Vol. 87 (1995) *ACTA PHYSICA POLONICA A* No. 1

Proceedings of the XXIII International School of Semiconducting Compounds, Jaszowiec 1994

CHARGE CARRIER TRANSPORT IN ARTIFICIALLY STRUCTURED TWO-DIMENSIONAL SEMICONDUCTOR SYSTEMS*

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General aspects of the electronic transport in two-dimensional and quasi--three-dimensional semiconductor systems are discussed. Contributions of different scattering processes to the total electron and hole mobilities in various types of modulation doped heterostructures are calculated. It is shown that in a wide temperature range phonon scattering is the principal scattering mechanism limiting electron and hole mobilities in high quality AlGaAs/GaAs modulation doped heterostructures. Scattering from rough walls in wide parabolic wells is briefly reviewed.

PACS numbers: 73.50.Bk, 73.40.Kp

1. Introduction

Development of the modern epitaxial techniques such as molecular beam epitaxy, metalorganic chemical vapor deposition and numerous variations of these two growth methods allows atomic scale control of the growth process. All the epitaxial growth methods provide excellent control of composition and doping along the growth direction, therefore they are perfect tools to fabricate two-dimensional structures.

Low-dimensional semiconductor systems have become fertile ground for basic research. The discoveries of the quantum Hall effect [1] and the fractional quantum Hall effect [2] were major developments in fundamental solid state physics in the last several years. The flexibility with which various structures could be designed and practically realized has led to new concepts of charge transport in

*This work was supported by the Director, Office of Energy Research, Office of Basic Energy Sciences, Materials Science Division of the U.S. Department of Energy under contract No. DE-AC03-76SF00098.

mesoscopic systems. Also, a wealth of new linear and nonlinear optical effects has been observed in semiconductor quantum wells [3].

It was evident from the beginning that the introduction of artificially structured 2D systems would open an opportunity to study basic transport phenomena in new and in many respects unusual material systems [4]. Using the concept of modulation or selective doping it has been possible, for the first time, to separate charge carriers from the parent impurities [4, 5]. This concept led to a very substantial reduction of impurity scattering and allowed the study of charge transport in almost perfectly pure semiconductors where phonon scattering plays a dominant role down to very low temperatures.

In this paper we will briefly review recent theoretical and experimental results on electronic transport in 2D and quasi-3D modulation doped heterostructures. We will focus our attention on 2D electron or hole gases confined at heterointerfaces of different semiconductors. However, many of the concepts and results will be directly applicable to charge transport in any two-dimensional system. The theoretical calculations will be compared with experimental results on the most extensively studied material systems.

2. Electronic structure

Quantum confinement of electrons and holes in 2D planes can be achieved by several methods [6]. However, the method most widely used to produce 2D systems utilizes band offsets at semiconductor heterointerfaces [7]. The band offsets can be used to confine electrons or holes in a thin square quantum well or at an interface between two different semiconductors.

In order to achieve 2D confinement the system has to satisfy certain conditions. First, the thickness of the well has to be smaller than the electron or hole de Broglie wavelength. For a 3D electron or hole gas of concentration n the de Broglie wavelength at the Fermi energy is $\lambda_F = 2\pi/k_F$, where $k_F = (3\pi^2 n)^{1/3}$. Hence the condition to observe 2D confinement of such gas is that the thickness w of the well satisfies the condition

$$w < 2\left(\frac{\pi}{3n}\right)^{1/3}. \tag{1}$$

It should be emphasized that this is a universal condition which does not depend on any semiconductor material parameters.

Another characteristic length for an electron or hole gas is the mean free path, i.e., the distance an electron or a hole can travel between momentum randomizing scattering events. For a 2D gas the mean free path l_p has to satisfy the condition,

$$l_p = v_F \tau = \hbar k_F \mu / e = \hbar (3\pi^2 n)^{1/3} \mu / e > w, \tag{2}$$

where v_F is the carrier velocity at the Fermi level, τ is the relaxation time and μ — the mobility. The above condition has a simple physical interpretation: it states that in a 2D system electrons or holes interact with the confinement walls more frequently than with random scattering centers.

Recently a new type of structure which connects 2D with 3D limits has been proposed and practically realized. In so-called parabolic quantum wells a wide well can be obtained by a combination of proper design of the alloy composition in the

well with remote doping [8, 9]. The width of such wells can be of the order of 1000 Å, i.e., it is larger than the de Broglie wavelength. Therefore, although the carrier motion is not quantized the mean free path in such structure can be larger than the width of the well. Consequently, one has to account for an interaction of free carriers with the confinement walls.

Among the variety of possible 2D semiconductor systems the single quantum well modulation doped heterostructures (SQW–MDH) are the semiconductor structures most frequently used to study transport of 2D electrons and/or hole gases. In such structures, schematically shown in Fig. 1, the shallow donors or acceptors are located in the barrier forming semiconductor $S2$. The carriers are

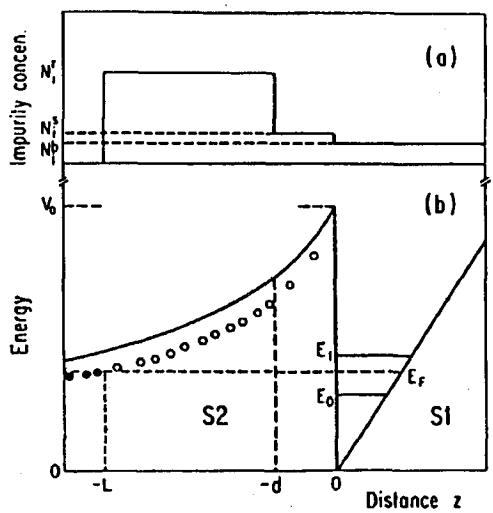

Fig. 1. Schematic representation of (a) the doping profile and (b) the conduction band energy for an n-type, single quantum well modulation doped heterostructure. $S1$ and $S2$ represent well- and barrier-forming semiconductor, respectively.

transferred from the parent dopants into the well forming semiconductor $S1$. The resulting electric field confines the mobile charges in a narrow quasi-triangular well at the heterointerface. By changing the distance d separating the dopants from the quantum well one can control the concentration of the electrons or holes in the well. Also, by increasing the separation one is able to very substantially enhance the carrier mobility by reducing the effectiveness of the ionized impurity scattering. Practical implementation of this idea has resulted in n-type AlGaAs/GaAs MDHs with low temperature electron mobilities exceeding 10^7 cm^2/(V·s) [10, 11] and p-type structures with hole mobilities approaching 4×10^5 cm^2/(V·s) [12]. The principal objective of all theoretical calculations of the 2D transport is to understand the scattering mechanisms limiting electron and hole mobilities in such structures. The starting point of the theory is to provide an accurate description of the electronic structure of electrons or holes confined in a quasi-triangular quantum well at the heterointerface.

2.1. n-type MDH

The wave function of an electron gas confined in the z-direction can be written in the form

$$\Psi_{n,k}(r,z) = \frac{1}{L^2}\chi_n(z)\exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}), \tag{3}$$

where $\boldsymbol{R} = (r,z)$, $r = (x,y)$ and $\boldsymbol{k} = (k_x, k_y)$. The wave function $\chi_n(z)$ is given by the solution of coupled Schrödinger and Poisson equations [13, 14]:

$$-\frac{\hbar^2}{2m^*}\frac{\mathrm{d}^2}{\mathrm{d}z^2}\chi_n(z) + [V_0\theta(-z) - e\phi(z)]\chi_n(z) = E_n\chi_n(z), \tag{4}$$

$$\frac{\mathrm{d}^2}{\mathrm{d}z^2}\phi(z) = \frac{4\pi e^2}{\varepsilon_0}\left[\sum_{i=0}^{m} N_i\chi_i(z) + N_\mathrm{A}(z) - N_\mathrm{D}(z)\right]. \tag{5}$$

Here $E_n(k) = E_n + \hbar^2k^2/2m^*$ is the dispersion relation for the n-th subband. $V_0\theta(-z)$ represents a step-like band offset at $z = 0$. $N_\mathrm{D}(z)$ and $N_\mathrm{A}(z)$ are the functions representing the distribution of shallow donors and acceptors respectively, N_i is the density of electrons in the i-th subband. The distribution of localized charges is schematically represented in Fig. 1.

The wave function of the ground subband can be represented by [14]:

$$\chi_0(z) = \begin{cases} Bb^{1/2}(bz+\beta)\exp(-bz/2), & z > 0, \\ B'b'^{1/2}\exp(+b'z/2), & z < 0, \end{cases} \tag{6}$$

where B, b, B', b' and β are variational parameters related to each other through the boundary conditions at the heterointerface, and the normalization condition for $\chi_0(z)$. Therefore the parameters B, B' and β can be expressed in terms of b and b' [15]. The corresponding energy E_0 of the bottom of the ground subband depends in a complex way on the variational parameters and the details of the carrier and impurity distribution in MDH [15].

The part of the wave function for $z < 0$ represents the finite penetration of the electron gas into the barrier. Incorporation of the penetration is important for calculations of the alloy disorder and surface roughness scatterings in GaAlAs/GaAs MDHs. The variational wave function (7) is very frequently used in the calculations of the electronic transport at low electron densities when only the ground subband is occupied [14, 15]. At higher electron densities or at elevated temperatures one needs to consider also the transport in higher lying excited subbands [16]. An exact treatment of such a problem is rather difficult and requires extensive numerical calculations.

2.2. p-type MDH

Transport of a 2D hole gas has been much less extensively studied both theoretically and experimentally. The complex nature of the valence Γ_8 band maxima in group III–V semiconductors makes a detailed analysis of the electronic structure of 2D holes difficult and numerically involved. The main difference in the description of electron and hole electronic structures is that in the case of holes one has to consider the fourfold degenerate valence band. Numerical calculations of the

band structure for specific p-type MDHs have been performed by several groups [17–19]. The main conclusion of these calculations was that the electronic structure of the fourfold degenerate Γ_8 valence band splits into a number of subbands. For $k_x = k_y = 0$ these subbands are twofold spin degenerate. It has been shown in the case of a p-type AlGaAs/GaAs MDH that the energy dispersion relations for the light and heavy holes are described by nonparabolic energy dependent effective masses and that the constant energy surfaces are warped [19]. An accurate description of the hole transport in such systems would require extensive numerical calculations. However, under certain conditions, one can use an approximation which can significantly simplify the problem.

Detailed calculations for a typical p-type AlGaAs/GaAs MDH have shown [19] that the first excited subband is located at about 10 meV below the ground subband. Therefore, for all practically achievable hole concentrations, the Fermi energy is low enough so that only the ground subbands are occupied. Consequently, at low temperatures one has to consider transport within the ground spin-up and spin-down subbands only [20]. Under such approximations one can use an approach previously described for electrons in n-type MDHs with the hole wave function similar to that given by Eq. (6).

3. Charge scattering mechanisms and comparison with experiment

Most of the theoretical descriptions of charge transport are based on the solution of the Boltzmann equation [21, 22]. For elastic, momentum randomizing scattering processes, the solution of the Boltzmann equation can be expressed in terms of an energy dependent relaxation time. For inelastic scattering processes, i.e., the processes in which the electron or hole loses or gains energy comparable or larger than $k_B T$, a different method to solve the Boltzmann equation has to be used. The most frequently used approach is based on either the variational principle [21] or an iterative method used e.g. by Rode [22].

All the major scattering processes limiting the electron and hole mobilities in compound semiconductors are now well established [22]. Among the different scattering mechanisms, only the scattering by ionized impurities and by alloy disorder can be considered as strictly elastic processes. Scattering by phonons always results in an exchange of energy. However, in the case of acoustic phonons the energy of phonons for small phonon wave vectors is very low. Therefore, for all practical purposes the scattering by acoustic phonons can be treated as an elastic process for the temperatures higher than ≈ 4 K.

A proper treatment of optical phonon scattering is by far most complex problem of charge transport in 2D systems. The large optical phonon energy (30 meV to 40 meV) makes the scattering process highly inelastic even at room temperature. It has been argued that since the optical phonons probe a wide range of subbands, therefore, the density of states participating in transport is an average over all those subbands. It can be shown that the total density of states for several subbands resemble the density of state of 3D gas. Consequently, one can use a 3D approximation to calculate the optical phonon scattering in 2D MDHs [16].

There are certain features which distinguish electron transport in two and

three dimensions. As shown in Fig. 1 in the case of ionized impurity scattering electrons can be scattered by remote impurities located within the doped region of the $S2$ semiconductor as well as by residual impurities and/or charged defects in the $S1$ semiconductor. Also, there is the possibility of charge scattering by structural rough interfaces [23, 24].

For MDH involving ternary compounds, an additional scattering from random alloy-disorder potential has to be included [25]. Two distinctly different types of MDHs containing ternary compounds are possible [16, 26]. In the first one the well is formed by a binary compound and the barrier is formed by a ternary alloy. In such MDH there is no significant alloy scattering. The only contribution to this scattering process is through the scattering of the charge carriers penetrating into the barrier. In the other type of structure with the well formed by the ternary alloy the charge carriers are very efficiently scattered by the disordered alloy in the well.

3.1. n-type MDH

The calculated temperature dependence of the electron mobility in $Al_{0.3}Ga_{0.7}As/GaAs$ MDH is shown in Fig. 2. Comparison of these calculations with available experimental data [10, 11] on high quality MDHs indicates that in the wide temperature range of 4 K to 300 K the electron mobility is determined by phonon scattering. The optical phonons dominate at $T > 70$ K and the acoustic phonon scattering plays a major role in the range 4 K to 40 K. At even lower temperatures the mobility levels off due to the scattering from remote impurities in the barrier and residual impurities or charged defects in nominally undoped quantum wells. The alloy disorder scattering of the electrons penetrating the AlGaAs barrier is very small and amounts to about 4% of the total scattering in MDHs with an electron mobility of 10^7 cm^2/(V·s). In the MDH measured in Ref. [11] with a spacer width of 750 Å additional scattering from the background impurities with concentrations of only 2×10^{13} cm^{-3} is required to account for the maximum mobility of 1.05×10^7 cm^2/(V·s).

In InP/InGaAs and InAlAs/InGaAs MDHs the well-forming $In_xGa_{1-x}As$ is lattice matched to InP and InAlAs for $x = 0.53$. There is one important difference between the charge transport in GaAs and in InGaAs. In the latter case the electrons are very efficiently scattered by the alloy-disorder potential in the well. Early experimental results on the 2D electron gas mobilities have shown that the mobility is independent of temperature for $T < 50$ K [27]. Also, the highest reported mobilities were limited to about 10^5 cm^2/(V·s). Theoretical calculations demonstrate that the mobility at these low temperatures is determined by the alloy disorder scattering in the well [16, 26]. Figure 3 shows the comparison of the theoretical calculation with the experimental data of Ref. [27]. Because of high electron density in the MDH studied [27], the calculations included the effects of the first excited subband using the approximate approach discussed in Ref. [16]. An analysis of the low temperature mobility data was used to determine the alloy-disorder parameter $\langle V \rangle$. It has been found that the experimental results can be explained assuming $\langle V \rangle$ to be in the range of 0.55 eV to 0.63 eV.

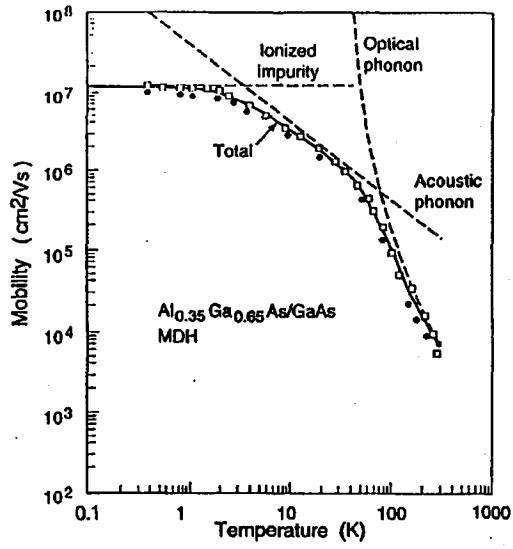

Fig. 2. Contribution of various scattering mechanisms to the total mobility in AlGaAs/GaAs MDH with a spacer width of 700 Å. Points are experimental data of Ref. [10] (□) and Ref. [11] (•) for the spacer width 700 Å and 750 Å, respectively.

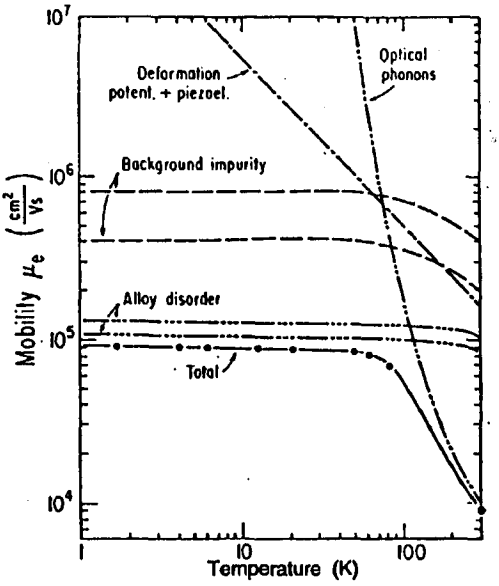

Fig. 3. Electron mobility in $In_{0.48}Ga_{0.52}As/In_{0.53}Ga_{0.47}As$ MDH with an 80 Å spacer. Experimental points are from Ref. [27]. The upper and lower background impurity mobilities correspond to the background impurity concentration of 5×10^{15} cm^{-3} and 1×10^{16} cm^{-3}, respectively.

3.2. p-type MDH

The available experimental data on 2D hole transport is restricted to AlGaAs/GaAs MDHs [12, 28, 29]. Also, the only existing theoretical treatment of the 2D hole transport is limited to a simple approach proposed by us and based on the assumption of decoupled spin-up and spin-down subbands [20, 30, 31]. It has been argued that since the light holes in the spin-down subband are very efficiently scattered by the heavy holes in spin-up subband, the mobility of holes in spin-down states is much lower. This, combined with a much smaller concentration of light holes in spin-down band, provides justification for neglecting the light hole contribution to the total conductivity. Under such circumstances the mobility of a 2D hole gas can be described in terms of carrier transport in a single subband. This allows use of the methods previously developed for a single parabolic electronic subband with one important modification which takes into account the p-type symmetry of the valence band Bloch wave functions [31].

Theoretical calculations of the hole mobility in a p-type AlGaAs/GaAs MDH with the hole density of 2×10^{11} cm^{-2} are shown in Fig. 4 [31]. Very good agreement between the calculated mobility and the experimental data of Ref. [29] is obtained. In the temperature range 4 K to 80 K the mobility is determined by phonon scattering. The largest contribution to the scattering is coming from the acoustic phonon scattering which is the dominant scattering mechanism up to the temperature of $\approx$ 60 K. The discrepancy between theory and experiment for $T < 4$ K can be attributed to the background ionized impurity scattering. This scattering mechanism was not included in the calculations.

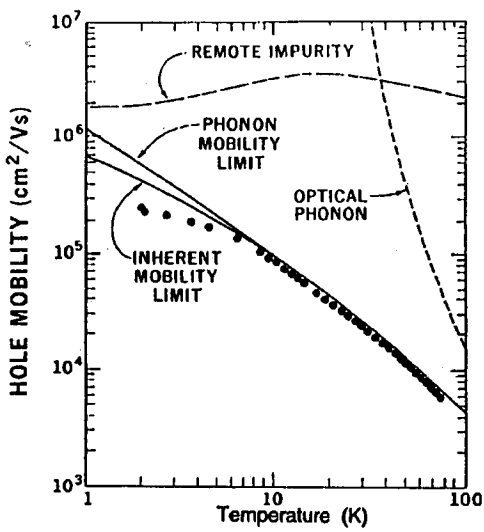

Fig. 4. Calculated hole mobility in p-type $Al_{0.5}Ga_{0.5}As/GaAs$ MDH. The points are the experimental data of Ref. [29] for the hole density of 2×10^{11} cm^{-2}.

3.3. Wide quasi-3D parabolic wells

So far we have considered 2D systems in which charge carriers are confined in one direction, and can freely move in a 2D plane. Such systems satisfy both conditions (1) and (2), necessary for a fully quantized 2D motion of the charge. Also, modulation (or remote) doping allows for a dramatic reduction of ionized impurity scattering. In standard 3D structures the ionized impurities and charge carriers are not spatially separated and ionized impurity scattering is the dominant process limiting the mobility at low temperatures.

Recent progress in the epitaxial growth of AlGaAs films allowed a realization of a new type of structure which has all the basic features of 3D systems and still has impurities removed from the immediate vicinity of the charge carriers [8, 9]. In modulation (or remotely) doped wide parabolic wells the composition of $Al_xGa_{1-x}As$ in the well is parabolically varied with the distance. If such a structure is doped in the regions outside the well, the electrons are transferred to the well. The resulting electrostatic potential flattens the bottom of the well. Consequently, one obtains a structure in which electrons are confined in a wide well and are separated from their parent donors. This design allows preparation of wells with a thickness of the order of 1000 Å and with the electron concentration of about 10^{16} cm^{-3} [32].

Such system can be considered a model of modulation doped 3D electron gas, which should exhibit an enhanced low temperature electron mobility. In fact, mobilities as high as 3×10^5 cm^2/(V·s) were reported in AlGaAs/GaAs wide parabolic wells [33]. Although such mobilities are much higher than those observed in standard 3D semiconductors, they are still much lower than mobilities in 2D MDII or what one would expect in any modulation doped system.

The reason for this lower than expected mobility lies in nonspecular scattering of the electrons from rough confinement walls. As has been discussed before, in addition to condition (1), one also has to consider condition (2), which in general is less restrictive, and is easily satisfied in 2D MDHs. In wide parabolic wells with $\mu \approx 3 \times 10^5$ cm^2/(V·s) and $n \approx 3 \times 10^{16}$ cm^{-3}/(V·s),

$$l_p \approx 10^4 \text{ Å} > w_e = 10^3 \text{ Å}. \tag{7}$$

This means that although the electron motion is not quantized in the parabolic well the mean free path of the electron is much larger than the well width. The transport of electrons in the well will be affected by the interaction with the confining walls.

The effects of electron interaction with the confinement walls in wide parabolic wells has been considered in Ref. [33]. It was assumed that a typical size of the roughness parameter is limited by the screening length. Calculations of the electron mobility in quasi-3D wells were performed adopting the approach previously developed for thin metallic films [34]. Results of the calculations are shown in Fig. 5. They indicate that the nonspecular scattering reduces the electron mobility by a factor of 2 to 3. It is also seen in Fig. 5 that incorporation of nonspecular scattering satisfactorily accounts for the experimentally observed temperature dependence of the mobility.

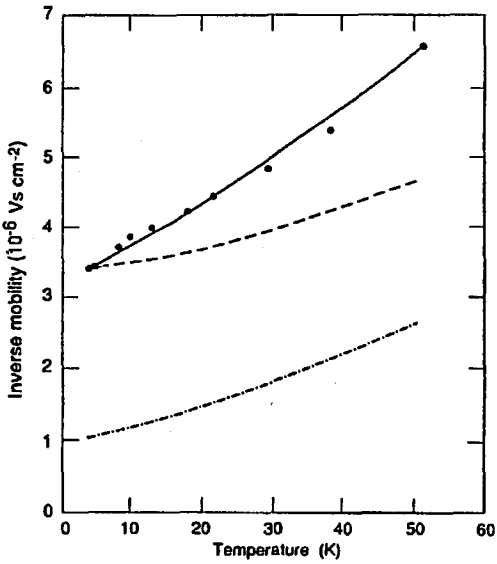

Fig. 5. Temperature dependent inverse mobility in a wide parabolic AlGaAs/GaAs well. The solid line represents the mobility for the background ionized impurity concentration of $N_i^b = 2.3 \times 10^{14}$ cm^{-3}, in which the scattering from the rough walls has been included. The dashed and dashed-point lines are the calculated mobilities without the scattering from the confinement walls with the N_i^b equal to 10^{15} cm^{-3} and 2.3×10^{14} cm^{-3}, respectively.

4. Conclusions

In this paper we have reviewed basic aspects of electron and hole transport in artificially structured 2D systems. The concept of modulation (or selective) doping has provided structures with extremely high electron and hole mobilities. Very significant reductions of impurity scattering in modulation doped systems allowed extensive studies of phonon scattering down to very low temperatures. At higher temperatures of $T > 100$ K charge transport in 2D systems is very similar to that observed in 3D high purity semiconductors.

Although this review was restricted to lattice matched semiconductor systems, most of the concepts and methods can be easily adopted to lattice mismatched and pseudomorphic systems. At strained semiconductor interfaces an important complication arises from the fact that one has to consider the effect of planar strain on the electronic structure. The effects of the strain are especially complex in the case of the degenerate valence bands. Also, the electronic transport depends on whether the strained layer is unrelaxed, partially, or fully relaxed, since it can be affected by structural defects at the interfaces. All these issues are of great importance for strained GaAs/InGaAs and Si/SiGe heterostructures which are considered the most promising systems for a high performance heterojunction bipolar transistors.

Charge transport in 2D systems is now a mature research area with well

developed experimental and theoretical methods. Progress in material preparation techniques have made possible to study charge transport in 1D (quantum wires), as well as unusual properties of QD (quantum dot) systems. An intense effort in several laboratories into development of these new methods of preparation of strongly confined low-dimensional systems has already produced a wealth of new results and certainly will be the research area actively pursued in the future.

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