Electrons in Heterojunctions

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Properties of electrons - and, in a few cases, of holes - in heterojunctions are described, with emphasis on simple treatments of energy levels and low-temperature transport properties in $Al_xGa_{1-x}As/GaAs$ heterojunctions. A few related aspects of electrons in quantum wells are also described.

1. Introduction

Although heterojunctions have been structures of basic interest and of device potential for many years, [1] the rapid developments in recent years have been spurred by the availability of growth techniques for making nearly ideal structures and by the superlattice proposal of Esaki and Tsu, subjects covered in other lectures at this School. The two-dimensional aspects of the properties of electrons in heterojunctions had as a forerunner the related properties of electrons in semiconductor inversion and accumulation layers, a field that was in some sense opened by the experiment of Fowler, Fang, Howard, and Stiles [2], although there was a considerable body of related work on that system and on thin films even earlier. For the purpose of these lectures I will not discuss these earlier developments, some of which are described in the review article by Ando et al.[3]. The reader should recognize that much of the elementary physics of electrons in heterojunctions is taken bodily, or in some cases adapted, from the earlier literature.

First, a few basic results. The density of states in a two-dimensional electrons gas is given by :

$$\rho_0(E) = m/\pi\hbar^2 \tag{1}$$

where m is the density-of-states effective mass for motion along the interface and where a spin degeneracy of 2 and a valley degeneracy of 1 have been assumed. When, as described below, there is a ladder of subbands i, with energies beginning at E_i, then the total density of electrons is given, with Fermi-Dirac statistics, by

$$N_s = \frac{mk_BT}{\pi\hbar^2} \sum_i \log \; 1 + \exp \left(\frac{E_F-E_i}{k_BT}\right) \tag{2}$$

where the density-of-states mass has been taken to be a constant, an approximation which ignores the nonparabolicity of the conduction band of GaAs. The simple notion of a constant, isotropic effective mass fails altogether for holes, as will be discussed in the lectures by Altarelli [4].

2. Heterojunction in Equilibrium

The simple, ungated heterojunction considered here is shown in Fig. 1. This figure omits the band bending associated with a gate or with Fermi level pinning at the outer surface of a real device, and therefore applies to structures in which the $Al_xGa_{1-x}As$ layer is sufficiently thick that these influences are absent. The additional effects induced by a gate will be discussed in the lectures by Vinter [5].

In most high-mobility heterojunctions, electrons are supplied to the GaAs channel by donors in the $Al_xGa_{1-x}As$ [6,7]. In a heterojunction in equilibrium, the Fermi level must be constant across the junction, leading to the condition

$$V_b = E_{Db} + V_l + V_{sp} + E_o + (E_F - E_o) \tag{3}$$

where V_b is the conduction band offset at the interface, E_{Db} is the donor binding energy in the $Al_xGa_{1-x}As$, V_l and V_{sp} are the potential energy drops across the ionized part of the doped layer and across the undoped spacer layer, respectively, E_o is the lowest quantum level in the GaAs channel, and E_F-E_o is the Fermi energy in the GaAs channel measured from the bottom of the lowest subband.

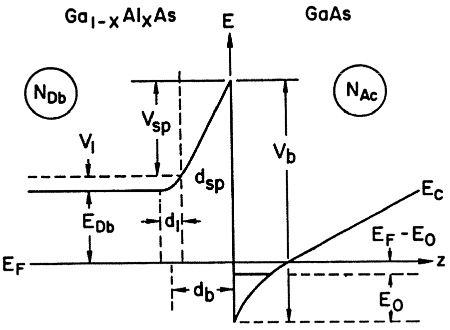

Fig.1 Schematic conduction band diagram for $Al_xGa_{1-x}As$/GaAs heterojunction at low temperature. The doping levels in the barrier region and in the GaAs are N_{Db} and N_{Ac}, respectively, and the thickness of the nominally undoped spacer is d_{sp}. The Fermi level in the barrier is assumed to be fixed by the donor binding energy E_{Db}.

Although the considerations leading to Eq. (3) are well known [8,9], this equation will be discussed here briefly, because it has turned out to be one way to determine band offsets, as applied to holes in $Al_xGa_{1-x}As$/GaAs heterojunctions by Wang et al. [10,11] and to electrons in GaInAs/AlInAs heterojunctions by Chaudhuri et al. [12]. The case shown in Fig. 1 assumes that the donor binding energy in $Al_xGa_{1-x}As$ is deep enough for the Fermi level to be pinned at the impurity level at low temperatures. That implies that any shallow donor levels, if present, are outnumbered by the residual acceptors often found in $Al_xGa_{1-x}As$. If the AlAs mole fraction x is small, or in the presence of light, Eq. (3) must be modified to account for a Fermi level above the conduction band edge in the $Al_xGa_{1-x}As$ [13].

The potential energy changes V_l and V_{sp} of Fig. 1 are given by

$$V_l = e(N_d + N_s)^2/2\varepsilon_b N_{Db}, \tag{4}$$

$$V_{sp} = e d_{sp}(N_d + N_s)/\varepsilon_b, \tag{5}$$

where ε_b is the permittivity of the $Al_xGa_{1-x}As$, N_{Db} is the net donor impurity concentration in the $Al_xGa_{1-x}As$, N_s is the channel electron density, and N_d is the density of fixed charges in the GaAs, given approximately by

$$N_d = (2\phi_d \varepsilon_c N_{Ac}/e)^{1/2}, \tag{6}$$

where ε_c is the permittivity of GaAs, N_{Ac} is the net acceptor concentration in the GaAs, and $e\phi_d$ is the energy difference between the conduction band edge in the bulk of the GaAs and the Fermi level (or the quasi-Fermi-level in the bulk, if there is a substrate bias or back gate bias). A more complete discussion is given, for example, in Sec. III.A.1 of Ref. 3.

The last term in Eq. (3) is simply given from the channel density N_s and the density of states, Eq. (1) or, for temperatures above absolute zero, from Eq. (2). The quantum energy E_o is found from methods like those outlined in the following section. The channel density itself is determined from a Hall effect measurement or from analysis of the magnetoconductance oscillations. If Eq. (3) is to be used to determine the band offset V_b, the remaining unknowns are the donor binding energy and N_d, the density of fixed charges. N_d is difficult to determine accurately because the impurity concentration in the GaAs may not be well known, especially for relatively pure samples. Fortunately, in those cases N_d is often small compared to N_s. It may be possible to measure N_d using back gate bias [14] or to infer it from measured subband splittings in conjunction with theoretical calculations [15,16].

The donor binding energy in $Al_xGa_{1-x}As$ has been known for many years to have a strong dependence on composition [17,24] and is difficult to measure accurately. Wang et al. [10,11] used p-type samples to determine the valence band offset from the valence band analog of Eq. (3). This has advantages over the corresponding procedure for n-type samples,because the acceptor binding energy in $Al_xGa_{1-x}As$ varies more gradually with composition than the donor binding energy, and because p-type samples are relatively free of the persistent photoconductance [25,32] that complicates many measurements on n-type samples. Wang et al. [10,11] studied p-$Al_xGa_{1-x}As$/GaAs heterojunctions with $x = 0.5$ and $x = 1$. They found that the valence band offset is given approximately by 0.45x (in eV) although other measurements, some of which are noted in Ref. 11, give values closer to 0.5 x. Most of the recent values (see Ref. 11 for a partial compilation) are considerably larger than the valence band offsets ($\sim$ 0.2 x, in eV) originally found by Dingle et al. [33] from analysis of quantum well optical absorption spectra, which were generally accepted for many years.

This abbreviated discussion does not cover the possible sources of error, both theoretical and experimental, that may affect this so-called charge transfer method of determining band offsets, nor does it describe the other methods that have been used. It shows, however, that very simple physics can sometimes lead to unexpected and useful results.

3. Subband Structure

The energy level structure of quasi-two-dimensional systems is easily calculated within the framework of effective mass approximation, provided that the complications associated with valley degeneracy, effective mass anisotropy, and with the complex valence band structure of most III-V and group IV semiconductors are put aside. We assume that the electron states (the simple considerations that follow are generally not valid for holes) have effective mass m and are derived from a single conduction band minimum. Then the one-electron wave function can be written as a product

$$\psi(x,y,z) = \zeta_i(z)\, u(r) \exp(iK.R), \tag{7}$$

where $\zeta_i(z)$ is the envelope wave function for the ith subband, u(r) is the periodic Bloch function associated with the bottom of the conduction band, and K and R are vectors in two-dimensional wave-vector and configuration space, respectively.

Within the spirit of effective mass approximation, the Schrödinger equation for the envelope function is

$$\frac{-\hbar^2}{2m_3}\frac{d^2\xi_i}{dz^2} + [V(z) - E_i]\,\xi_i(z) = 0 \tag{8}$$

where m_3 is the effective mass for motion normal to the interface and V(z) is the effective potential, which can contain both electrostatic contributions and contributions due to band structure variations. The energy levels measured from the bottom of the conduction band are

$$E = E_i + \hbar^2K^2/2m, \tag{9}$$

where m is the effective mass, assumed isotropic, for motion parallel to the interface.

For silicon inversion layers, where V(z) is very large (≈3eV) in the oxide, one can usually assume that only the semiconductor region, with $z > 0$, enters in the Schrödinger equation, and use the boundary condition $\zeta_i(0) = 0$. In heterojunctions and quantum wells, where the interface barrier height is smaller and wave functions can spread into regions with varying effective mass, a modified Schrödinger equation [34]

$$\frac{-\hbar^2}{2}\,\frac{d}{dz}\,\frac{1}{m_3}\,\frac{d\xi_i}{dz} + [V(z) - E_i]\,\xi_i(z) = 0 \qquad (10)$$

can be used provided there is no change in conduction band character across the interface. This form conserves probability current.

It is clear that some kind of grading is present in an electronic sense even for crystallographically ideal surfaces, as indicated schematically in Fig. 2. There must be at least one layer of atoms with bonding - and therefore also other electronic properties such as energy levels and polarizability - different from that of either of the adjoining materials. Equation (10) is an approximate way of dealing with such a transition layer. Other methods have been discussed, for example, by Kroemer and Zhu [35] and by White et al [36]. Stern and Schulman [37] used both the effective mass approach of Eq. (10) and a tight-binding approach to study energy levels in quantum wells, and found that a modest amount of grading has a relatively small effect on the energy levels.

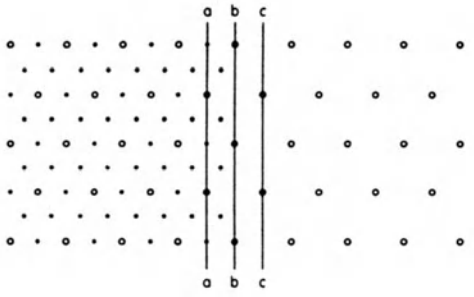

Fig.2 Schematic illustration of a crystallographically ideal interface. Atoms on the line b-b have bonding different from that of atoms on either side of the interface.

Some interesting formal consequences of a modified Schrödinger equation with a rapidly but continuously varying effective mass in a graded transition layer have been discussed by Price and Stern [38]. Interface boundary conditions enter in a crucial way in the coupling of the two valleys for a (001) Si surface, as reviewed by Ando [39]. Interface boundary conditions and general aspects of the effective mass approximation will be discussed in the lectures by Altarelli [4].

Solutions of the Schrödinger equation within the simple effective mass approximation have been given by many authors. The potential energy V(z) includes a term which depends on the eigenfunctions $\zeta_i(z)$, and the Schrödinger equation and Poisson's equation must therefore be solved self-consistently. The Hartree approximation, in which many-body effects are ignored, has been used by Stern and Howard [40] for silicon inversion layers and similar systems , including the effects of effective mass anisotropy, and detailed results have been given by Stern [41]. Many-body effects must, however, be included to give agreement with experiment. These effects have been treated by many authors, including Vinter [42], Jonson [43], and Ando [44]. A discussion of many-body effects in relation to the temperature dependence of energy levels has been given by Kalia et al [45,46]. Experimental tests of theory are provided by optical absorption measurements (see, for example, [3] , but the absorption peaks are not expected to coincide with the calculated energy differences. The necessary corrections have been reviewed by Ando [47]. Results for (001) Si inversion layers show good agreement with the theory, but recent measurements [48] on other Si surfaces are in less satisfactory agreement with the theory [49]. Subband separations can also be found from Raman scattering measurements, a subject covered in the lectures by Abstreiter [50].

Self-consistent solutions of the Schrödinger equation and Poisson's equation are required unless there is negligible charge in the channel. The band bending and the envelope wave function for the lowest subband in an $Al_xGa_{1-x}As/GaAs$ heterojunction are shown in Fig. 3, from a self-consistent calculation by Ando [9].

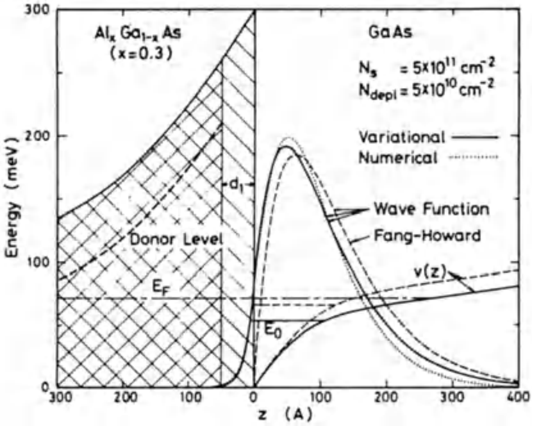

Fig.3 Self-consistent results for an $Al_xGa_{1-x}As/GaAs$ heterojunction calculated using both variational (full and dashed curves) and numerical (dotted curve) envelope functions (after Ando, Ref. 9)

Self-consistency may also be important in a quantum well if carriers are introduced by adding impurities in the barrier. In relatively wide wells and for sufficiently high carrier densities, the quantum well then approaches the character of two isolated heterojunctions, and the lowest energies occur in pairs, with symmetric and antisymmetric envelope functions. The evolution of the eigenvalue spectrum for such a situation is shown in Fig. 4.

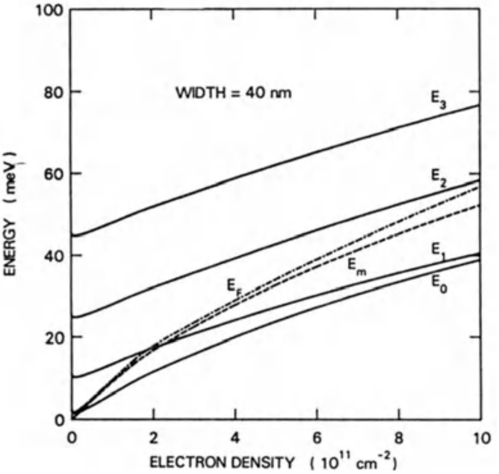

Fig.4 The four lowest calculated energy levels in an $Al_{0.4}Ga_{0.6}As$-GaAs-$Al_{0.4}Ga_{0.6}As$ quantum well 40 nm wide versus the density of electrons in the well. Also shown are the Fermi energy E_F and the maximum energy E_m of the self-consistent potential in the well. All energies are measured from the bottom of the empty well. Many-body effects, which have been included via a local-density scheme as in Ref. 16, account for the dip at low electron densities (after Stern and Schulman, Ref. 37).

4. Static Screening

A system with mobile charges will respond to changes in the energies of electronic states in such a way as to screen out fluctuations. The conventional treatment of such systems assumes that the fluctuations are sufficiently small that Poisson's equation can be linearized. Let us assume that we are dealing with an electron system that is two-dimensional in a quantum sense, so that at low enough temperatures only one subband is occupied, and that the charge distribution of electrons is given by

$$g(z) = \zeta_0^2(z), \tag{11}$$

where $\zeta_0(z)$ is the normalized envelope wave function for the lowest subband. Suppose that some perturbation, for example a charged impurity, induces a weak perturbing potential $\psi(r)$. Then the physically relevant potential to be screened by the two-dimensional electron system is the average potential in the electron layer,

$$\phi_{av}(R) = \int \phi(r) g(z) dz,$$

where $R \equiv (x,y)$. Poisson's equation for the perturbing potential is [40]

$$\nabla^2\phi(r) - 2q_s\phi_{av}(R)g_0(z) = -\rho_{ext}(r)/\varepsilon, \tag{12}$$

where the screening parameter q_s is

$$q_s = \frac{me^2}{2\pi\varepsilon\hbar^2\,[1 + \exp(-y)]}, \tag{13}$$

and $y = (E_F - E_0)/k_BT$. (As before, we assume a valley degeneracy of 1 here). At low temperatures, the bracketed expression in Eq. (13) approaches unity. At high temperatures, Eq. (13) gives $q_s = N_s e^2/2\varepsilon k_BT$, but this result and the simplified one-subband picture used here become invalid when carriers in higher subbands contribute to the screening.

Equation (13) gives the two-dimensional screening effect for static potentials and long-wavelength perturbations. The linear response under more general conditions, the two-dimensional analog of the Lindhard [51] dielectric response of a free electron gas, has been derived by Stern [52]. In the limit of long wavelengths and zero frequency, his result is equivalent to the long-wavelength treatment given above, but for wave vectors greater than $2k_F$ it leads to a rapid decrease in the screening parameter with increasing q [52]. Screening, like other aspects of two-dimensional physics, sometimes has a different character from that which might be expected from intuition based on physics in three dimensions. The wave-vector independence of screening for $q < 2k_F$ is one example. Another is the fact that the screening does not depend on electron density, at least for an ideal two-dimensional system at absolute zero. A treatment of the dielectric response of a two-dimensional electron system, including its nonlocal character, was given by Dahl and Sham [53].

5. Scattering Mechanisms

Although many of the aspects of transport in two-dimensional systems are worthy of detailed examination, the discussion here concentrates on the simplest case, the Coulomb scattering that limits the mobility in GaAs-based heterojunctions at low temperatures, and refers only briefly to other mechanisms.

Scattering by a charge outside a sheet of electrons is most simply described in Born approximation, which gives the cross-section for scattering through an angle θ as [40]

$$\sigma(\theta) = (me^2/2\pi\hbar^3 v)\,|(\psi_f\,|\phi(r)|\,\psi_i)|^2, \tag{14}$$

where v is the carrier velocity. The perturbing potential - $e\phi(r)$ reflects both the external charge and the screening effect of the carrier in the two-dimensional layer. If we simplify the problem further by assuming that the electrons lie in a sheet of zero thickness in the plane z = 0 and that the surrounding media have permittivity ε, then the screened Coulomb potential in the electron plane associated with a charge Ze located a distance d away is

$$\phi(R) = (Ze/4\pi\varepsilon) \int_0^\infty q(q+q_s)^{-1} J_0(qR)\exp(-qd)dq, \tag{15}$$

where J_0 is the Bessel function of order zero, R is the distance from the point in the layer closest to the charge, and q_s is the screening parameter given in Eq. (13). A more complete expression that takes both the finite thickness of the electron layer and the dielectric discontinuity into account was first given by Stern and Howard [40] using the Fang-Howard [54] variational envelope function. They showed that, at least for silicon inversion layers, the Born approximation is not seriously in error. To the best of my knowledge, a similar analysis of the validity of the Born approximation has not been carried out for GaAs-based heterojunctions. The most detailed calculation of Coulomb scattering is that of Vinter [55], who went beyond the linear screening approximation and found somewhat smaller mobilities for silicon inversion layers than those deduced from the model indicated here, based on linear screening and the Born approximation.

The dominant Coulomb scatterers in silicon inversion layers are thought to be residual charged impurities at the Si-SiO_2 interface, with impurities in the Si itself making a negligible contribution in the samples typically used. In GaAs heterojunctions, on the other hand, the Coulomb scatterers arise both from the impurities that donate electrons to the channel and from residual impurities in the GaAs itself.

The effect of an interface on the conductance of a bulk semiconductor has long been discussed in terms of specular and diffuse scattering by the boundary. For a dynamically two-dimensional system, the notion of specularity has no meaning because the carriers have no component of velocity in the direction normal to the interface. Instead, the scattering must be treated microscopically. This subject has been discussed in some detail in Ref. 3, primarily with silicon inversion layers in mind. For GaAs-based heterojunctions and quantum wells, there are several experiments showing that the interface is quite smooth, with lateral correlation lengths greater than 10 nm and vertical steps of atomic dimensions. Because interface scattering increases strongly with electron density, and the densities in these structures are generally smaller than in silicon inversion layers, interface scattering is not believed to play an important role in limiting the mobility in heterojunction devices [9], as opposed to the strong role played by this mechanism in silicon inversion layers at high electron densities. Alloy scattering connected with penetration of the wave function into the $Al_xGa_{1-x}As$ is also weak [9], but may be important in other systems in which the material on the channel side of the heterojunction is an alloy, as discussed, for example, by Bastard [56].

In GaAs-based heterojunctions, where interface scattering is believed to be relatively unimportant in limiting the mobility, the principal low-temperature scattering mechanism in good samples arises from the ionized impurities in the barrier that contribute charges to the channel and from residual impurities in the GaAs itself. A calculation of the combined effect of these two contributions [57], shown in Fig. 5, gives a peak mobility of order 10^6 $cm^2V^{-1}s^{-1}$, close to the highest values that have been measured in $Al_xGa_{1-x}As$/GaAs heterojunctions in the dark (see, for example, [58]). The predicted peak mobility depends mainly on the residual ionized impurity concentration in the GaAs, and the measured values indicate that this is of order 10^{14} cm^{-3} in the best samples. Further improvement in the mobility of ungated heterojunctions would appear to require even purer GaAs.

When carriers occupy more than one subband, the factors that influence the mobility change in at least two ways. First, the screening is changed by the presence of carriers in the second subband. Here the wave vector dependence of

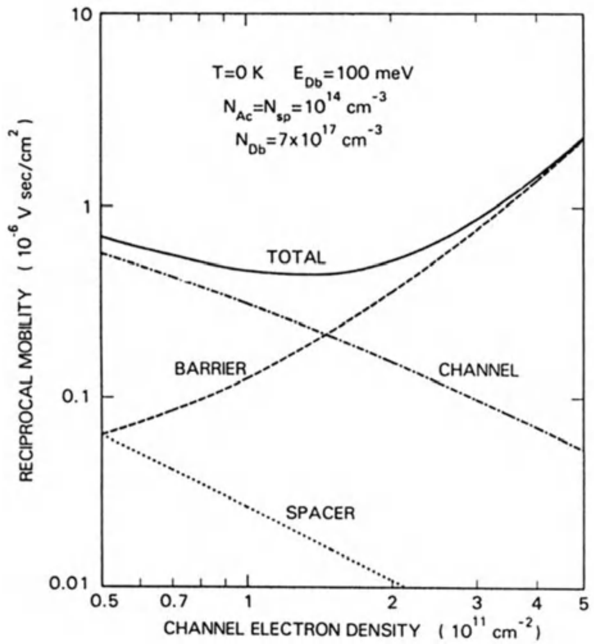

Fig.5 Calculated low-temperature mobility of elecrons in $Al_x Ga_{1-x}As/GaAs$ heterojunctions as limited by Coulomb scattering (after Stern, [57])

screening [52], noted briefly above, becomes nontrivial because the Fermi wave vectors in the two subbands are generally different. Second, the presence of the second subband may open a new scattering channel. The first of these effects appears to increase the mobility [59], while the second reduces it [60]. For GaAs-based heterojunctions, mobility reduction is expected [9] and observed [61].

Although temperature dependence of mobility in semiconductors outside the range of strong or weak localization is usually attributed to phonon scattering, the temperature dependence of screening can lead to a decrease of mobility with increasing temperature. This effect was first pointed our for silicon inversion layers by Stern [62]. His calculation gave a linear dependence on temperature, consistent with experiments of Cham and Wheeler [63]. Kawaguchi et al. [64], however, found a more nearly quadratic dependence. Theoretical attempts to resolve this are still inconclusive [65].

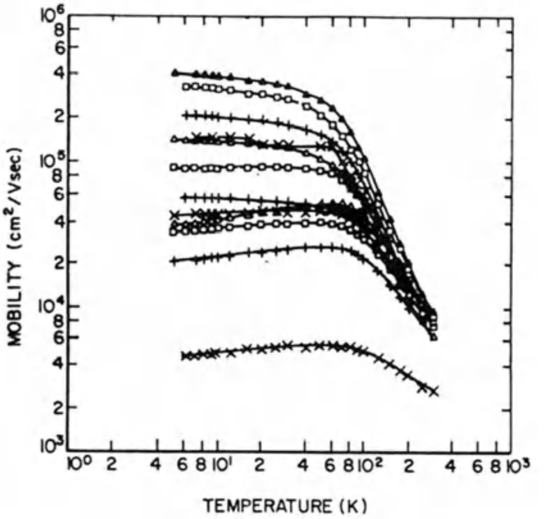

Fig.6 Temperature dependence of electron mobility in a series of $Al_xGa_{1-x}As$ / GaAs heterojunction samples (after Lin, [69])

For electrons in GaAs-based heterojunctions the situation is quite different. The Coulomb scattering is primarily forward scattering because the screening is relatively weak (in part because of the small electron effective mass). Thus the mechanism described above is not effective. Instead, in very high mobility samples the mobility decreases with increasing temperature, [66-68] whereas in low mobility samples it first increases [67,68]. These effects are illustrated in Fig. 6, from the Ph.D. thesis of Lin [69]. The former effect is attributed to phonon scattering, including a piezoelectric contribution [66]. The mobility increase is thought to result from averaging of the relaxation time over the thermal distribution of carrier energies, [65,68,69]. At temperatures above $\sim$10 K the mobility in the best sample is dominated by phonon scattering, including polar optical phonons. The theory of phonon scattering has been discussed, for example, by Price [70], and will be covered in part in the lectures by Vinter [5].

Acknowledgments

I am indebted to the organizers of the Winter School on Heterojunctions and Superlattices in Semiconductors for the opportunity to participate and thank B.J.F. Lin for permission to include the as yet unpublished results of Fig. 6. I also thank many of my colleagues for useful discussions, particularly P.M. Mooney, M.I. Nathan, T.N. Theis, and D.J. Wolford for discussions of deep donors and persistent photoconductance.

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