of a correction term due to the particle-hole ladder diagrams. More details on the calculational model and the analytical expressions for the broadening of the states and conductivity can be found elsewhere.

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The physical model employed in these calculations includes scattering with all bulk phonons (acoustic and nonpolar optical), surface-roughness scattering, and Coulomb scattering from both ionized impurities in the depletion region and interface/oxide charges. For intervalley scattering (zero-order and first-order interactions), we use the same phonon energies and coupling constants as those relevant for bulk silicon. The anisotropy of the deformation potential interaction is also accounted for. More details about the model can be found in the Appendix.

In Fig. 1, we compare our simulation results for the mobility with the experimental effective mobility data for n-channel metal-oxide-semiconductor field-effect transistors (MOSFETs) fabricated on (100) Si wafers. Filled circles and triangles represent the experimental effective mobility data derived from drain conductance measurements. The inversion charge density has been determined from the gate-channel capacitance measurements. Solid (dashed) lines are the corresponding simulation results when depletion charge scattering is included (omitted) in the calculations. A total of four subbands (three from the unprimed and one from the primed ladder of subbands) are taken into account. We use an exponential model for the surface-roughness autocorrelation function. We find that the rms height of the bumps is 0.26 nm (0.25 nm) for the device with lower (higher) doping. For both devices, roughness correlation length is estimated to be 1.4 nm.

III. SILICON INVERSION LAYERS WITH HIGH DOPING PROFILES

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IV. In$_{0.4}$Al$_{0.6}$As-In$_{0.4}$Ga$_{0.6}$As MODULATION DOPED HETEROSTRUCTURES

At low temperatures, the dominant scattering mechanisms in the In$_{0.4}$Al$_{0.6}$As-In$_{0.4}$Ga$_{0.6}$As MDH shown in Fig. 3 are: remote impurity (from the δ-depletion layer), interface-trap, alloy disorder, interface-roughness and deformation potential, and piezoelectric-coupled acoustic mode scattering. Polar optical phonon scattering is found not to play any significant role at 1.6 K. Screening of the alloy disorder and deformation potential scattering potentials by the free carriers is also neglected because of their short-range nature. This effect should certainly have been included for the long-range electron-piezoelectric acoustic phonon interaction, but since this scattering process is extremely weak at 1.6 K, its matrix element is also left unscreened. Assuming that deformation potential scattering is an elastic process, one has $\hbar \omega / k_B T$...
Gate

<table>
<thead>
<tr>
<th>Layer Description</th>
<th>Material Composition</th>
</tr>
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<tbody>
<tr>
<td>30 nm und In\textsubscript{0.4}Al\textsubscript{0.6}As (barrier layer)</td>
<td></td>
</tr>
<tr>
<td>10 nm und In\textsubscript{0.4}Al\textsubscript{0.6}As (spacer)</td>
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<tr>
<td>50 nm und In\textsubscript{0.4}Ga\textsubscript{0.6}As (well)</td>
<td></td>
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<tr>
<td>0.1 μm und In\textsubscript{0.4}Al\textsubscript{0.6}As (buffer layer)</td>
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<td>0.1 μm und In\textsubscript{0.4}Al\textsubscript{0.6}As (buffer layer)</td>
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<tr>
<td>0.1 μm und In\textsubscript{0.4}Al\textsubscript{0.6}As (buffer layer)</td>
<td></td>
</tr>
<tr>
<td>Semi-insulating GaAs substrate</td>
<td></td>
</tr>
</tbody>
</table>

FIG. 3. Cross-sectional view of the δ-doped In\textsubscript{0.4}Al\textsubscript{0.6}As-In\textsubscript{0.4}Ga\textsubscript{0.6}As heterostructure on (100)-oriented semi-insulating GaAs substrate with intermediate, undoped, and compositionally step-graded buffer layers.

\[ \frac{3^{\frac{1}{2}}\alpha_0 \sqrt{m^* \beta^2 m_e T}}{\sqrt{\pi}} = \sqrt{4 \beta m_e T}, \]  

where \( \alpha_0 \) is the phonon frequency, \( k_B \) is the Boltzmann constant, \( \epsilon_L \) is the longitudinal elastic constant, \( m^* \) is the effective mass, and \( \rho \) is the crystal density. Using the material parameters summarized in Table I, we find that the equivalent temperature is \( T_e \approx 0.22 \) K. Thus, the equipartition approximation can be assumed to hold for temperatures above 1 K for the acoustic mode scattering of thermal electrons. The matrix elements for surface roughness, acoustic phonon, and alloy disorder scattering can be found elsewhere. For the wavevector dependent matrix element for scattering between subband \( n \) and \( m \) due to Coulomb charges located at a distance \( z_i \) from the interface (in the InAlAs layer), we use the following expression:

\[
\langle n | U(q, z_i) | m \rangle = \frac{e^2}{2q\epsilon_b} \int_{-\infty}^{0} dz \psi_m(z) e^{-q|z-z_i|} + \frac{e_b e_w}{\epsilon_b + \epsilon_w} e^{-q|z+z_i|} \psi_m(z) + e^2 \int_{-\infty}^{0} dz \psi_n(z) e^{-q|z-z_i|} \psi_m(z) \tag{1}
\]

in which the image term due to the difference of the static dielectric constants in the well (\( \epsilon_w \)) and in the barrier layer (\( \epsilon_b \)) is properly taken into account. The effective mass enhancement with increasing gate voltage due to conduction band nonparabolicity is also taken into account.

When solving for the subband structure, the number of the self-consistent field iterations was considerably decreased when using the analytical solutions of the Poisson equation. We calculate that in equilibrium, the electron transfer from the δ-doped region to the well (see Fig. 3) is governed by

\[
E_F + \Phi_0 - eV_G = \Delta E_c + \frac{e^2 N_D L}{\epsilon_b} \sum_i \int_{-\infty}^{0} z \psi_i^2(z) dz - \frac{e^2}{\epsilon_b} (W + L) \sum_i \left\{ N_i^0 \left[ 1 - \int_{-\infty}^{0} \psi_i^2(z) dz \right] + N_i^0 \int_{-\infty}^{0} \psi_i^2(z) dz \right\}, \tag{2}
\]

where \( L = 30 \) nm and \( W = 10 \) nm are the widths of the barrier and spacer layers, \( E_F \) is the Fermi level, \( \Phi_0 = 0.8 \) eV is the Shottky barrier height, \( V_G \) is the gate voltage, \( \Delta E_c = 0.52 \) eV is the conduction band offset, \( N_D = 3 \times 10^{22} \) cm\(^{-2} \) is the Si δ-doping sheet, and \( N_i^0 (N_i^0) \) is the sheet electron density of the \( i \)th subband in the barrier (quantum well).
Self-consistent results for the gate-voltage dependent electron densities are shown in Fig. 4. We observe good agreement between the experimental data derived from the Hall effect and SdH measurements and the theoretical calculations for all gate voltages. Our simulation results are also in agreement with the theoretical calculations reported by Wieder et al. We find that the significant effective mass enhancement (see the inset of Fig. 4) due to conduction band nonparabolicity prevents the population of the third subband until \( V_G > 0.4 \) V. We also find that, in contrast to silicon inversion layers where exchange-correlation effects are significant even at room temperature, many-body corrections do not considerably affect the subband structure in the MDH because of the small effective mass.

Gate-voltage dependence of the low-temperature theoretical mobilities is shown in Fig. 5. Although the average mobility is \( \mu = \frac{1}{N_i \mu_i} \), measured mobilities shown in Fig. 5 are Hall mobilities so that for a multisubband case, the expression \( \frac{1}{N_i \mu_i} = \frac{\mu_i}{N_i} \) is more suitable for comparing the experimental results with the theoretical calculations. To take into account the diffusion effects, the \( \delta \)-doping sheet is modeled as a 4 nm wide layer centered 8 nm away from the interface with Si doping density of \( 7.52 \times 10^{18} \) cm\(^{-3} \). Interface-roughness scattering is assumed to exist at both heterointerfaces of the quantum well. We assume that the rms height of the roughness is one monolayer (ML) \( \Delta = 2.83 \) Å. The lateral spread of the interface roughness is taken to be \( \zeta = 100 \) Å. For this particular heterostructure, we find that surface-roughness and acoustic phonon limited component mobilities (not shown on the figure) are of the order of \( (0.5 - 1) \times 10^6 \) and \( 10^7 \) cm\(^2\)/V s, respectively. By fitting the calculated mobilities at high gate voltages to the experimental data, we were able to determine the alloy-disorder scattering parameter in the system to be in the range 0.5–0.55.

Component mobility results presented in Fig. 5 suggest that the inclusion of alloy scattering, in addition to Coulomb scattering (from the ionized donors in the \( \delta \)-doped region and interface traps), leads to good agreement between the theoretical calculations and the experimental data. The dip in the theoretical mobility at \( V_G = -0.85 \) V signals that a new channel (second subband) for scattering opens in the MDH which leads to a sudden increase in phase space for scattering between the two subbands to occur. Since the carriers residing in the first excited subband are at about four times larger average distance from the heterointerface (compared to those in the ground subband), they do not feel as much the Coulomb scattering potentials and exhibit about two times higher mobility.

V. CONCLUSIONS

Our results suggest that depletion charge scattering, which has been ignored in some previous theoretical studies, is responsible for the deviation of the mobility from the universal curves near the threshold voltage. At high gate voltages (high values of \( N_i \)), due to the closer confinement of the carriers to the interface, the magnitude of the mobility in these highly doped samples is considerably reduced by surface-roughness scattering, in addition to the still significant intervalley scattering. We also find that the weighting coefficients \( a \) and \( b \) that appear in the definition of the average electric field—show a pronounced doping dependence. For the In\(_{0.4}\)Al\(_{0.6}\)As-In\(_{0.4}\)Ga\(_{0.6}\)As MDH, we find that at \( T = 1.6 \) K the magnitude of the mobility is limited by Coulomb and alloy scattering. From the subband structure (gate-voltage dependence of the electron density) and mobility simulations, we calculate that the relevant effective mass at the conduction band minima of the In\(_{0.4}\)Ga\(_{0.6}\)As ternary alloy is \( m^* = 0.058 \) \( m_0 \). An observed effective mass enhancement suggests that nonparabolicity effects are considerable in this MDH and must be taken into account if accurate mobility results are desired. The effect of the many-body interactions, calculated in the local density-functional approximation, is found not to be important for the MDH.

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APPENDIX

The expression for the matrix elements for scattering between subbands \( n \) and \( m \) due to a Coulomb charge in the depletion region, in the oxide, or right at the interface, in the presence of a different dielectric medium, can be found in the review article by Ando, Fowler, and Stern. For the surface-roughness matrix element, we use the result obtained by Ando who corrected the result obtained by Matsumoto and Uemura by taking into account the change in the electron density distribution and the effective dipole moment of

![Graph showing cumulative and component theoretical mobilities vs gate voltage.](image)
the deformed Si–SiO₂ surface in addition to the usual local potential energy term that equals the linear term of the Taylor expansion of the surface potential.

For anisotropic elastic continuum such as silicon, for which the deformation potential constant Ξ is a tensor,²⁹ matrix element squared for scattering between subbands n and m due to acoustic phonons, in the usual equipartition approximation, equals to²¹

$$\langle n | U^{eq}_{\lambda}(q) | m \rangle^2 = \frac{k_B T}{\rho V \nu_{\lambda}} \left[ \Delta^{eff}_{\lambda, nm}(q) \right]^2 F_{nm},$$  \hspace{1cm} (A1)

where

$$F_{nm} = \int_0^\infty dz \, \psi_n^*(z) \psi_m(z),$$  \hspace{1cm} (A2)

νₐ is the sound velocity, and ρ is the Si mass density. The effective deformation potential constant that appears in expression (A1) is calculated from

$$\left[ \Delta^{eff}_{\lambda, nm}(q) \right]^2 = \frac{1}{F_{nm}} \int_0^\infty dz \, \Delta^{\lambda}_{nm}(q) \mathcal{S}_{nm}(z),$$  \hspace{1cm} (A3)

where

$$\mathcal{S}_{nm}(z) = \int_0^\infty dz \, \psi_n(z) e^{i q z} \psi_m(z)$$  \hspace{1cm} (A4)

and $\theta_Q$ is the angle between the wave vector Q of the emitted (absorbed) phonon and the longitudinal axis of the valley. According to Hirring and Vogt,²⁹ the effective deformation potentials $\Delta_{\lambda}(\theta_Q)$ ($\lambda$=LA or TA) that appear in Eq. (A3) are given by

$$\Delta_{LA}(\theta_Q) = \Xi_d + \Xi_a \cos^2(\theta_Q),$$  \hspace{1cm} (A5a)

$$\Delta_{TA}(\theta_Q) = \Xi_a \cos(\theta_Q) \sin(\theta_Q).$$  \hspace{1cm} (A5b)

In Eqs. (A5a) and (A5b), $\Xi_a$ is the uniaxial shear potential, and $\Xi_d$ is the dilatation potential that are believed to have values of approximately 9.0 and −11.7 eV, respectively.²¹,³⁰ It is important to point out that Eq. (A5b) accounts for the contribution of both TA branches.

The matrix element for nonpolar optical phonon scattering is generally found from a deformable ion model. The zero-order process, which describes a perturbation that can be associated with the local dilatation or compression of the lattice which produces local fluctuation in the electron energy, dominates at moderately high electron energies. The matrix elements for scattering between subbands n and m (that belong to α and β valleys) due to a zero-order interaction is given by

$$\langle n | U^{eq}_{\alpha}(q) | m \rangle^2 = \frac{\hbar D_{\lambda}^2}{2 \rho V \omega_{\lambda}} F_{nm},$$  \hspace{1cm} (A6)

where $D_{\lambda}$ is the deformation field and $\omega_{\lambda}$ is the frequency of the phonon mode.

When the zero-order matrix element for the optical or intervalley interaction vanishes, then $D_{\lambda}$ is identically zero. In this case, one has to consider the first-order term of the interaction. The squared matrix element for scattering between subbands n (α valley) and m (β valley) due to this first-order process is given by³¹

$$\langle n | U^{eq}_{\alpha}(1) | m \rangle^2 = \frac{\hbar D_{\lambda}^2}{2 \rho V \omega_{\lambda}} (q^2 F_{nm} + c_{nm}),$$  \hspace{1cm} (A7)

where

$$c_{nm} = \int_0^\infty dz \left\{ \frac{d}{dz} \left[ \psi_n^*(z) \psi_m(z) \right] \right\}^2.$$  \hspace{1cm} (A8)

In the scattering among the equivalent valleys, there are two types of phonons that might be involved in the process. The first type, the so-called g phonon couples the two valleys along opposite ends of the same axis, i.e., (100) to (100). This is an umklapp process and has a net phonon wavevector $0.3 \pi/\alpha$. The so-called h phonons couple the (100) valley with (010), (001), etc. Hence, the reciprocal lattice vector involved in the g-process is $G_{100}$ and that for an h process is $G_{111}$.

Within a four subband approximation, scattering between the two valleys in the $e_0$, $e_1$, and $e_2$ subbands involves only g-type phonons. The scattering between these three minima is treated by using a high-energy phonon of 750 K activation temperature (treated as zero-order interaction) and 134 K phonon treated via first order interaction. Scattering between the $e_0$, $e_1$, and $e_2$ subbands and the four $e_0'$ subbands involves f phonons with activation temperatures of 630 and 230 K treated via zero-order and first-order interactions, respectively. Scattering between the $e_0'$ subbands involves both g and f phonons with activation temperatures of 630 K (zero-order interaction) and 190 K (first-order interaction). All of the high-energy phonons are assumed to be coupled with a value of $D_{\lambda} = 9 \times 10^8$ eV/cm, and all of the first-order coupled phonons are assumed to be coupled with $D_{\lambda} = 5.6$ eV. These values are consistent with the results given in Refs. 20 and 32.

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