

MEYER W E

ELECTRICAL CHARACTERIZATION OF SEMICONDUCTOR
HETEROSTRUCTURES

MSc (Physics)

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Electrical characterization of semiconductor heterostructures

WE Meyer

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by

Walter Ernst Meyer

Submitted in partial fulfilment of the requirements for the degree

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in the

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University of Pretoria

Pretoria

December 1992

Supervisor: Prof F D Auret

Co-supervisor: Dr H W Kunert

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Advances in growth techniques for semiconductor microstructures have led to a demand for more sophisticated characterization techniques, suitable for more accurate characterization of microstructures.

Capacitance-voltage (*CV*) profiling provides a relatively inexpensive technique suitable for the characterization of doping profiles, isotype heterojunctions, and delta doped structures. Furthermore this technique can easily be adapted to measure a large number of samples on a routine basis. In this dissertation the application of the *CV* profiling technique to isotype heterostructures and delta doped structures is described. The results obtained by *CV* measurements on delta doped structures are compared to those obtained by secondary ion mass spectroscopy (SIMS).

Elektriese karakterisering van halfgeleier heterostrukture

deur

Walter Ernst Meyer

Voorgelê ter gedeeltelike vervulling van die vereistes vir die
graad

MSc (Fisika)

aan die

Universiteit van Pretoria

Studieleier: Prof F D Auret

Mede-studieleier: Dr H W Kunert

As gevolg van die vordering op die gebied van groei-tegnieke vir halfgeleier mikrostrukture, is dit tans moontlik om kristalle te kweek waarin die samestelling binne atoom-afstande variëer. Hierdie vermoë het gelei tot 'n behoefte aan karakteriseringstegnieke wat geskik is om sulke mikrostrukture akkuraat te karakteriseer.

Kapasitansie-spanning (*CV*)-diepteprofiel metings bied 'n relatief goedkoop alternatief tot duurder tegnieke soos sekondêre ioon massa spektroskopie (*SIMS*) vir die analisering van doteringprofile, isotipe heterolasse, asook delta gedoteerde strukture. In hierdie verhandeling word die *CV*-tegniek en sy beperkings bespreek. Daar word ook 'n vergelyking getref tussen die resultate verkry deur *CV*-metings en die resultate verkry deur *SIMS*-metings van delta gedoteerde monsters.

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1

Introduction

Most electronic devices currently used in commercial applications, are fabricated by means of planar techniques on a single semiconductor substrate. Doping is done by means of ion-implantation, where ions of the dopant material are accelerated through high voltages onto the surface of the semiconductor. By varying the energy of the ions, the penetration depth can be adjusted, so that structures, in which the doping varies with depth, can be grown. In order to selectively dope specific regions of the substrate, masks to screen areas not to be doped are applied before ion implantation. Although this technique is suitable for the mass production of many devices, it is very difficult to obtain abrupt changes in the doping profile and impossible to change the semiconductor composition.

As the search for devices operating at higher speeds with higher efficiencies continued, it became increasingly important to specify doping profiles with higher accuracy and with sharper changes. Lately heterostructures, in which different types of semiconductors with different band gaps are used in the same device, have become increasingly useful. For instance, it was found that by sandwiching a layer of semiconductor with a lower band gap between two layers of a semiconductor with a higher band gap, it was possible to create the equivalent of the textbook “quantum well”. Such a quantum well could be useful for two reasons. Firstly, it can act as a well by allowing electrons to flow into it and accumulate at the bottom of the well with a higher density than in the surrounding semiconductor. The second property of the quantum well is that the charges trapped in the well, behave as predicted by quantum mechanics textbooks: the momenta in the direction perpendicular to the well become quantized. This causes the electrons in the well to behave like a two-dimensional gas. Such a gas has a number of properties that make it especially useful for the production of semiconductor lasers.

Recent advances in growth techniques have made it possible to grow semiconductor structures in which the doping concentration and composition can be changed abruptly within the dimensions of a few atomic layers. Coupled with this capability, came the necessity to characterize these structures with increasing accuracy. A number of characterization techniques have been developed for such structures. The most important of these are photoluminescence (PL), secondary ion mass spectroscopy (SIMS), transmission electron microscopy (TEM), Hall effect measurements, deep level transient spectroscopy (DLTS), and capacitance voltage (CV) profiling.

These characterization techniques can broadly be divided into two categories:

- 1) Methods relying on determining the chemical composition of the sample, such as SIMS, TEM, and helium ion (Rutherford) backscattering spectroscopy (RBS).
- 2) Methods relying on the electronic properties of the semiconductors. These methods include PL, CV, DLTS, and Hall effect measurements.

The techniques in category 1 are generally only suited to samples with high doping levels ($>10^{16} \text{ cm}^{-3}$), and require very expensive equipment. Furthermore, in many cases these techniques require special sample preparation or calibration, which makes them unsuitable for cost-effective assessment of a large number of samples. In contrast to many of the techniques relying on chemical composition, CV profiling can in many cases provide accurate results, and be used for routine testing of a large number of samples at relatively low cost.

In this dissertation a detailed study of the CV profiling technique has been made, and the results of a number of measurements made on test samples are presented. The term “heterojunction” has been interpreted in its wider sense, so as to include delta doped, and semiconductors with doping steps. For some samples the CV results are also compared with SIMS results.

Chapters 2 to 5 consider the general properties of semiconductors and semiconductor contacts. This is not intended to be a complete study of the theory of semiconductors, but rather to highlight a number of topics which will be referred to at a later stage. In the second part (Chapters 6 and 7), the theory and limitations of CV profiling on semiconductors is discussed in detail. The experimental equipment, procedures and results are discussed in chapter 8. Chapter 9 contains general conclusions.

2

An overview of the properties of semiconductors

The properties of semiconductors are adequately described in a number of textbooks. For this reason only a short description of the most important properties of semiconductors is given in this chapter. For a more complete introduction to the properties of semiconductors, the reader is referred to textbooks e.g. Ridley (1988), Sze (1981), Smith (1978), and Henisch (1989). Topics referred to in this dissertation are discussed in more detail.

2.1 Crystalline solids

In crystalline solids the atoms, ions, or molecules, of which the solid is composed, are arranged in a regular, repeated, three-dimensional pattern. In large, high purity single crystals, as used for most semiconductor devices, this pattern is repeated millions of times throughout the crystal, with very few deviations. Such a pattern, according to which the atoms of a crystal are arranged, is called the crystal structure. This pattern can be produced by repeating a simple pattern at regular intervals. These elementary building blocks are called unit cells. In many cases these unit cells consist of simpler arrangements, which, when repeated also make up the crystal structure. If these simpler arrangements can not be divided any further, they are referred to as primitive unit cells.

Mathematically, the structure can be described by a lattice, defined by the set of vectors

$$\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3, \quad (2.1)$$

where the n_i are integers, and the vectors $\mathbf{a}_i$ are referred to as the basis vectors. The crystal structure can now be obtained by placing a set of atoms (an atomic basis) at every lattice point. This leads to a structure that has translational symmetry, i.e. it will remain invariant under a translation by any vector $\mathbf{R}$, as defined above.

In general, the crystal structure is highly symmetric, i.e. there exist a large number of operations that, when performed on the arrangement, leaves it essentially unchanged. The set of all symmetry operations that can be performed on a specific crystal structure (together with the operation of combination) conforms to the requirements of a mathematical group (see for example Hamermesh 1960). If each of the symmetry operations in a group leaves at least one point unchanged, the group is referred to as a point group. If the translational

symmetry of the crystal is added to that of the point group, so-called space groups are formed, which completely describe the symmetry of the crystal.

It is sometimes necessary to refer to a specific plane in a crystal structure. This is done by means of Miller indices. These are obtained by first finding the intercepts of the plane with the three basis axes in terms of the lattice constants, taking the reciprocals of these numbers, and then reducing them to the smallest three integers having the same ratio. The result is enclosed in parentheses and indicated as (hkl) . The notation $\{hkl\}$ is used to denote all planes which, because of the symmetry of the crystal, are equivalent to (hkl) . Directions in the crystal structure are indicated by finding a vector in the direction to be indicated, and reducing its components to the smallest set of three integers having the same ratio. The direction is then indicated as $[hkl]$, meaning a specific direction, or $\langle hkl \rangle$ to indicate a set of equivalent directions.

The semiconductors silicon and germanium both crystallize according to the diamond lattice. This lattice can be derived from the face centered cubic (fcc) lattice. Formally it may be described as being built up from two interpenetrating fcc lattices, which are offset from one another along the body diagonal by one quarter of its length. In this arrangement each atom is at the centre of a tetrahedron, connecting it to its four equally spaced nearest neighbours. The structure of such a lattice is shown in figure 2.1. Also shown is the outline of a cube, corresponding to one of the two f.c.c. sub-lattices.

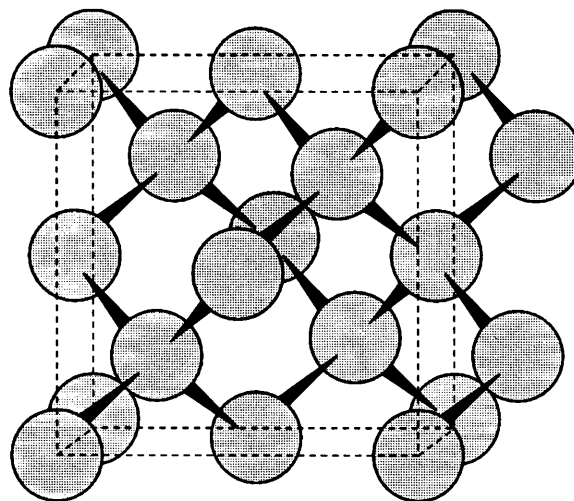


Figure 2.1: The structure of the diamond lattice. The dotted outline indicates a cube corresponding to one of the f.c.c. sub-lattices.

If the sites on the two interpenetrating lattices are occupied by two different elements, say A and B , the atoms on different sub-lattices are no longer equivalent. In this case they will still be arranged in a similar tetrahedral structure, but now every atom of element A is bonded to four atoms of element B and vice-versa. The arrangement that is formed in this way is called

the zincblende structure. Most III-V semiconductors (like GaAs) crystallize according to this structure. The zincblende structure, as typified by GaAs, is shown in figure 2.2. It is essentially identical to the diamond lattice, except that lattice sites are apportioned equally between two different atomic species. Ga atoms occupy the sites on one of two interpenetrating fcc sub-lattices while the other fcc sub-lattice is populated by As.

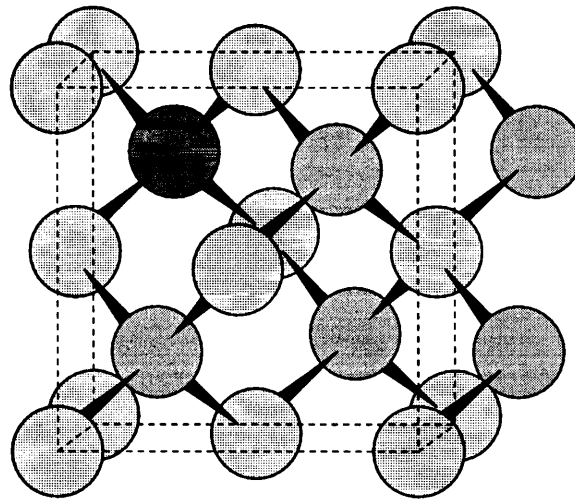


Figure 2.2: The zincblende structure, as typified by GaAs. A cube corresponding to one of the fcc sub-lattices is indicated.

In the quantum mechanical description of crystals, it is frequently necessary to transform between the so-called $\mathbf{r}$ -space and the $\mathbf{k}$ -space. In the $\mathbf{k}$ -space the periodicity of the crystal structure is described by the reciprocal lattice. The basis of the reciprocal lattice is given by

$$\mathbf{b}_i = \frac{2\pi \mathbf{a}_j \times \mathbf{a}_k}{(\mathbf{a}_1 \times \mathbf{a}_2) \cdot \mathbf{a}_3} \quad (2.2)$$

where i, j and k are assigned cyclic permutations of the values 1, 2 and 3.

The unit cell of the reciprocal lattice can be represented by a Wigner-Seitz unit cell. This unit cell is constructed by drawing the perpendicular bi-sector planes of lines connecting the chosen center of the unit cell to the nearest equivalent reciprocal lattice sites. The Wigner-Seitz cell for the diamond and zincblende lattices is shown in figure 2.3. Also shown are the high symmetry points and lines.

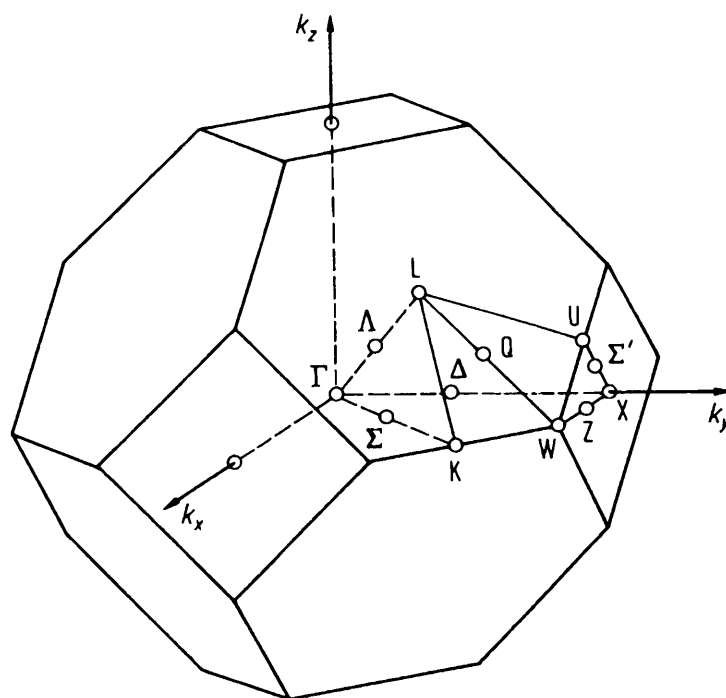


Figure 2.3: The Brillouin zone for diamond and zincblende lattices. The high symmetry points and lines are also indicated: Γ : $(0,0,0)$, zone centre; L : $2\pi/a (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$, zone edge along $\langle 111 \rangle$ axes Λ ; X : $2\pi/a (0,0,1)$, zone edge along $\langle 100 \rangle$ axes Δ ; K : $2\pi/a (\frac{3}{4}, \frac{3}{4}, 0)$, zone edge along $\langle 110 \rangle$ axes Σ . (After Brillouin 1963)

2.2 Electronic states in crystalline materials

To understand the physical properties of a crystal, it is necessary to understand how the behaviour of isolated atoms is changed, when they are placed in a regular arrangement, such as a crystal lattice.

Consider Si as an example. In the isolated state, the K - and L -shells (consisting of the $1s$, and $2s$ - and $2p$ -orbitals respectively) of the Si atom are filled, while the M -shell (consisting of the $3s$ -, $3p$ - and $3d$ -orbitals) contains 4 electrons. The highest filled shell, in this case the M -shell, is called the valence shell, while the electrons in the inner filled shells are referred to as core electrons. Generally the core electrons are bound much tighter and stay much closer to the nucleus than the valence electrons.

When the atoms are bound together to form a crystalline lattice, the orbitals of the valence shell overlap, and the electrons in these orbitals are responsible for the formation of a chemical bond. The orbitals of the core electrons, however, do not overlap, and remain essentially unchanged. The core electrons thus remain closely bonded to the nucleus, and do not directly affect the physical properties of the crystal. The nucleus and core electrons can thus be seen as a unit, with a nett positive charge.

Because the mass of an ion is at least a factor 10^4 greater than that of an electron, the ions move more than 10^4 times slower than the electrons. The ions can thus be regarded as being stationary, with the valence electrons moving freely among them, without affecting their positions. The electrons can thus be seen as moving in a periodic potential formed by the positively charged ions, as illustrated in figure 2.4

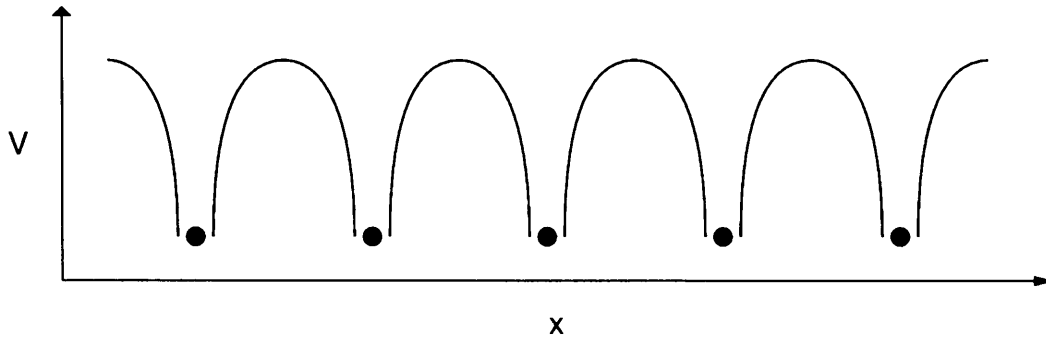


Figure 2.4: A schematic illustration of the potential of the crystal lattice felt by the "free" electrons.

2.3 Energy bands

A complete description of a crystal can be obtained by solving the Schrödinger equation for the whole crystal

$$\mathbf{H}\Psi = \mathbf{E}\Psi, \quad (2.3)$$

where the Hamiltonian consists of the sum of the Hamiltonians of all the particles in the crystal

$$\mathbf{H} = \sum_i \left(-\frac{\hbar^2}{2m_i} \nabla_i^2 \right) + \frac{1}{2} \sum_j \sum_{i \neq j} \frac{e_i e_j}{4\pi\epsilon_0 |r_i - r_j|} \quad (2.4)$$

and i ranges over all the particles in the crystal.

As shown previously, this model can be simplified by assuming that the nuclei and the core electrons are stationary. This problem is, however, still extremely difficult to solve. Generally it is also assumed that the wave function of each electron in the crystal is the same as that of a single electron moving in a potential formed by the stationary ions, and all the other electrons in the crystal.

Thus the band structure can be obtained by solving the Schrödinger equation for an approximate one-electron problem, where the influence of all the other electrons is combined

in a total, effective, periodic potential $V(\mathbf{r})$:

$$\left[\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) \right] \phi_{\mathbf{k}}(\mathbf{r}) = E_{\mathbf{k}} \phi_{\mathbf{k}}(\mathbf{r}) \quad (2.5)$$

Because of the translational symmetry of the crystal (and thus also of the potential $V(\mathbf{r})$), it follows that all physical quantities should be unchanged after the application of a translational symmetry operation. From this statement Bloch's theorem can be proven (Callaway 1984), which states that all the solutions of the above equation can be written as

$$\phi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k} \cdot \mathbf{r}} U_{n,\mathbf{k}}(\mathbf{r}) \quad (2.6)$$

where $U_{n,\mathbf{k}}(\mathbf{r})$ is periodic in $\mathbf{r}$ with the periodicity of the direct lattice, and n is the band index. It can furthermore be shown that the energy, $E_{\mathbf{k}}$, is periodic in the reciprocal lattice with $E_{\mathbf{k}} = E_{\mathbf{k}+\mathbf{G}}$, where $\mathbf{G}$ is any reciprocal lattice vector. Thus, to label the energy for a specific band uniquely it is sufficient to use only $\mathbf{k}$'s in a primitive cell of the reciprocal lattice. Conventionally this primitive cell, also known as the Brillouin zone, is chosen as the Wigner-Seitz cell. The dependence of the energy E on $\mathbf{k}$ for a specific solid is known as its band structure.

The Brillouin zone for the diamond and zincblende structures is identical to that of an fcc lattice, as illustrated in figure 2.3. Also shown are a number of symmetry points, which are: Γ , center of the zone; L , zone edge along $\langle 111 \rangle$ axes; X , zone edge along $\langle 100 \rangle$ axes; and K , zone edge along $\langle 110 \rangle$ axes. The symmetry lines are Λ ($\langle 111 \rangle$ axes), Δ ($\langle 100 \rangle$ axes) and Σ ($\langle 110 \rangle$ axes). For a discussion of the symmetry properties and their effect on the band structure of semiconductors see for instance Parmenter (1955).

There exist a large number of methods according to which the band structure of semiconductors can be determined. The $\mathbf{k} \cdot \mathbf{p}$ method for calculating the band structure of semiconductors is quite successful in describing the band structure of diamond lattice semiconductors such as Si and Ge. Although this is not the ideal method to calculate the band structure of GaAs, it can be used very elegantly to calculate the approximate band structure in a quantum well, as will be discussed in chapter 5.

2.4 Calculation of energy band structure using the $\mathbf{k} \cdot \mathbf{p}$ method

When equation (2.6) for the Bloch wave-functions is substituted in the Schrödinger equation, one obtains after some simplification (Kane 1956, Callaway 1984)

$$\left\{ \frac{\mathbf{p}^2}{2m} + \frac{\hbar}{2m} \mathbf{k} \cdot \mathbf{p} + \frac{\hbar^2 \mathbf{k}^2}{2m} + V(\mathbf{r}) \right\} U_{n,\mathbf{k}}(\mathbf{r}) = E_{\mathbf{k}} U_{n,\mathbf{k}}(\mathbf{r}) . \quad (2.7)$$

Clearly this equation is a normal Schrödinger equation, with the terms $(\hbar/2m) \mathbf{k} \cdot \mathbf{p}$ and $\hbar^2 \mathbf{k}^2 / 2m$

added to the Hamiltonian. The second term is constant for a given $\mathbf{k}$, and can thus easily be taken into account. The $\mathbf{k} \cdot \mathbf{p}$ term, however, is not constant. This term can be treated as a perturbation of the original Hamiltonian.

By applying second order perturbation theory to the above equation (in many cases the first order terms disappear due to symmetry), an expression can be found that describes the band structure of the crystal, in terms of a number of experimentally determinable values.

A further term that is generally also taken into account is the spin-orbit interaction (Dresselhaus 1955). This is done by adding a term $\mathbf{H}_{so} = (\hbar/4m^2c^2)[(\nabla V \times \mathbf{p}) \cdot \boldsymbol{\sigma}]$ (where $\boldsymbol{\sigma}$ is the electron spin operator) to the Hamiltonian (or more correctly, using the Dirac equation and ignoring negligible terms). This results in the splitting of some bands into two bands, depending on the spin of the relevant electrons.

The band structure, of Si and GaAs is shown in figure 2.5 and 2.6 respectively. Here it can clearly be seen that there is an energy region in which no states are allowed. In an intrinsic semiconductor all the states below this band gap are filled at 0 K. These states are referred to as the valence band, while the states above the forbidden band gap are referred to as the conduction band. The energy difference between the lowest states of the conduction band, and the highest states in the valence band is called the band gap, E_g . The energy at the bottom of the conduction band is designated E_C , while the energy at the top of the valence band is E_V . The energy of electrons is generally defined to be positive, when measured upwards, while the energy of holes (a hole is an unoccupied state, acting like a particle with a positive charge) is considered positive when measured downwards.

In the zincblende structure, the valence band consists of four sub-bands (spin excluded). At $k = 0$, the top three bands are degenerate, and form the upper edge of the band. The two top valence bands are referred to as the heavy (the wider band with less curvature) and the light (the narrower band with the higher curvature) holes. The mass referred to here is the effective mass. The effective mass is a tensor quantity, defined as

$$\frac{1}{m_{ij}^*} = \frac{1}{\hbar} \frac{\partial^2 E(\mathbf{k})}{\partial k_i \partial k_j}. \quad (2.8)$$

This tensor replaces the mass of a free electron in most equations, and describes how the behaviour of the electron is changed because of the interaction with the periodic lattice. For instance, instead of the free electron mass, the effective mass is used to calculate the acceleration of an electron under an external field, and to determine the density of states in the specific band. It is generally expressed as a fraction of the free electron rest mass m_e . Some values are given in chapter 3.

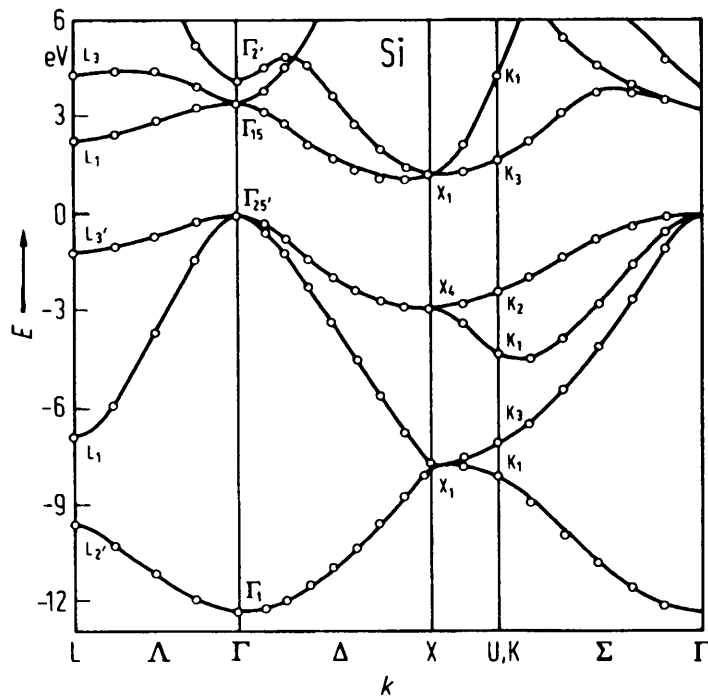


Figure 2.5: Band structure of Si as calculated by non-local, energy-dependent pseudopotential method (solid line) and localized atomic orbital method (circles) by Sieh (1985).

The conduction band also consists of a number of sub-bands, but this varies greatly between different zincblende semiconductors. If the minimum in the conduction band occurs at the same k as the maximum in the valence band, as in the case of GaAs, the band gap is said to be direct. For GaAs the conduction band minimum is at the centre of the Brillouin zone, Γ , thus there is only one conduction band minimum in the Brillouin zone. This minimum is more or less spherically symmetric.

Silicon is an indirect band gap semiconductor. Here the minimum in the conduction band is situated along the $\langle 100 \rangle$ axis, about three-quarters of the distance to the Brillouin zone edge. As there are six equivalent $\langle 100 \rangle$ axes, it follows that silicon has six equivalent minima in its Brillouin zone.

In summary, it can be seen that the single energy levels of isolated atoms, are spread out to form energy bands when the atoms are placed together in a crystal lattice. In semiconductors there is a gap between the lowest band filled at 0 K (the valence band) and the band directly above it (the conduction band).

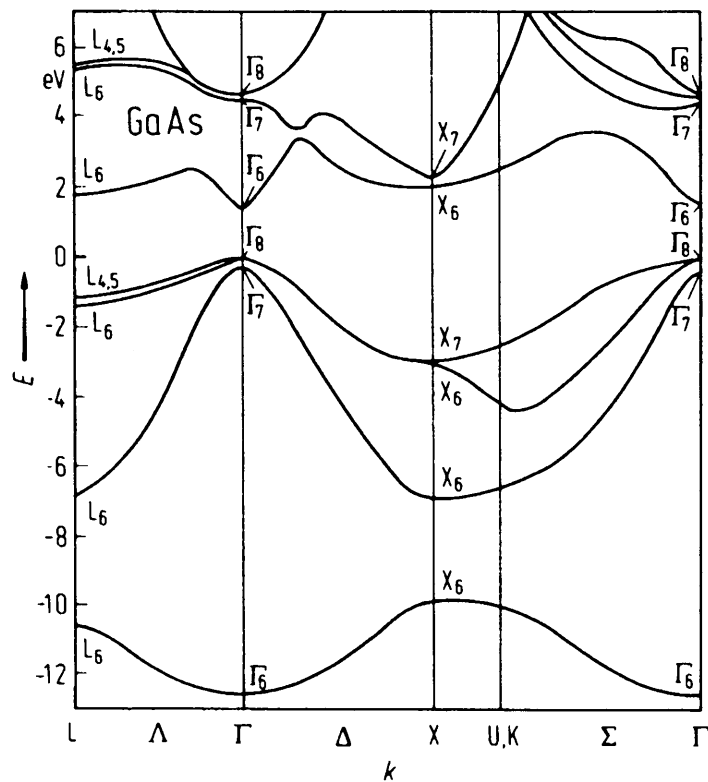


Figure 2.6: Band structure of GaAs as calculated by non-local, energy-dependent pseudopotential calculations by Chelikowsky (1976).

2.5 Occupancy of states in the valence and conduction bands

In a pure, defect-free semiconductor, the amount of electrons in the crystal is just enough to fill all the states in the valence band. If this is true to a good approximation, the semiconductor is called intrinsic. In this case, the only electrons in the conduction band are electrons that have been excited from the valence band. Similarly, the only holes in the valence band are those that have been left because electrons have been excited to the conduction band.

In order to make a useful device, it is in many cases necessary to “add” or “remove” electrons from the semiconductor. This can be done by doping the semiconductor with a very low concentration of an impurity atom. For instance, by replacing an atom in a silicon crystal by a group V element like phosphorus, an extra electron is added to the crystal. This electron is a valence electron, and is therefore not strongly bound to the phosphorus atom. The electron is thus easily freed from the phosphorus atom, so that it can move freely in the crystal, with the other valence electrons. An atom like the phosphorus atom is referred to as a donor. Similarly, if a silicon atom is replaced by a group III element like boron, it will contribute only three electrons instead of the usual four. This means that an extra electron

can be accommodated in the valence band of the semiconductor. These atoms are referred to as acceptors.

The total number of electrons in the conduction band of the semiconductor is given by

$$n = \int_{E_c}^{E_{top}} N(E) F(E) dE, \quad (2.9)$$

where $N(E)$ is the density of states in the conduction band, and $F(E)$ is the probability that a given state is occupied. E_{top} is the energy at the top of the conduction band. The density of states in the conduction band for low energies can be approximated by

$$N(E) = M_c \frac{\sqrt{2}}{\pi^2} \frac{(E - E_c)^{1/2}}{\hbar^3} (m_{de})^{3/2}, \quad (2.10)$$

where M_c is the number of equivalent minima, and m_{de} is the geometric mean of the effective masses along the principal axes of the ellipsoidal energy surface. The probability that a state is occupied is given by the Fermi-Dirac distribution

$$F(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{kT}\right)}, \quad (2.11)$$

where k is Boltzmann's constant, T is the absolute temperature, and E_F is the Fermi energy.

The integral (2.9) can be evaluated to yield

$$n = N_C \frac{2}{\sqrt{\pi}} F_{1/2}\left(\frac{E_F - E_C}{kT}\right), \quad (2.12)$$

where N_C is the effective density of states in the conduction band defined by

$$N_C \equiv 2 \left(\frac{2\pi m_{de} kT}{h^2} \right)^{3/2} M_C \quad (2.13)$$

and $F_{1/2}(\eta_f)$ is Fermi-Dirac integral

$$F_{1/2}(\eta_f) \equiv \int_0^\infty \frac{\eta^{1/2}}{1 + e^{(\eta - \eta_f)}} d\eta. \quad (2.14)$$

If the Fermi level is several kT below the conduction band, the Fermi distribution can be

approximated by a Boltzmann distribution. In this case the integral (2.14) approaches the value $\sqrt{\pi} e^{\eta}/2$, and equation (2.12) becomes

$$n = N_C \exp\left(-\frac{E_C - E_F}{kT}\right). \quad (2.15)$$

However, there are cases when this approximation is not valid. Other, more exact, approximations for integral (2.14) will be discussed later in chapter 7.

For the hole density in the valence band, similar equations can be derived:

$$p = N_V \frac{2}{\sqrt{\pi}} F_{1/2}\left(\frac{E_V - E_F}{kT}\right), \quad (2.16)$$

where N_V is the effective density of states in the valence band, given by

$$N_V \equiv 2 \left(\frac{2\pi m_{dh} kT}{h^2} \right)^{3/2}, \quad (2.17)$$

where m_{dh} is the density of states effective mass of the valence band. In the case of semiconductors with a typical zincblende valence band, the density of states is given by

$$m_{dh} = (m_{lh}^{3/2} + m_{hh}^{3/2})^{2/3}, \quad (2.18)$$

where m_{lh} and m_{hh} refer to the “light” and “heavy” holes respectively. Under non-degenerate conditions, the above equation can be approximated by

$$p = N_V \exp\left(-\frac{E_F - E_V}{kT}\right). \quad (2.19)$$

In the derivation of the previous equations, the probability that a given state is occupied, was assumed to be given by the Fermi-distribution. It is thus not surprising that the occupancy of states in the semiconductor strongly depends on the value of the Fermi-energy, E_F . The position of the Fermi level in a semiconductor can be determined by making use of the charge-neutrality condition. By equating the number of holes in the valence band to the number of electrons in the conduction band, one obtains

$$N_C \exp\left(-\frac{E_C - E_F}{kT}\right) = N_V \exp\left(-\frac{E_F - E_V}{kT}\right), \quad (2.20)$$

and by solving for E_F an expression of the Fermi-energy can be obtained

$$E_F = \frac{E_C + E_V}{2} + \frac{kT}{2} \ln\left(\frac{N_V}{N_C}\right). \quad (2.21)$$

At room temperature kT has a value of only 0.03 eV, and since N_V and N_C seldom differ by more than a factor of 100, it follows that the Fermi level in an undoped (intrinsic) semiconductor lies close to the middle of the band gap.

When a semiconductor is doped with impurity atoms, these impurities cause energy levels in the band gap of the semiconductor. A donor level is defined as being neutral when filled by an electron, and positive when empty. A level that is neutral when empty, and negative when occupied by an electron, is called an acceptor level.

The probability of a donor level being empty (i.e. having donated its electron) can be calculated from the Fermi-distribution. In general the bound state of the donor atom is twofold degenerate (because of spin). With this taken into account, the density of ionized donors is given by

$$N_D^+ = N_D \left[1 - \frac{1}{1 + \frac{1}{g} \exp\left(\frac{E_D - E_F}{kT}\right)} \right] \quad (2.22)$$

where N_D is the density of donor atoms, and g is the ground state degeneracy of the donor impurity level. For acceptor impurities the equivalent expression is

$$N_A^- = N_A \left[\frac{1}{1 + g \exp\left(\frac{E_A - E_F}{kT}\right)} \right] \quad (2.23)$$

where the ground state degeneracy factor, g , is 4 for acceptor levels. This is because in Ge, Si and GaAs the valence band is fourfold degenerate (spin included) at $\mathbf{k} = 0$.

2.6 Determining the position of the Fermi level for doped semiconductors

The position of the Fermi level in an extrinsic semiconductor can be determined in a similar way as was used in the intrinsic case. For a given set of N_C , N_D , N_A , N_V , E_C , E_D , E_A , E_V and T the position of the Fermi level can be uniquely determined from charge neutrality

$$n + N_A^- = p + N_D^+ \quad (2.24)$$

In general this leads to a non-linear equation in E_F . In complicated cases this equation has to be solved numerically, but in many simple cases this equation can be solved by making relevant assumptions. For instance, if the concentration of donors is much higher than that of acceptors, the effect of the acceptors can be ignored in most cases. In this case it is found

that the Fermi level moves upwards from the middle of the band gap towards the conduction band. By substituting the relevant values in equation (2.24) it can be shown that the distance between the Fermi level and the conduction band edge, often referred to as ξ , is

$$\xi = E_C - E_F = kT \ln \left(\frac{N_C}{N_D} \right). \quad (2.25)$$

Similarly, if the acceptor concentration is dominant, the Fermi level will move downwards, towards the valence band.

2.7 Ternary and quaternary alloy semiconductors

In an attempt to “tune” the band gap of semiconductors, semiconductor alloys were developed. For instance, by making an alloy of GaAs and AlAs it is possible to change the band gap continuously from the band gap of GaAs, of about 1.4 eV, to the band gap of AlAs of about 2.2 eV. Other parameters such as the lattice constant a change in a similar way. Alloys like this are generally indicated as $\text{Ga}_{1-x}\text{Al}_x\text{As}$, where x indicates the concentration of AlAs in the alloy. In addition to ternary alloys such as $\text{Ga}_{1-x}\text{Al}_x\text{As}$, quaternary alloys such as $\text{Ga}_{1-x}\text{In}_x\text{As}_{1-y}\text{P}_y$ have been developed. With these alloys it is possible to specify two parameters. For instance, it is possible to choose x and y in such a way that, within certain limits, a semiconductor with any band gap and any lattice parameter can be created. This is especially important when semiconductor heterojunctions are made. Here one semiconductor is grown on top of another. In general, if one of the semiconductors is an alloy, it is possible to vary its composition in such a way that both semiconductors have the same lattice parameter. In this case it is possible to grow heterojunctions with very few interfacial defects.

Figure 2.7 (on the next page) illustrates the lattice parameter vs. energy gap for a number of semiconductors and their alloys. Lines connecting the pure III-V compounds illustrate the relationship between the band gap and the lattice parameter of their alloys. The shaded areas indicate the combination of band gaps and lattice parameters which are possible with quaternary semiconductors. Note that the lattice parameter of $\text{Ga}_{1-x}\text{Al}_x\text{As}$ changes only very slightly as x is varied from 0 to 1. It will be seen later that it is this property that makes it very suitable for the growth of heterostructures.

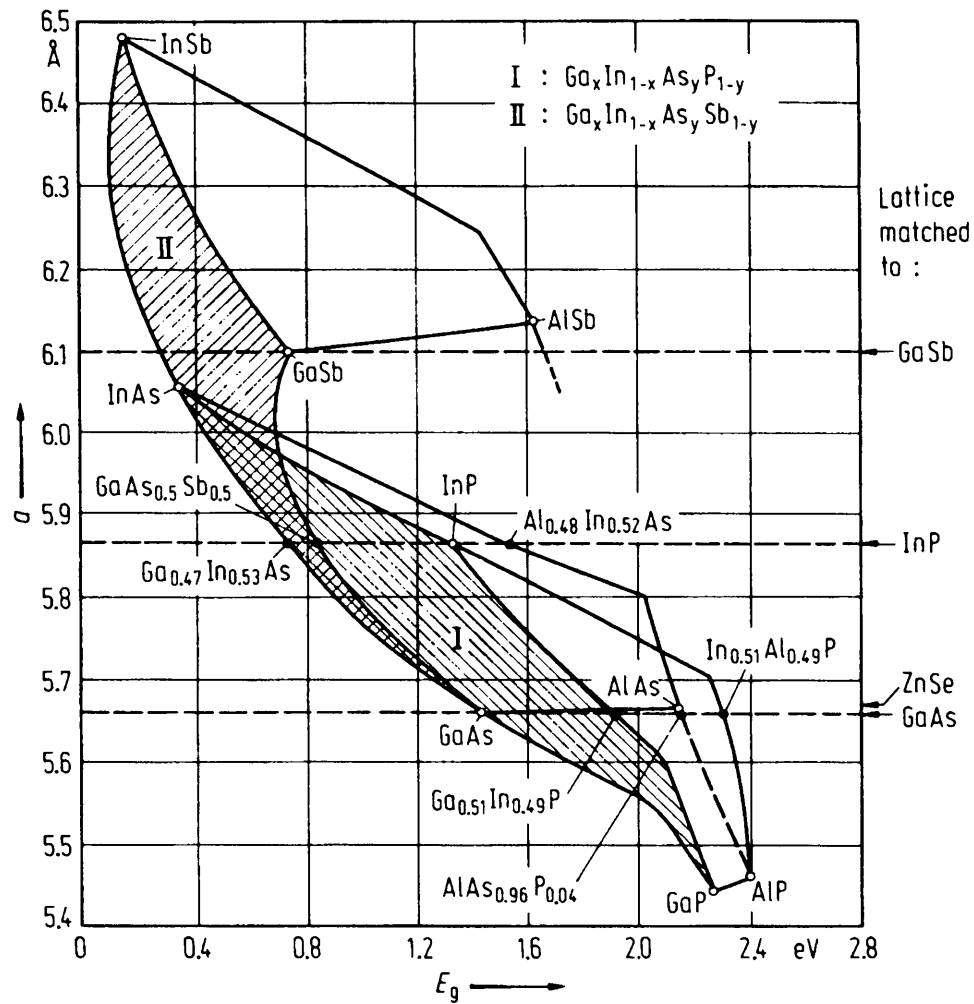


Figure 2.7. Lattice parameter vs. energy gap for various III-V compounds and their alloys (Madelung 1991)

3

Properties of some III-V semiconductors

The purpose of this chapter is to give a quick overview of the properties of some of the semiconductors that are discussed in this dissertation. For a more complete list of the properties of a very large number of semiconductors the reader is referred to reference works such as those by Madelung (1991) (from which much of the data in this chapter was obtained) or the appropriate volumes of the Landolt-Börnstein series, in which a number of appropriate references are cited.

Ga_{1-x}Al_xAs is a very popular material for the fabrication of semiconductor heterostructures. Because its lattice constant is very close to that of GaAs, heterojunctions between GaAs and Ga_{1-x}Al_xAs have relatively few interfacial defects.

GaAs, AlAs and Ga_{1-x}Al_xAs all crystallize according to the zincblende structure, as described in chapter 2. GaAs has a direct gap, while AlAs has an indirect gap. The properties of Ga_{1-x}Al_xAs depend strongly on x . For $x < 0.3$ Ga_{1-x}Al_xAs has similar properties than GaAs, except that its band gap increases and lattice parameter decreases slightly with increasing x . For $x > 0.5$, Ga_{1-x}Al_xAs has an indirect band gap, and its properties correspond more closely to those of AlAs.

More complete information can be found in a number of excellent review papers summarizing the properties of GaAs, AlAs, and Ga_{1-x}Al_xAs (see for instance Adachi 1985 and Chand *et al* 1984).

3.1 Gallium arsenide (GaAs)

GaAs is a direct band gap semiconductor, with the conduction band minimum situated at Γ . The band structure is shown in the previous chapter, figure 2.6. The band gap at 300 K is 1.424 eV. At other temperatures in the range 0 to 800 K the band gap can be calculated from (Blakemore 1982)

$$E_g = 1.519 - 5.408 \times 10^{-4} T^2 / (T + 204) \text{ eV.} \quad (3.1)$$

The density of states effective masses of holes and electrons in units of m_e are $m_{p,ds} = 0.53$ and $m_{n,ds} = 0.063$, and the effective density of states in the conduction band N_C is 4.7×10^{17} , while the effective density of states in the valence band N_V is 7.0×10^{18} at 300 K. The values

for the effective masses do not seem to vary by more than a few percent under the influence of temperature in the range 10 - 300 K.

The dielectric constant ϵ_s is 12.8 times ϵ_0 at 300 K, and at other temperatures can be calculated from

$$\epsilon_s/\epsilon_0 = 12.40 \times (1 + 1.2 \times 10^{-4}T). \quad (3.2)$$

There seems to be some controversy regarding this result, and some authors quote a value of 13.1 at 300 K (Adachi 1985). The breakdown field of GaAs is about 4×10^7 V/m. The most important *n*-type dopant is Si, which forms a donor band 5.84 meV below the conduction band edge. In GaAs, most donor levels are very close to the conduction band.

3.2 Aluminium arsenide (AlAs)

The band structure of AlAs is shown in figure 3.1. AlAs has an indirect band gap, with the minima situated near the *X* points of the Brillouin zone, and a band gap of 2.153 eV at 300 K. The density of states effective masses of electrons in the *X*, *L* and Γ minima are $m_{n,ds}(X) = 0.71$, $m_{n,ds}(L) = 0.66$, and $m_{n,ds}(\Gamma) = 0.150$ respectively, while the density of states effective mass for holes $m_{h,ds} = 0.174$. The low frequency dielectric constant is 10.06 times ϵ_0 . The binding energy of Si donors is approximately 57 meV.

3.3 Aluminium gallium arsenide ($\text{Ga}_{1-x}\text{Al}_x\text{As}$)

The band structure of $\text{Ga}_{1-x}\text{Al}_x\text{As}$ is characterized by a crossover from the sequence $\Gamma - L - X$ in GaAs to $X - L - \Gamma$ in AlAs. While *x* is smaller than about 0.35, the band structure of $\text{Ga}_{1-x}\text{Al}_x\text{As}$ remains similar to GaAs, with the conduction band minima in the same sequence. When *x* = 0.35, the *L* and *X* bands have the same energy, and for larger *x* their order is interchanged when compared to GaAs. For *x* larger than 0.43, the Γ -band has a higher energy than the *X*-band, causing the semiconductor to have an indirect band gap. In the region where *x* is smaller than 0.3, the composition dependence of the band gap at 300 K, is given by (Saxena 1981)

$$E_g(\Gamma) = 1.420 + 1.087x + 0.438x^2 \text{ eV}, \quad (3.3)$$

while the lattice parameter is given by (Adachi 1985)

$$a = 5.6533 + 0.0078x \text{ \AA}. \quad (3.4)$$

According to Adachi (1985) the dielectric constant and effective masses can be determined to a good approximation by assuming a linear compositional dependence. However, it should be noted that when there is a possibility that more than one conduction band minimum could contribute towards conduction (eg. when *x* is in the region of 0.43), the

effect of all the contributing minima should be taken into account. This procedure is described in detail by Chand *et al* (1984).

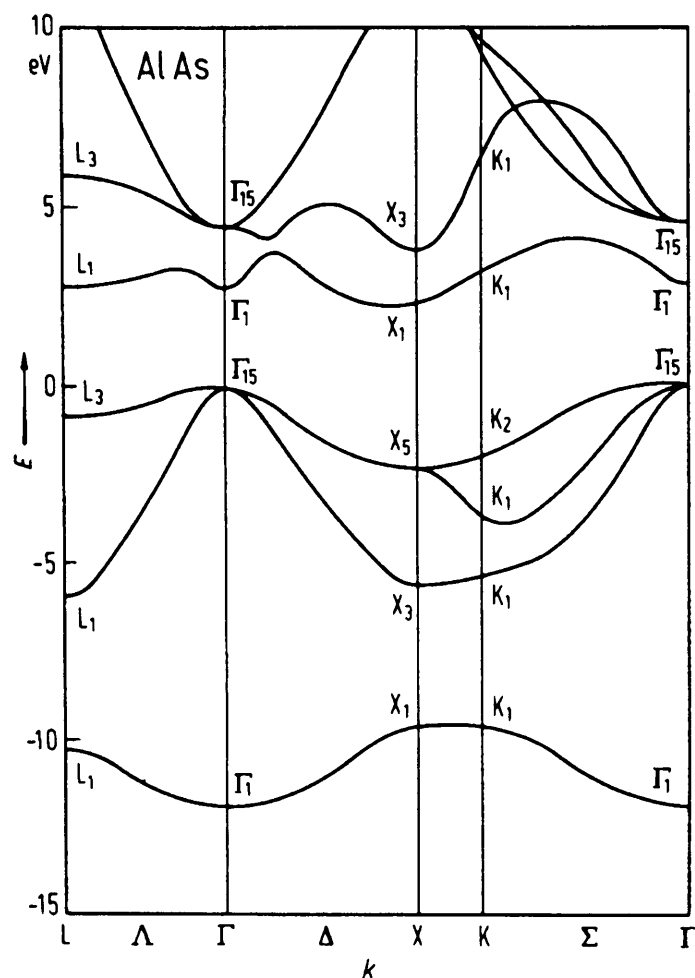


Figure 3.1. Band structure of AlAs as calculated by means of an orthogonalized LCAO method (Haung 1986).

The impurity levels in AlGaAs are an irregular function of x . The case of Si has been investigated by Chand *et al* (1984). Si is almost an ideal dopant, since it has a sticking coefficient of almost unity, a small diffusivity, and allows good optical and electrical properties to be obtained. For this reason Si is a very popular dopant in GaAs-AlGaAs heterostructures. According to Chand *et al* (1984), E_D remains constant at about 10 meV for $x < 0.2$, but starts rising at $x \sim 0.2$ to a value of about 60 meV at $x = 0.3$, reaching a maximum of about 160 meV at $x \sim 0.48$, where the band gap changes from direct to indirect. Hereafter

E_D decreases monotonically to a value of about 57 meV in AlAs. In the region $0.22 < x < 0.40$, which is the most often used region, E_D can be expressed as

$$E_D \cong 707x - 146 \text{ meV}. \quad (3.5)$$

4

Metal-semiconductor junctions

A number of early researchers have noted that the total resistance of a metal-semiconductor junction depends on the polarity of the applied voltage. This effect was researched further and later used in point contact rectifiers. A number of models, according to which these junctions operate, have been suggested. In this chapter, the model proposed by Schottky (1942) will be discussed in detail. This model describes an ideal case, where the metal and the semiconductor are in intimate contact, without the presence of any interface states. In practice it is possible to fabricate contacts which approach this limit. The Bardeen model describes a more general case where the effects of an interfacial layer and interface states are taken into account. A detailed discussion of the Bardeen model is given in Bardeen (1947) and Rhoderick (1988). Currently metal-semiconductor junctions are important because they are used in devices, and also as tools in the analysis of physical parameters of semiconductors. For this reason metal-semiconductor junctions have been studied extensively.

4.1 The structure of a Schottky barrier

When a metal contact is evaporated onto the surface of a semiconductor, a potential barrier is formed at the metal-semiconductor interface. Here, only the case for an n -type semiconductor will be considered. The formation of a Schottky barrier on p -type material occurs similarly.

4.2 The Formation of a Schottky Barrier in an ideal case

Qualitatively the formation of a Schottky barrier can be described by first considering the metal and the semiconductor in their isolated, electrically neutral states, as shown in figure 4.1(a). Here χ_s is the electron affinity of the semiconductor. (The electron affinity of a substance is the energy released when an electron is added to the material - i.e. in this case the difference between the vacuum level and the conduction band edge.) ϕ_m and ϕ_s are the work functions of the metal and the semiconductor respectively. (The work function of a material is the energy required to remove an electron from the material to the vacuum level - i.e. the difference between the vacuum level and the Fermi level.) Figure 4.1 illustrates the case where the work function of the metal is larger than that of the semiconductor, which, in practice, is the most important case. This relationship between the two work functions causes the Fermi level of the metal to be lower than that of the semiconductor.

Now, if the metal and the semiconductor were connected by means of a thin wire, electrons would flow from the semiconductor to the metal. Because of this flow of electrons, a positive charge builds up on the surface of the semiconductor, while a negative charge builds up on the surface of the metal, causing an electric field in the gap between the metal and the semiconductor. This electric field opposes the flow of electrons. The equilibrium condition is reached when the Fermi levels of the two materials coincide. This implies that the potential difference between the metal and the bulk of the semiconductor is equal to the difference in their Fermi levels.

The negative charge that builds up on the surface of the metal is caused by extra electrons that are accommodated within the Thomas-Fermi screening distance of about $0.5 \text{ \AA}$. In the semiconductor, however, the only electrons close to the Fermi level that can be removed, are those in the conduction band, which are provided by the ionized donor atoms. Thus the positive charge in the semiconductor is provided by the uncompensated donor atoms, left after electrons have flowed from the conduction band. The concentration of these donor atoms is much lower than the concentration of electrons in the metal. This means that electrons are depleted from the conduction band up to an appreciable depth, w . For carrier densities of 10^{16} cm^{-3} the thickness of this so-called depletion layer, is generally in the order of a micron. Because the charge in the depletion region is distributed over a finite distance, the potential changes slowly over the depletion region, and causes the bands to bend upwards as shown in figure 4.1(b).

The difference between the electrostatic potentials at the surfaces of the metal and the semiconductor is given by $V_i = \delta E_i$, where δ is the distance between the metal and the semiconductor, and E_i is the electric field in the gap. As the gap, δ , is decreased, the electric field stays finite (figure 4.1(c)), and causes V_i to tend towards zero as the gap disappears. When ideal contact is made, the barrier due to the vacuum disappears completely (figure 4.1(d)), and the only barrier seen by electrons, is that caused by the bending of the bands in the semiconductor. The height of this barrier measured relative to the Fermi level is given by

$$\phi_b = \phi_m - \chi_s. \quad (4.1)$$

The height of the barrier relative to the position of the conduction band in the neutral region of the semiconductor is called the diffusion potential, and is indicated by V_d .

In practice it is very difficult to fabricate Schottky diodes by conventional vacuum deposition without a thin insulating layer of oxide about 10 to 20 $\text{\AA}$ thick forming on the surface of the semiconductor. This layer is often referred to as the interfacial layer. A practical Schottky diode is therefore better represented by figure 4.1 (c). The interfacial layer is usually very thin, so that electrons can easily tunnel through it, causing this case to be almost indistinguishable from the ideal case illustrated in figure 4.1 (d). Furthermore, the potential drop V_i is so small that equation (4.1) remains a reasonable approximation.

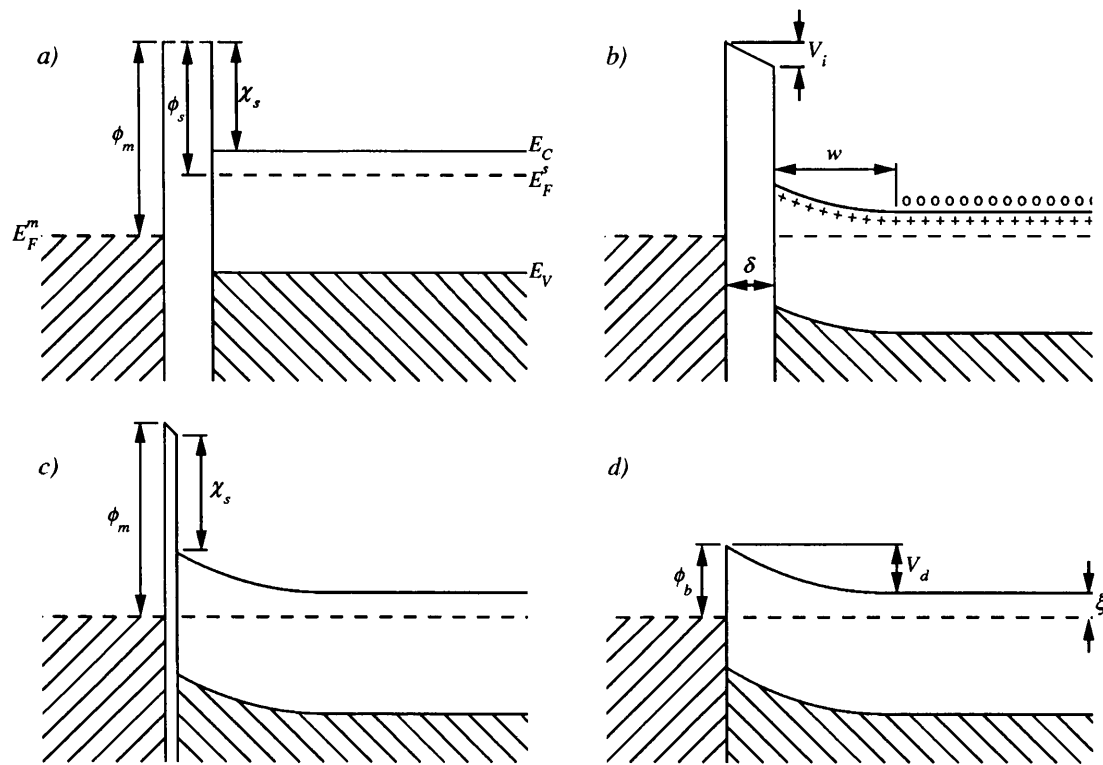


Figure 4.1: The formation of a Schottky barrier. a) The metal and the semiconductor in their isolated states, b) electrically connected, c) separated by a narrow gap, d) in perfect contact. (After Rhoderick 1988)

In this discussion we have assumed that the properties of the semiconductor stay “bulk like” right up to the interface. This, however, is seldom the case. Since the atoms close to the surface have neighbours on one side only, they tend to have a different symmetry in comparison to atoms in the bulk of the semiconductor, in the direction perpendicular to the surface. This process is called relaxation. Thus the high symmetry of the crystal is suddenly terminated at the surface, causing the conditions that led to the creation of a band gap in the bulk of the crystal not to exist at the surface. Thus it is possible that states exist at the surface of the semiconductor with energies in the band gap. These states can also contribute to the charge in the contact region, thus affecting the barrier height (Cowley *et al* 1965). Another source of localized states in the interfacial region are so-called metal induced gap states (MIGS) which are caused by the wave function of the electron states in the metal extending into the semiconductor. These states decay exponentially into the semiconductor within a couple of Angstroms. A more detailed discussion is given by Rhoderick (1988). Another assumption that might not be valid is that ϕ_m and χ_s remain constant right up to the interface. In practice these factors cause significant deviations from the predictions made by equation (4.1).

4.3 Behaviour of the barrier under forward and reverse bias

When a bias is applied across the barrier, the relationship between the Fermi levels in the semiconductor and the metal is changed. Under zero bias conditions, the electrons from both sides of the junction “see” the same barrier height. As a result there is no nett flow of electrons over the barrier in the one or the other direction.

However, if a forward bias is applied (i.e. negative side is connected to the semiconductor), the position of the Fermi level in the semiconductor is raised relative to that of the metal. This decreases the amount of band bending, causing electrons in the semiconductor to “see” a lower barrier than those in the metal. This causes a nett flow of electrons from the semiconductor to the metal. As the forward bias is increased, the barrier presented to the electrons decreases, causing an increase in the current flowing over the junction.

Under reverse bias, the Fermi level of the semiconductor is lowered relative to that of the metal, causing more band bending and an increase in the barrier seen by electrons in the semiconductor. This also increases the length of the depletion region. The barrier experienced by electrons from the metal, however, stays constant. Thus the current from the semiconductor to the metal stays constant, as the current from the semiconductor to the metal decreases. This causes the current under reverse bias to tend toward a limit as the reverse bias is increased. This continues until the electric field in the depletion region increases beyond the dielectric strength of the semiconductor, causing the semiconductor to break down suddenly, leading to a large current flowing across the barrier. This could cause irreversible damage to the device.

4.4 Current-transport across the barrier

There are a number of mechanisms according to which electrons can be transported across the barrier. These are discussed in detail by Rhoderick (1988). In “almost ideal” Schottky diodes, fabricated on GaAs with doping concentrations in the $10^{14} - 10^{16} \text{ cm}^{-3}$ range, the dominant mechanism for reverse bias and small forward bias is thermionic emission. According to this theory, the current flowing through the contact is limited only by the flow of electrons across the barrier due to the bending of the bands. By assuming that the electrons in the conduction band have a Maxwellian distribution, it can be shown that the current density, J , flowing across the barrier is given by

$$J = A^{**} T^2 \exp(-q\phi_b/kT) \{ \exp(qV/nkT) - 1 \} \quad (4.2)$$

where A^{**} is the Richardson constant, T is the temperature, q is the electron charge, ϕ_b is the barrier height, k is the Boltzmann constant, V is the applied bias, and n is the so-called ideality factor. For an ideal case n should be equal to one, but because of effects like the voltage dependence of the barrier height, it is in many cases larger than unity. Equation (4.2) is valid for both forward and reverse bias. For large forward bias, however, the series

resistance of the contact becomes the limiting factor, causing the current through the diode to be less than predicted by the thermionic emission model.

There are other mechanisms which also contribute to current flow across the Schottky barrier. These mechanisms, e.g. tunnelling and recombination, are only significant when the current flow due to thermionic emission is very low, as in the reverse and low forward bias regions. For this reason they are only mentioned in this study. A good description of these mechanisms can be found in Rhoderick (1988) or Sze (1981).

4.5 Calculation of the electric field in a Schottky barrier

The form of the band edge profiles can be calculated by solving Poisson's equation, subject to certain boundary conditions. The first boundary condition is obtained from the barrier height, while the second is obtained by assuming that there is no electric field in the bulk of the semiconductor. By choosing $x = 0$ at the interface, the boundary conditions can be written as $E(\infty) = 0$, and $V(0) = V_d$. These relationships serve as boundary conditions for the solution of Poisson's equation in the semiconductor, which can be written in the one-dimensional case as

$$\frac{d^2V}{dx^2} = \frac{1}{\epsilon_s} \rho(x), \quad (4.3)$$

where $\rho(x)$ is the total charge density in the semiconductor and ϵ_s is the permittivity of the semiconductor. In general, contributions from the valence band, the conduction band, ionized donors and acceptors and deep levels in the band gap should be taken into account. This however leads to a very complicated equation, that can only be solved numerically. The equation can be simplified by making use of the depletion approximation.

According to the abrupt or depletion approximation, it is assumed that it is possible to divide the semiconductor into two regions: the depletion region, directly below the metal, which is devoid of free carriers, and the bulk of the semiconductor, which is electrically neutral, and in which no electric field exists. In the depletion region, where there are no electrons in the conduction band, the charge density, ρ , is qN_D . If the width of the depletion region is w , the charge density in the semiconductor can be written as

$$\rho(x) = \begin{cases} qN_D & \text{if } x \leq w \\ 0 & \text{if } x > w \end{cases} \quad (4.4)$$

By integrating this equation twice, and applying the boundary conditions, the width of the depletion region can be obtained as

$$w = \sqrt{\frac{2\epsilon_s V_d}{qN_D}} \quad (4.5)$$

while the electric field and the potential in the depletion region are given by

$$E(x) = - \frac{qN_D (w - x)}{\epsilon_s} \quad (4.6)$$

and

$$V(x) = - \frac{qN_D}{2\epsilon_s} (w - x)^2. \quad (4.7)$$

From the above equations it can be seen that the magnitude of V rises quadratically as the metal is approached, to a maximum value of $qN_D w^2/2\epsilon_s$ at the interface, which is equal to the diffusion potential V_d . The electric field strength increases linearly, and reaches a maximum value, E_{max} , at the interface. The magnitude of the field at the interface is

$$|E_{max}| = qN_D w / \epsilon_s = Q_d / \epsilon_s, \quad (4.8)$$

where Q_d is the total charge per unit area due to uncompensated donors in the depletion region, which can also be written as

$$Q_d = qN_D w = \sqrt{2\epsilon_s qN_D V_d}. \quad (4.9)$$

From this the diode's capacitance per unit area can be determined as

$$C = \frac{\partial Q_d}{\partial V_d} = \sqrt{\frac{\epsilon_s qN_D}{2V_d}} = \frac{\epsilon_s}{w}. \quad (4.10)$$

In this approximation the depletion region of a reverse biased Schottky diode can be seen as the two plates of a parallel plate capacitor. Here the depletion region, which is depleted of free carriers and thus acts as an insulator, acts as a dielectric between the plates. In most cases the depletion approximation yields acceptable results, but when higher accuracy is required, a more accurate charge distribution model should be used.

4.6 A more exact analysis of the electric field in a Schottky barrier

The depletion approximation implies an abrupt transition between the depletion region and the bulk of the semiconductor. In general, however, the majority carrier concentration changes gradually over a finite transition region. The effect of this, and of minority carriers accumulating close to the interface has been investigated by Atalla (1966), and has been reported in many textbooks e.g. Rhoderick (1988). In this derivation it is assumed that the Fermi level stays approximately flat, right up to the interface. (This assumption is controversial. However, it can always be assumed that the Fermi level in the depletion

region will be far enough from the conduction band, so that the number of conduction electrons in the depletion region remains negligible. It is thus only the hole concentration at the surface, p_s , which is affected. A detailed discussion is given later, in chapter 6. Now, if the potential is chosen so that the bottom of the conduction band in the neutral region of the semiconductor is equal to zero, i.e. so that $V(\infty) = 0$, and the electron concentration in the neutral region is n_o , the electron concentration in the depletion region is given by $n = n_o \exp[-qV(x)/kT]$. A similar equation can be written down for the hole concentration, p

$$p = p_s \exp\{q[V_d + V(x)]/kT\} . \quad (4.11)$$

where V_d is the diffusion potential (at zero bias) and p_s is the hole concentration at $x=0$. The net charge density is then given by

$$\rho = q(N_D + p - n) . \quad (4.12)$$

This charge density can now be substituted in Poisson's equation. After some manipulation the resulting equation can be integrated to yield an expression for the electric field at the metal-semiconductor interface, E_{max}

$$E_{max}^2 = \frac{2q}{\epsilon_s} \left\{ N_D \left(V_d - \frac{kT}{q} \right) + \frac{p_s kT}{q} \left[1 - \exp\left(-\frac{qV_d}{kT}\right) \right] + \frac{kTN_D}{q} \exp\left(-\frac{qV_d}{kT}\right) \right\} . \quad (4.13)$$

If the barrier height is much larger than kT/q , but small enough so that the term involving p_s is negligible, the above equation can be simplified to

$$E_{max}^2 = \frac{2qN_D}{\epsilon_s} \left(V_d - \frac{kT}{q} \right) . \quad (4.14)$$

This equation is similar to equation (4.8), which was derived for the depletion approximation, except for the term kT/q , on the right. This term is a correction due to the transition region (also called the Debye tail, or incorrectly, the reserve layer) in which the electron density falls from n_o to a negligible value. In this case the equation for the capacitance per unit area of the junction becomes

$$C = \sqrt{\frac{\epsilon_s q N_D}{2(V_d - kT/q)}} . \quad (4.15)$$

A number of other papers have also appeared, applying better approximations to the problem of calculating the capacitance of a Schottky diode. Recently Van Mieghem *et al* (1990) have calculated the capacitance of an abrupt diode where Fermi-Dirac statistics have been used with a parabolic band, instead of the usual approximation of Boltzmann statistics. Another approach that has become more popular, as the processing power of computers has increased, is computer simulation techniques. Some of the papers dealing with this technique are described in chapter 7.

5

Heterojunctions

In general, a heterojunction is defined as the interface between two dissimilar materials. Its usage in semiconductor research is usually restricted to a junction between two different monocrystalline semiconductor materials. It has, however, also been used to refer to metal-semiconductor junctions and to steps in the doping profile in semiconductors. In this chapter only junctions between two different monocrystalline semiconductors will be discussed.

Heterojunctions can be classified as abrupt or graded according to the distance over which the transition from the one material to the other is made. Furthermore heterojunctions are also classified according to the type of conductivity of the two semiconductor materials. If both semiconductors have the same type of conductivity, the junction is referred to as an *isotype* heterojunction, otherwise it is called an *anisotype* heterojunction.

Semiconductor heterojunctions were first theoretically analysed by Gubanov (1952), but research was only taken up after Kroemer (1957) suggested that anisotype heterojunctions might exhibit extremely high injection efficiencies in comparison to homojunctions. The first isotype and anisotype heterojunctions were manufactured by Anderson in 1960.

Since *CV* techniques are generally suitable for characterising isotype heterojunctions only, only these will be discussed in this chapter. A discussion of the properties of anisotype heterojunctions is given in Sharma (1974).

5.1 Band edge profiles of abrupt isotype heterojunctions

As in our previous model, developed for metal-semiconductor interfaces, we shall assume that the band structure and other properties of each of the semiconductors remain unchanged right up to the interface plane, where they change abruptly into the bulk properties of the other semiconductor. This assumption is reasonable when both the constituent semiconductors have a similar structure. Fortunately, many of the technologically important semiconductors have zincblende or diamond structures, and thus they are quite compatible, as long as their lattice constants are similar.

The band edge profile of two isolated, intrinsic semiconductors with band gaps E_{g1} and E_{g2} is shown in figure 5.1(a). When the two semiconductors are joined to form a heterojunction, charge will flow from the one semiconductor to the other until their Fermi levels coincide. In the intrinsic case we assume that the effect of any charge transfer is negligible and that no

band bending occurs. It can be seen that the sum of the valence and conduction band discontinuities, ΔE_V and ΔE_C , and the band gap of the second semiconductor, E_{g2} , should be equal to the band gap of the first semiconductor, E_{g1} . If both semiconductors are intrinsic, their Fermi levels lie in the middle of the band gap. From this it follows that the valence band offset equals the conduction band offset, or that $\Delta E_V = \Delta E_C = (E_{g1} - E_{g2})/2$. This relationship seems to be obeyed reasonably well in practice for a number of heterojunctions (Jaros 1989). However, as was the case with metal-semiconductor junctions, there are many other factors, such as interface states, that influence the band line-up. A number of attempts have been made to predict the band offsets of heterojunctions (see Mailhiot *et al* 1986 and Pollard 1991). However, as was the case with Schottky diodes, none of the techniques seem to be able to predict the band offset of all heterojunctions reliably.

A large amount of work has been done to determine the ratio between the conduction band and valence band discontinuity of heterojunctions. However, even widely used heterojunctions such as GaAs-AlGaAs heterojunctions, there is still uncertainty, with a number of different values quoted in the literature. A recent discussion on the conduction band offset of a GaAs-AlGaAs heterojunction is given by Okumura *et al* (1985)

Another point to note is that the band gaps mentioned above, refer to the smallest distance between the conduction band and the valence band, the so-called principal band gap. In general, electrons moving in different directions would experience different steps in the conduction band. For instance, consider a GaAs-AlAs heterojunction. In GaAs, which is a direct gap semiconductor, the X-minimum lies about 0.5 eV above the Γ -minimum. In AlAs, however, the absolute minimum in the conduction band is positioned on the X symmetry line, while the minimum at Γ is 0.5 eV above the X-minimum. This implies that, if the valence band discontinuity is chosen correctly, there is a region in which electrons in the Γ -minimum experience an upward step while moving from GaAs to AlAs, while the electrons in the X-minimum experience a downward step. This effect becomes important when current transport across the heterojunction is considered. In a stationary problem, where current flow is assumed to be negligible, the effect of higher valleys becomes less important and usually only the lowest valley is filled at room temperature.

In the previous paragraphs it was assumed that the two semiconductors forming the heterojunction were intrinsic. If one or both of the semiconductors are doped, it follows that the position of the Fermi level in the band gap would change. As a result of the dopants, a space charge region that leads to band bending is established. This leads to the forming of the so-called "spike". The extent of the space charge region may be calculated in a similar manner as was used for Schottky diodes. Except for the depletion region forming on the one side of the heterojunction, it is also possible that a so-called accumulation region could form on the other side of the junction, forming a "notch" in the conduction band. In some cases the bands are bent below the Fermi level. If the bands are bent far enough, it is possible for a number of discrete confined states to occur in the notch region. These states have been observed in a number of heterojunction systems, see for instance Matsumoto (1982). Here quantum mechanical effects begin to play a significant role.

The band edge profile depicted below, illustrates the case where $\chi_1 > \chi_2$ and $E_{g1} < E_{g2}$, so that the band gap of the smaller band gap semiconductor lies within the band gap of the larger band gap semiconductor (the so-called type I heterojunctions). This is most common in practice. Other possible cases, less frequently observed, are discussed by Jaros (1989) and Sharma (1974).

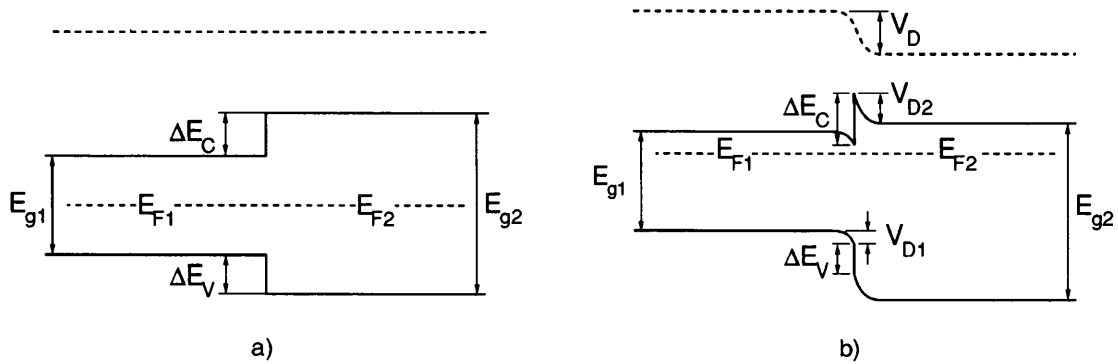


Figure 5.1: Band edge profiles of abrupt heterojunctions: a) Intrinsic case, b) n-type isotype heterojunction.

A typical example that agrees with the band diagram shown in figure 5.1 is an n -AlGaAs/ n -GaAs heterojunction. $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$ has a band gap of approximately 1.79 eV, while the band gap of GaAs is about 1.42 eV at room temperature. Hence the sum of the valence and conduction band discontinuities should be about 0.37 eV. In practice it was found that this discontinuity is shared in the ratio 62:38 (Kroemer *et al* 1984) between the conduction band and the valence band. Therefore the conduction band discontinuity ΔE_C is expected to be about 0.23 eV, while the valence band discontinuity ΔE_V should be about 0.14 eV.

The energy band profile in the interface region of an isotype heterojunction can be calculated by solving for the electric field strength (E) on either side of the interface, and equating the electric displacement on both sides of the interface, i.e. $\epsilon_1 E_1(x_0) = \epsilon_2 E_2(x_0)$. If it is assumed that the electrons are distributed according to a Boltzmann distribution, an analytical expression for the relation between the two built-in voltages V_{D1} and V_{D2} can be found (Anderson 1962)

$$V_{D2} = \frac{\epsilon_1 N_{D1}}{\epsilon_2 N_{D2}} \left[\frac{kT}{q} \left\{ \exp\left(\frac{qV_{D1}}{kT}\right) - 1 \right\} - V_{D1} \right] \quad (5.1)$$

From this equation it can be seen that if the total built-in voltage, $V_D = V_{D1} + V_{D2}$, is at least several kT and the doping concentration on both sides of the junction is similar, V_{D2} will be much larger than V_{D1} . Thus it can be assumed that the notch, V_{D1} , will be of the order of only a couple of kT .

The relationship between the conduction band offset and the built-in voltage V_D can be determined by making use of the relationship between the Fermi level and the conduction band. Because the Fermi level remains flat under zero-bias conditions, it follows that

$$\xi_1 + \Delta E_C - V_D = \xi_2 \quad (5.2)$$

where ξ_1 and ξ_2 are the distances between the Fermi level and the conduction bands of the first and second semiconductors respectively. Assuming that all the donors are ionized, and the number of acceptors is negligible, ξ can be approximated by equation (2.25). In this case it can be shown that

$$\Delta V = \frac{kT}{q} \ln \left[\frac{N_{D2}/N_{C2}}{N_{D1}/N_{C1}} \right] + \Delta E_C, \quad (5.3)$$

where N_{D1} and N_{D2} are the doping densities, and N_{C1} and N_{C2} are the effective density of states in the respective materials. This relationship, together with equation (5.1) can be used to uniquely determine the built-in potentials V_{D1} and V_{D2} for any two semiconductors, in the absence of interface charges.

5.2 Current-voltage characteristics

The thermionic emission of carriers across the heterojunction barrier can be described in a similar way as was the case with metal-semiconductor junctions. Here the height of the spike is assumed to be the barrier across which emission takes place. According to this theory the current through the heterojunction is given by

$$I = B \exp \left(-\frac{qV_{D2}}{kT} \right) \left[\exp \left(\frac{qV_2}{kT} \right) - \exp \left(-\frac{qV_1}{kT} \right) \right], \quad (5.4)$$

where $V = V_1 + V_2$ is the applied voltage, $B = aqXN_{D2}(kT/2\pi m^*)^{1/2}$, a is the area of the junction, and X is the transmission coefficient for electrons across the interface. The bias is said to be forward if it reduces the built-in voltage. As mentioned previously, V_{D1} and V_1 are much smaller than V_{D2} and V_2 . In this case equation (5.4) can be reduced to

$$I = B \exp \left(-\frac{qV_{D2}}{kT} \right) \left[\exp \left(\frac{qV_2}{kT} \right) - 1 \right]. \quad (5.5)$$

This method can be used to determine the height of the spike, in a similar way as was used for Schottky diodes. The size of the conduction band discontinuity can be determined from the height of the spike. However, this technique is unreliable, since the built-in voltage, and consequently the region over which equation (5.3) is valid, is very small compared to that of a Schottky diode. Furthermore, a number of other conduction mechanisms are possible. These include diffusion, tunnelling and recombination in the interfacial region.

5.3 Interface states

As mentioned previously, abrupt semiconductor heterojunctions are manufactured by growing layers of different semiconductor materials onto a single crystal semiconductor with identical or completely different crystallographic structures. The interface between the two semiconductors usually has a large number of defects. This is especially true if the two semiconductors do not have the same crystal structure, or if there is a large difference between their lattice parameters. Many of these interfacial defects are electrically active, and produce energy levels within the forbidden gap, thus influencing the electrical properties of the heterojunction. In most cases the effects of these interfacial defects is undesirable, and much work has been done in an effort to reduce them to the minimum.

Van der Merwe (1964) has shown that the strain caused by the lattice mismatch may be relaxed by the formation of misfit dislocations, as shown in figure 5.2. These dislocations form crossed grids with the symmetry of the plane in which the junction is formed. They accommodate the change in lattice parameter at the heterojunction by providing extra half-planes of atoms in the material with the smaller lattice parameter.

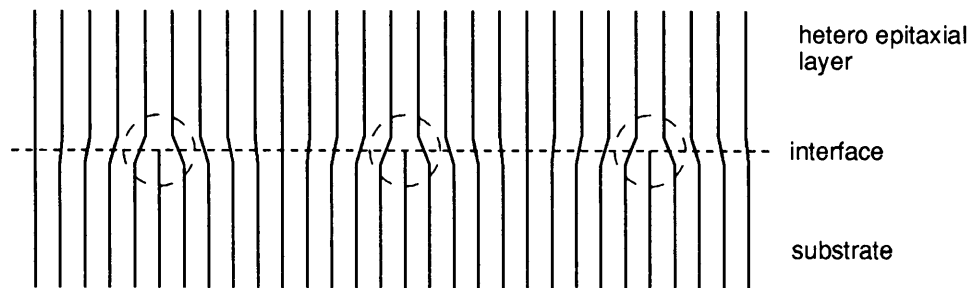


Figure 5.2: Schematic representation of misfit dislocations at a heterojunction interface (after Sharma et al 1974)

The number of dislocations at an abrupt heterojunction interface can be estimated by calculating the difference between the surface density of dangling bonds of the two semiconductors. By using this method the spacing between misfit dislocations along any direction is given by the expression (Van der Merwe 1964)

$$p = \frac{ab}{(b-a)}, \quad (5.6)$$

where a is the repeat distance in the given direction in the material with the smaller lattice constant and b is the corresponding distance in the other material.

Using these methods, the theoretical number of misfit dislocations can be calculated for a

number of different combinations of semiconductors. The values range from approximately 10^{14} cm^{-2} for semiconductors with a relatively large mismatch such as Ge/Si (4% mismatch) to approximately 10^{12} cm^{-2} for semiconductors with little mismatch, such as GaAs/AlAs (0.2% mismatch). This calculated density of misfit dislocations can be used as an order of magnitude estimation of the density of interface states expected in the heterojunction.

There are a number of other factors which also influence the number of interface defects, and the values obtained using the techniques above, should be seen as estimates. For example, in thin layers of only a couple of lattice parameters thick, the lattice mismatch may be accommodated to a large extent by straining in the thin layer, causing considerably less defects than expected. On the other hand, the number of defects may be more than predicted by the above model due to a number of processes which may occur during the growth of the structure.

In the above discussion the room temperature lattice parameter was used. Since most crystals are grown at elevated temperatures, this assumption is not valid. If there is a large difference in the thermal expansion coefficients of two lattice matched semiconductors, they may no longer be lattice matched at elevated temperatures. Furthermore, the thermal mismatch may lead to the formation of more defects during cooling and, in extreme cases, may even result in cracking or peeling off of the grown layers.

Another phenomenon that could also give rise to an observed interface charge is interdiffusion. Except for changing the abrupt nature of the interface, it may also lead to the formation of homojunctions on one or both sides of the heterojunction interface, masking its true properties. For example, when GaAs is grown on Si, Si may diffuse into the GaAs where it acts as an *n*-type dopant. This however, can be avoided by growing such heterojunctions at lower temperature.

5.4 Quantum wells

In the previous sections we have seen that the electronic structure of a semiconductor heterojunction can be modelled as a step-like discontinuity in the conduction and valence band edges. The materials most frequently used to construct such heterojunctions are GaAs and $\text{Al}_x\text{Ga}_{1-x}\text{As}$. The aluminium mole fraction *x* is generally chosen between 0.30 and 0.35. In this range the conduction band discontinuity is large and the alloy is still a direct gap material. Furthermore, abrupt GaAs-AlGaAs interfaces can easily be grown by means of MBE and OMVPE techniques. Using these growth techniques, it is possible to grow more complicated systems consisting of several layers of such materials of well-controlled thickness. The simplest of these systems is shown in figure 5.3a). It consists of a thin layer of GaAs sandwiched between two thick layers of $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$. The band edge profile of the undoped device can be obtained by simply adding the results obtained previously for a single heterojunction, leading to a well shaped structure as shown in figure 5.3b). For this reason the device is often referred to as a quantum well.

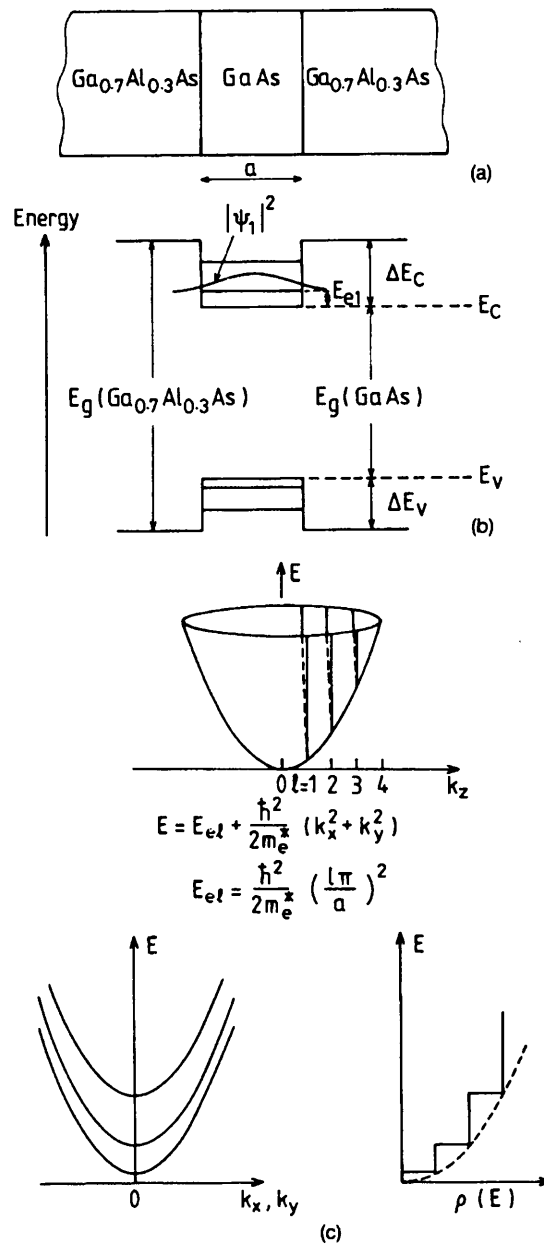


Figure 5.3: a) Schematic diagram of a quantum well, b) band diagram with bound states indicated. c) Density of states in the conduction band of the quantum well; z is the direction perpendicular to the interface, ρ is the density of states (the broken line indicates the density of states in the bulk crystal). (After Jaros 1989.)

If the quantum well is thick enough ($a > 20 \text{ \AA}$) that the layer has the properties of bulk GaAs, but still thinner than the mean free path of an electron ($a < 400 \text{ \AA}$) the electrons in the well can, to a good approximation, be modelled as free electrons with an energy

$E_C + (\hbar k)^2/2m_e^*$. The problem of finding the allowed states in the well is now reduced to the well-known “particle in the box” problem, where the Schrödinger equation is

$$\left\{ -\frac{\hbar^2}{2m} \frac{d}{dz^2} + V \right\} \phi = E\phi, \quad (5.7)$$

and

$$V = \begin{cases} -V_o & \text{if } |z| < a/2 \\ 0 & \text{if } |z| \geq a/2 \end{cases}. \quad (5.8)$$

Here a is the width of the well, V_o is the depth of the well, and z is the coordinate perpendicular to the interface.

The solution to this problem can be found in any elementary quantum mechanics textbook, therefore it will be discussed only briefly here. There always exists at least one (and if the well is deep enough, more) bound states in the well. Within the well the bound-state wave function has the form of a standing wave. Outside the GaAs well, the wave function decays exponentially towards zero. There is no simple analytical expression for the bound state energy levels, but as a first approximation, they can be calculated by assuming an infinitely deep well

$$E = \frac{\hbar^2}{2m^*} \left(\frac{\pi l}{a} \right)^2, \quad l = 1, 2, 3, 4, \dots, \quad (5.9)$$

where m^* is the effective mass of the particle, a is the width of the well, and l is the quantum number of the level. The exact solutions are shown in the graph in figure 5.4.

The “particle in a box” problem does not accurately describe the situation in a quantum well, because it neglects the periodic potential of the crystal structure in which the heterostructure is formed. It is therefore not surprising that the experimental results obtained differ from the results of this simple model. A more accurate approximation of the wave function of a particle (hole or electron) in a quantum well can be obtained by making use of the envelope wave function approximation. According to this approximation the wave function of the particle can be expressed as (Schuurmans *et al* 1985)

$$\psi^l = \sum_j F_j^l(z) u_j^l(\mathbf{r}), \quad (5.10)$$

where z is the growth direction and $u_j(\mathbf{r})$ is the periodic Bloch part of the wave function. $F_j(z)$ is the envelope of the wave function which is slowly varying on the scale of the lattice constant a , and has to be joined across the interfaces by suitable boundary conditions. The superscript l refers to the well material ($l = 1$) or the barrier material ($l = 2$). The label j runs over all the states in the material. However, in many cases it is necessary to use bands only

in the immediate (energy) vicinity of the state under consideration. In the most simple approximation only one band is used, and it is assumed that the envelope function F^I is continuous across the interfaces. This results in exactly the same problem as described in equations (5.7) and (5.8). For a more advanced analysis, see Schuurmans *et al* (1985), who have considered the eight Γ -point basis states in the Kane-type $\mathbf{k}\cdot\mathbf{p}$ analysis. They also cite a number of other papers describing other methods by means of which the energy of the confined states can be determined.

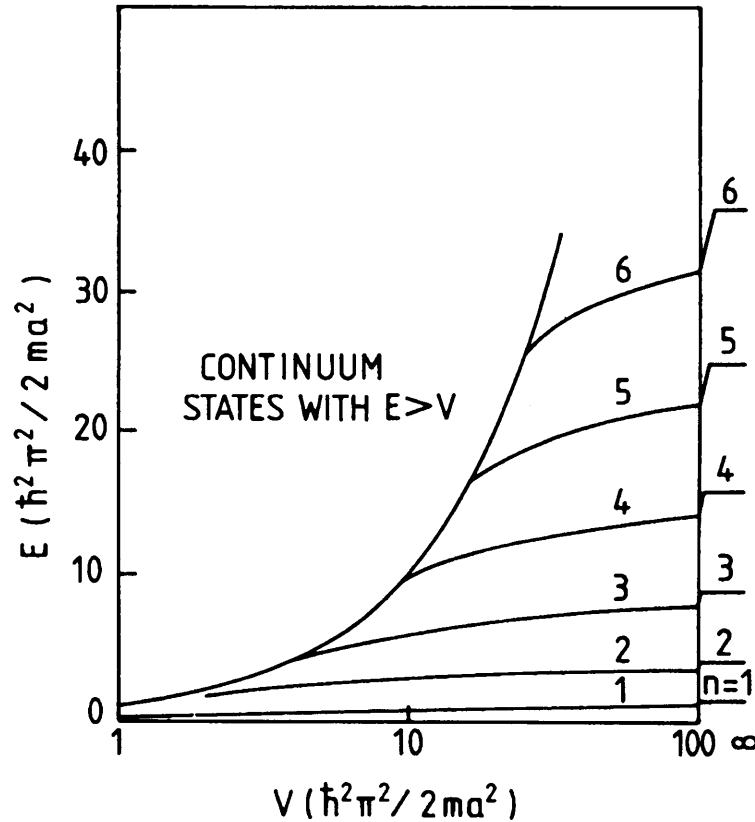


Figure 5.4: Exact solutions of the “particle in the box” problem for a one-dimensional potential well of width a and depth V . The solutions for an infinite well are shown at the right of the graph. (After Jaros 1989.)

5.5 Properties of a two-dimensional electron gas

As explained in the previous section, the movement of electrons in the z -direction (the direction perpendicular to the interface) is quantized. The motion in the plane however, is unaffected. Thus the electrons in the quantum well behave as though confined to two dimensions. This has a number of profound implications.

The most important property that distinguishes a two-dimensional (2D) gas from a three-dimensional (3D) gas is the density of states (DOS). The density of states for a 3D gas is calculated by considering the volume of a sphere in $\mathbf{k}$ -space, which varies as k^3 . (See for instance Pathria 1985). In the case of a 2D electron gas, the $\mathbf{k}$ -space is two-dimensional. In this case the sphere is replaced by a disk. Since the density of states in an n -dimensional wave-vector space is $(2\pi)^{-n}$, the number of states with $|\mathbf{k}| < k$ is given by

$$N(k) = g_v \pi k^2 (2\pi)^{-2}, \quad (5.11)$$

where g_v is the ground state degeneracy. From this it follows that the density of states is

$$D(E) = \frac{dN(E)}{dE} = \frac{dN}{dk} \frac{dk}{dE} = \frac{2\pi g_v}{(2\pi)^2} k \frac{dk}{dE}. \quad (5.12)$$

If it is assumed that the electron energy spectrum (in the 2D plane) is given by

$$E = E_0 + \frac{\hbar^2 k^2}{2m}, \quad (5.13)$$

where m is the effective mass, which in this case is assumed to be isotropic, equation (5.12) becomes

$$\begin{aligned} D(E) &= g_v \frac{m}{\pi \hbar^2}, \quad E > E_0 \\ &= 0, \quad E < E_0, \end{aligned} \quad (5.14)$$

This means that the density of states rises abruptly at the energy E_0 and is constant for higher energies. However, this derivation takes only one band into account. If there are other 2D bands at higher energy levels, there will be additional step increases in the density of states, so that the graph for the total density of states looks like a stepped parabola, as indicated in figure 5.3(c). It is also interesting to note the relationship between the density of states in the well (indicated by the solid line) and the density of states in the bulk of the semiconductor (indicated by the dotted line). It follows that for a given quantum state E_n , the DOS is independent of both the energy and the layer thickness. It is also clear that in the classical limit the 2D DOS and the 3D DOS become indistinguishable.

Another interesting feature of the 2D DOS is that the DOS remains finite at the lowest 2D level. This implies that all dynamic phenomena remain finite at low temperatures. This is one of the features that make quantum wells ideally suited for use in lasers.

5.6 Superlattices

Consider a structure that consists of a large number of alternating layers of GaAs and AlGaAs. If the AlGaAs layers are relatively thin, the wave functions of the confined states in the separate quantum wells penetrate far enough into the barrier for the wave functions to overlap. This means that electrons are able to tunnel through the barriers and move between different wells. The conduction band profile now resembles the potential in a crystal, as discussed in chapter 2. As a first approximation similar techniques as applied in chapter 2 can be used to calculate the band-structure of the system. This leads to the formation of so-called *minibands* separated by *minigaps* just as the periodicity of the crystal lattice leads to the formation of bands and band gaps in a crystal.

5.7 Delta-doped structures

By using modern growth techniques, it is possible to grow structures in which the dopant atoms are confined to a single atomic plane, as shown in figure 5.5. By confining the dopant atoms to such a narrow area, 2D carrier concentrations higher than $1 \times 10^{13} \text{ cm}^{-2}$ can be obtained. This high localization of carriers about the dopant plane screens the free carriers from the effect of ionized impurity scattering, resulting in enhanced carrier mobility. Also, the use of delta doping in modulation doping devices, such as MODFETs, has been shown to improve their transconductance.

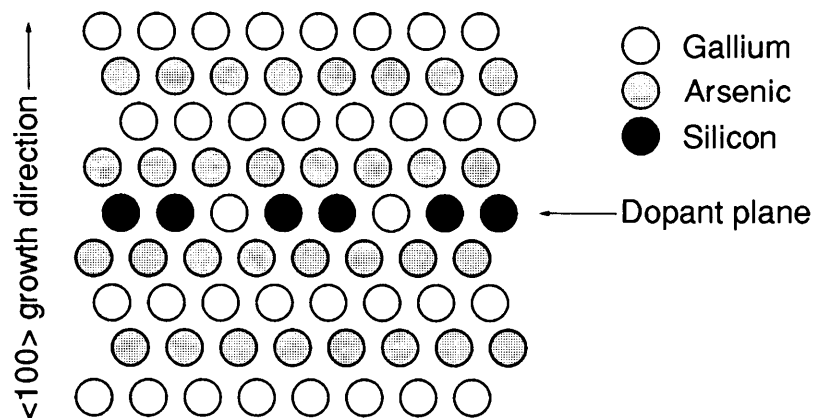


Figure 5.5: Atomic structure of a Si delta doping in GaAs as seen from the side. Here all the Si dopants are ideally deposited on a single plane during epitaxial growth interruption.

Because of the high concentration of donor atoms in the doping plane, there is a strong electric field in the adjacent region. This causes the conduction band edge to be bent in a V-shape, and allows for the formation of 2D-states in the doping plane, as shown in figure 5.4

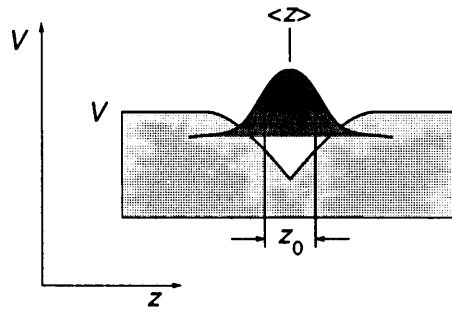


Figure 5.6: Band profiles in the region of a δ -doping spike. Also shown is the shape of the two-dimensional wave function.

5.8 “Doping” heterojunctions

Bychkovskii *et al* (1990) have shown that the band gap of a semiconductor is narrowed as a result of doping. This narrowing seems to be mainly as a result of the reduction of energy of majority and minority carriers due to their interaction with the dopant atoms and other majority carriers. They found that the reduction in the energy gap from the intrinsic case is in the order of 10 meV for 10^{17} cm^{-3} doped n -type Si at room temperature, but increases to 100 meV at a doping level of 10^{19} cm^{-3} .

5.9 Growth of semiconductor heterostructures

A number of techniques have been used for the growth of semiconductor heterostructures. Only those applicable to the growth of high quality III-V heterostructures will be considered. The most important techniques are liquid phase epitaxy (LPE), organometallic vapour phase epitaxy (OMVPE) and molecular beam epitaxy (MBE). The quality of interfaces produced by these techniques are compared by Garner *et al* (1979).

In the LPE method, layers are grown by keeping the substrate in contact with a saturated solution containing the compound to be grown. This solution is then cooled at a prescribed rate, so that a new layer is grown on the substrate. In the case of GaAs and AlGaAs, Ga is usually used as a solvent.

In the OMVPE technique, a number of gaseous compounds are mixed in a growth chamber containing the substrate. In the case of AlGaAs, the commonly used reagents are trimethylaluminium $(\text{CH}_3)_3\text{Al}$, trimethylgallium $(\text{CH}_3)_3\text{Ga}$ and arsine AsH_3 . When these compounds are mixed together in a hydrogen atmosphere, they decompose to form AlGaAs and methane (CH_4) . For n -type doping a small amount of silane (SiH_4) is added to the mixture. In a modern OMVPE system, the flow rates of these gasses are controlled by computer, thus allowing for accurate and repeatable growth conditions. Although interfaces grown by means of OMVPE are slightly graded (typically $60 \text{ \AA}$), the total cost of the apparatus is relatively low compared to MBE, and the technique yields good quality material.

Of the three growth techniques mentioned, MBE is the most advanced, and allows for the accurate growth of abrupt ($< 15 \text{ \AA}$) semiconductor interfaces. In MBE the substrate is mounted in a ultrahigh-vacuum chamber and exposed to a thermal beam of atoms and molecules. The molecular beams of each required species are supplied by a number of evaporation cells, each controlled by a separate heater and shutter. As is the case with OMVPE, the whole process is computer-controlled. In most cases other analytical instruments are built into the growth chamber. These include mass spectroscopy, Auger spectroscopy and electron diffractometry. A schematic illustration of a typical MBE reactor is shown in figure 5.7.

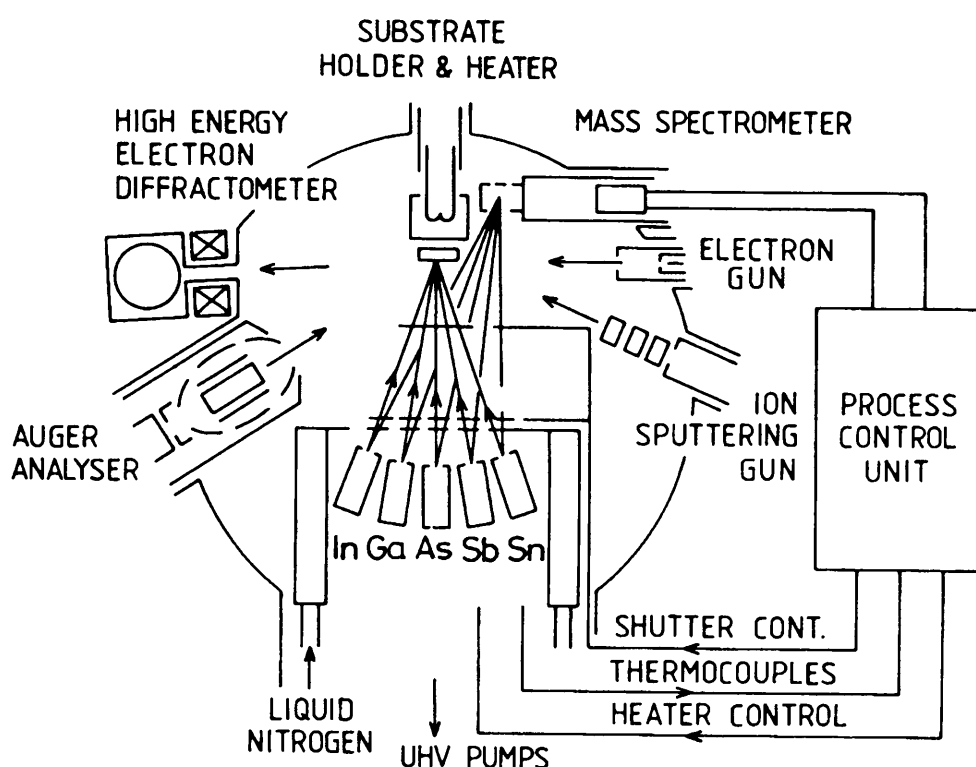


Figure 5.7: A schematic illustration of an MBE reactor for the epitaxial growth of semiconductor microstructures. (After Jaros, 1989)

6

Capacitance-voltage measurements

In chapter 4 the formation of the Schottky barrier has been discussed, and an expression for the capacitance per unit area of a Schottky diode as a function of applied bias has been found. This equation can be rewritten as

$$C^{-2} = \frac{2}{q\epsilon_s N_D} \left(V_{d0} + V_r - \frac{kT}{q} \right), \quad (6.1)$$

where V_{d0} is the diffusion voltage at zero bias and V_r is the applied bias. From this equation it follows that, if the dopant concentration N_D is constant, a graph of C^{-2} versus V_r should be a straight line, with a slope of $2/q\epsilon_s N_D$ and intercept on the C^{-2} axis of $V_{d0} + kT/q$. In general, however, there are a number of factors which influence the shape of the C^{-2} versus V_r graph, and could cause it to deviate from a straight line, even though the dopant concentration may be constant. These factors will be discussed later in this chapter.

6.1 Determination of doping concentrations by means of Capacitance-Voltage profiling

Consider a semiconductor with a non-homogeneous donor distribution, as indicated by the heavy line in figure 6.1. If a Schottky contact was fabricated on the surface at $x = 0$, a depletion region would be formed below the surface. According to the depletion approximation, there are no free carriers in the depletion region, and the carrier density in the bulk of the semiconductor is equal to the donor density, N_D . The carrier density is thus given by

$$n(x) = \begin{cases} 0 & 0 < x \leq w \\ N_D(x) & x > w \end{cases} \quad (6.2)$$

where $N_D(x)$ is the donor density in the semiconductor. The shape of the carrier density profile is shown by the thin line in figure 6.1. If the reverse bias is increased by a small amount, ΔV , the width of the depletion layer is increased by Δw . Let $n_1(x)$ and $n_2(x)$ be the distributions of free carriers before and after the increase in reverse bias. The change in the majority carrier concentration is now given by $\Delta n(x) = n_2(x) - n_1(x)$, and the charge removed per unit area is

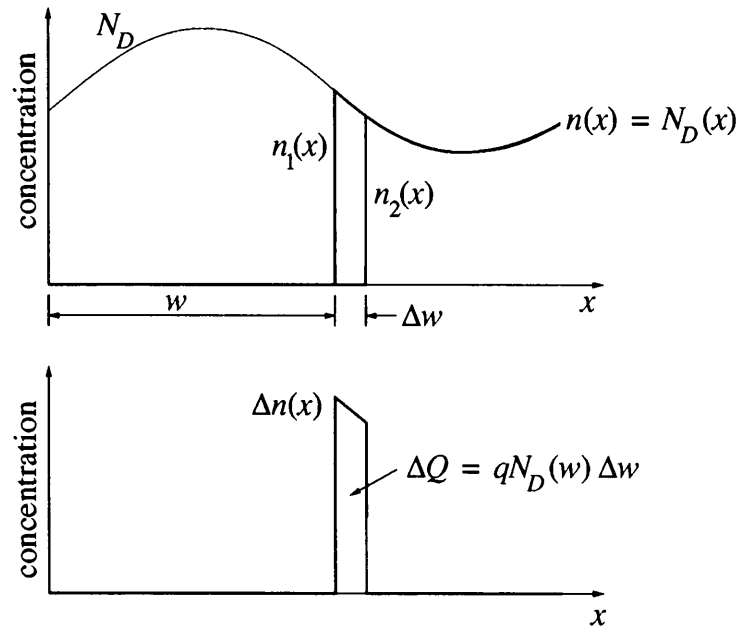


Figure 6.1: The charge distribution in the depletion region of a non-uniformly doped semiconductor.

$$\Delta Q = \int_0^{\infty} \Delta n(x) dx, \quad (6.3)$$

In the depletion approximation this simplifies to

$$\Delta Q = qN_D(w) \Delta w \quad (6.4)$$

for small Δw . The increase in the applied voltage can be found by calculating the increase in the potential at the interface due to the change in charge distribution, giving

$$\Delta V = w \Delta E = qN_D(w) w \Delta w / \epsilon_s. \quad (6.5)$$

According to the depletion region approximation, the capacitance per unit area of the depletion region, C , is given by ϵ_s/w . Thus the width of the depletion region is

$$w = \epsilon_s / C. \quad (6.6)$$

By substituting this relation in equation (6.5), an expression for the density of donor atoms in terms of the measured capacitance per unit area can be found

$$N_D(w) = -\frac{C^3}{q\epsilon_s} \left(\frac{dC}{dV} \right)^{-1}. \quad (6.7)$$

Thus by using equation (6.6) in conjunction with equation (6.7), it is possible to determine the doping profile in the semiconductor below a Schottky diode from its capacitance-voltage characteristics.

6.2 Factors influencing the accuracy of CV measurements

In the depletion approximation the assumption is made that the charge density in the depletion region is constant, and due only to the ionized donor atoms. This assumption implies that (Goodman 1963)

- the sum of the barrier height and the applied bias, $V_B + V$, must be sufficiently less than the band gap, E_g , to ensure that the minority carrier concentration remains negligible compared to N_D .
- the barrier height must be much larger than kT/q .
- there may be no deep levels in the band gap.
- the charge in the depletion region must be due only to ionized donor atoms.

A number of physical processes occurring in the semiconductor influence the accuracy of the measurements. These may be due to the inherent properties of the Schottky diode, the substrate on which the Schottky diode is manufactured, or the measurement apparatus.

Circuit considerations for capacitance measurements

Ideally, the Schottky diode should behave like an ideal capacitor. This however, is seldom the case, since the Schottky junction also has a leakage conductance G which becomes quite large especially when the diode is forward-biased. Furthermore, there is always a small series resistance present, consisting of the resistance of the semiconductor substrate, the resistance of the probe and metal contact system, as well as the leads to the test instruments. The effect of series resistance measurements has been investigated by Goodman (1963) and later by Wiley *et al* (1975).

The actual circuit of a Schottky contact may be represented by a fixed resistance r in series with a parallel combination of a voltage dependent capacitance C and a voltage dependent conductance G , as in figure 6.2. (Note: r , C and G can be either the measured values, or the values per unit area. Both cases lead to the same results, provided they are used consistently.)

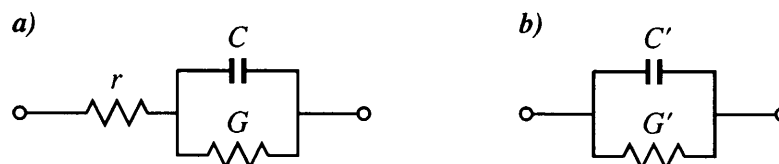


Figure 6.2: a) A simplified equivalent circuit of a Schottky contact with a high series resistance, and b) the equivalent circuit as measured by the capacitance meter.

Most modern capacitance meters are able to characterize the circuit in terms of only two parameters, e.g., the capacitance C' and the parallel conductance G' , which are calculated from the magnitude Z and the phase θ of the impedance at the (angular) test frequency ω according to

$$G' = \frac{1}{Z} \cos \theta, \quad (6.8)$$

and

$$C' = \frac{1}{Z\omega} \sin \theta. \quad (6.9)$$

To obtain accurate results, it is necessary to prepare the sample in such a way that either the series resistance r , or the parallel conductance G , or both, are negligible. It is not always possible to prepare such ideal samples. This problem has been investigated by Goodman (1963), who has found guidelines according to which corrections for a high series resistance can be made.

When a circuit as depicted in figure 6.2, is connected to a capacitance meter, and the capacitance and parallel conductance are measured, the bridge will measure the following values for G and C , as calculated from the impedance

$$G' = \frac{G(rG + 1) + \omega^2 r C^2}{(rG + 1)^2 + \omega^2 r^2 C^2}, \quad (6.10)$$

and

$$C' = \frac{C}{(rG + 1)^2 + \omega^2 r^2 C^2} \quad (6.11)$$

where ω is the test signal frequency. Clearly, if $rG \ll 1$ and $\omega r C \ll 1$, the measured capacitance will be equal to the capacitance of the device. This implies that the series resistance should be much smaller than the parallel resistance ($1/G$) and it should also be much smaller than the reactance of the capacitor ($1/\omega C$). It is generally possible to satisfy the condition $rG \ll 1$ for most Schottky diodes during reverse bias smaller than the breakdown voltage, and for a limited range of forward bias. The condition $\omega r C \ll 1$ is also satisfied in most cases except where the series resistance of the sample is unusually high and at very high measurement frequencies. For a measurement accuracy of 1%, it is necessary that $(rG + 1)^2 + \omega^2 r^2 C^2 \leq 1.005$. As a rough guide, the symbol $\ll$ in the above two equations, can be taken to imply a difference of more than an order of magnitude. In borderline cases where $0.05 \leq \omega r C \leq 0.5$, C can be approximated by inserting $rG = 0$ into equation (6.11), solving for C and ignoring higher order terms in C'

$$C = C'(1 + \omega^2 r^2 C'^2) \quad (6.12)$$

If r is independent of V , r may be estimated by biasing the contact far into the forward direction (resistance limited region) and measuring the differential resistance. In many cases however, the high series resistance is caused by a defect in the bulk of the semiconductor, and may be voltage dependent. An example of such a case is where a thin insulating layer is formed between the semiconductor substrate and the epilayer, because of compensation by impurities on the substrate. In such cases it is extremely difficult to isolate the junction capacitance, and to calculate an accurate carrier density profile.

The condition $rG \ll 1$ should always be adhered to. If not, the bias applied to the device is not equal to the voltage across the Schottky barrier. This effect is particularly noticeable when the diode is forward biased, and the parallel conductance, G , becomes large. Also, if the high series resistance is due to the resistance of the evaporated metal layer, a further complication arises: every point on the contact is not at the same potential. This could cause the CV profile to smear out, and reduce the achievable resolution (Auret *et al* 1993).

Another point, frequently ignored, is that the accuracy of the measured capacitance depends on the phase of the impedance. Even in the ideal case, when only the series resistance or the parallel conductance dominates, the accuracy of the measured capacitance decreases sharply if the effect of either of these causes the phase of the impedance to deviate sharply from 90° . The highest accuracy is obtained when the phase deviates from 90° by no more than one or two degrees. These values differ from one instrument to another, but generally the measurement error doubles when the phase deviates by more than 5° from 90° . Therefore measurements made when the phase is smaller than 45° are prone to very large errors. This point is discussed more fully later in this chapter.

More recently, the basic Goodman model has been extended by Chan *et al* (1990) (by adding an extra term to the Taylor series) to make even better corrections for larger series resistance. In an experiment where a resistor was placed in series with a good diode, this technique has provided excellent results. This model, however, is only necessary in extreme cases where the series resistance is very large (in the range of $500\ \Omega$ to $10\ \text{k}\Omega$). Such a high series resistance is in many cases an indication that the diode is defective in some way and may give inaccurate readings anyhow. Furthermore this technique does not take parallel conductance into account and consequently is of limited use.

Frequency dependence of the capacitance

It has been found that the measured capacitance depends on the frequency at which the capacitance is measured. This could be because of interface states, deep levels, or minority carriers. In most cases, however, this frequency dependence disappears completely at frequencies of 1 MHz and above. Since many capacitance bridges, used for semiconductor analysis, operate at a fixed frequency of 1 MHz, or are at their most accurate at 1 MHz, this frequency is generally used when measuring the capacitance of a Schottky diode. The frequency dependence of Schottky diodes, due to deep levels in the band gap, is discussed by Zohta (1973) and Berroth *et al* (1989). The effect of interface states is discussed by Card and Rhoderick (1971).

Trapping effects

Goodman (1962) has shown that a high concentration of deep traps in the band gap affects the measured CV carrier concentration. These effects have been investigated by Kimberling (1973) and Korol *et al* (1975), and more recently by Shiao *et al* (1986). In particular, it has been found that even devices which are known to be uniformly doped, display non-linear C^2 - V characteristics, because of the effect of deep levels. A number of procedures, by means of which the deviations can be “corrected” have been suggested (see, for instance Vasudev *et al* 1976 and Bryant *et al* 1986). In all these techniques, the analysis is greatly simplified if it is assumed the test signal frequency is high enough not to affect the occupancy of the deep levels. A frequency of 1MHz is sufficient in most cases. In this case the only effect of deep levels is that they contribute extra charge to the depletion region.

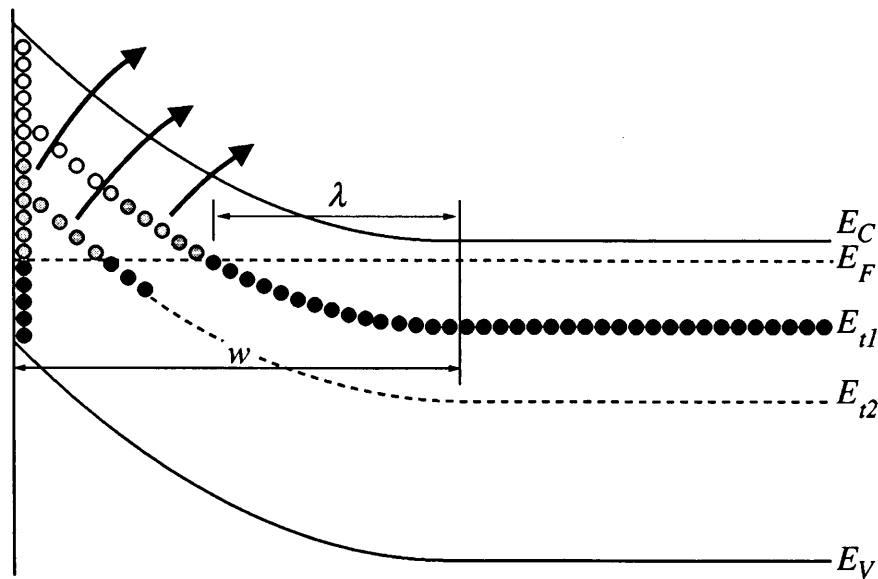


Figure 6.3: Band diagram of a Schottky diode with deep level defects and interface states within the band gap. When a reverse bias is applied to the diode, the deep levels empty and contribute to the charge in the depletion region. Note that the deep levels are only emptied when they cross the Fermi level. This happens a distance λ away from the depletion region edge.

The method of Bryant *et al* (1987) explains the effects of deep levels on the CV characteristics, and could be used in some cases to correct for the effect of deep levels. Consider the case as depicted in figure 6.3. For a uniform doping density N_D of uncompensated donors, and a uniform density N_t of deep traps which are neutral, when occupied, and positively charged, when unoccupied, the charge density is given by $\rho = q(N_D + N_t)$ for $0 < x < (w - \lambda)$

and by $\rho = q N_D$ for $(w - \lambda) < x < w$. Integration of Poisson's equation gives the total potential difference across the space charge region

$$V = \frac{q}{\epsilon_s} \left[\frac{N_D w^2}{2} + \frac{N_t (w - \lambda)^2}{2} \right]. \quad (6.13)$$

The charge in the depletion layer is given by

$$Q = q [N_D w + N_t (w - \lambda)]. \quad (6.14)$$

If we assume that the capacitance meter test signal frequency is sufficiently high not to induce a significant change in the occupancy of the traps, the measured capacitance is caused by the change in occupancy of the shallow donors only. In this case the capacitance per unit area is, as previously

$$C = \frac{\epsilon_s}{w}. \quad (6.15)$$

Substituting this relationship in equation (6.13) we obtain

$$V = \frac{q\epsilon_s}{2C^2} \left[N_D + N_t \left(1 - \frac{\lambda C}{\epsilon_s} \right) \right], \quad (6.16)$$

and

$$\frac{dV}{dC^2} = \frac{q\epsilon_s}{2} \left[N_D + N_t - \frac{\lambda N_t C}{\epsilon_s} \right]. \quad (6.17)$$

The deviation from the theoretical value is dependent on the density of traps N_t and the parameter λ , which is determined by the energy of the traps E_t relative to the Fermi energy E_F

$$\lambda = \sqrt{\frac{2\epsilon_s}{q N_D} (E_F - E_t)}. \quad (6.18)$$

However, if $w < \lambda$, (i.e. when $\lambda C/\epsilon_s > 1$), the trap level is always below the Fermi level, thus equation (6.16) reduces to

$$V = \frac{q\epsilon_s}{C^2} N_D, \quad (6.19)$$

which is the same as the case without the deep levels. Thus it follows that the values obtained for N_D when $q V_{bi} < E_t$, will not be affected by any deep traps lying further than $q V_{bi}$ from the conduction band. On the other hand, under large reverse bias, equation (6.16)

reduces to

$$V = \frac{q \epsilon_s}{2 C^2} [N_D + N_t]. \quad (6.20)$$

Between these two extremes, various techniques can be used to calculate the carrier density of the material. In the most simple case, the experimental carrier density is determined by simply adding a term $(q \epsilon_s / 2)(N_t - \lambda N_t C / \epsilon_s) = (N_t q \epsilon_s / 2)(1 - \lambda / w)$ for all points for which $w > \lambda$.

If, on the other hand, it is known that the doping and the trap densities are constant, the intercept at $C = 0$, of the dV/dC^2 vs C graph can be used to calculate $N_D + N_t$. If E_t is known from DLTS measurements, it is possible to calculate λ , and thus to estimate N_t from the slope of the graph.

In many cases it is possible to choose material with low defect concentrations, which will not influence the measurement. If this is not possible, or higher accuracy is required, the corrections discussed above could be applied.

For defects lying in the middle of the band gap or lower, like the EL2 in GaAs, another technique may be used. It has been found by Ma *et al* (1988) that, because of the Fermi level bending upwards in the depletion region, some defects may remain beneath the Fermi level for all reverse biases, rendering the defects invisible to DLTS studies. This effect is more pronounced with Schottky diodes having a lower barrier height. For instance the EL2 defect seems to disappear for Schottky diodes with a barrier height of less than 0.6 eV, such as those made with Mg contacts on *n*-GaAs. The bending of the Fermi level is discussed later in this chapter.

Variation of the effective surface area with depletion layer width

There are two reasons why the effective surface area of the Schottky barrier could change. The first is that some extra capacitance is measured across the junction due to edge effects (Willis 1990), as shown in figure 6.4. The capacitance due to the edge effect can be estimated to an order of magnitude by calculating the extra area of the depletion region edge and calculating the capacitance in the usual way. Using this technique the capacitance of the edge region, C_o is found to be

$$C_o = \epsilon_s \pi p / 2, \quad (6.21)$$

where p is the perimeter of the contact. As the surface area varies quadratically with the perimeter of the contact, it is possible to make the contact large enough so that the edge effects become negligible. If this is not possible, the capacitance should be corrected for the edge effects as described by Willis (1990).

Another way by which edge effects can be reduced is by using guard rings and similar structures. These and other techniques for the elimination of surface effects are discussed by Tove (1982).

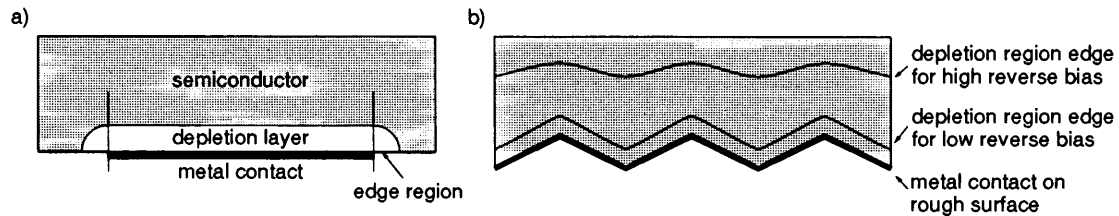


Figure 6.4: Variation of surface area with applied voltage: a) Edge effects in a Schottky diode, b) Surface roughness (After Goodman 1963)

Another reason why the surface area of the depletion region may change with applied bias, is surface roughness. Goodman (1963) found that for Schottky contacts, deposited on a well-etched CdS sample, the $1/C^2$ vs V plot was always concave upwards. It was also noted that the surface developed a “velvet” finish, due to the many irregularities caused by the etching process. As the depletion region widens, the irregularities tend to smooth out, thus reducing the effective contact area. This effect has been analysed mathematically (Goodman 1963), but clearly the most reliable way to eliminate it, is to use polished surfaces.

Insulating interfacial layer and interface states

Before Schottky diodes are fabricated on the surface of a semiconductor, the surface is usually cleaned by some or other technique, to remove impurities such as hydrocarbons and oxide films. However, as soon as the semiconductor has been cleaned, a new layer of impurities starts forming on the surface. This is particularly relevant if the semiconductor is cleaned by chemical means, when an oxide layer of several Angstroms may form on the surface of the semiconductor while it is transported to the vacuum chamber for evaporation. The capacitance of this insulating interfacial layer is effectively in series with that of the depletion region. However, there are a number of complications which are likely to arise.

At the interface between the metal and the semiconductor are a large number of interface states. These can be caused either by states within the insulator itself, or by surface relaxation, or by metal induced gap states (MIGS) as described in chapter 4. The effect of a thin interfacial layer and interface states on the capacitance has been analysed by Cowley (1966), who found that the capacitance of the Schottky diode can be written as (equations simplified by Rhoderick 1988)

$$\frac{1}{C} = \frac{1}{C_d} + \frac{1}{C_{ox} + C_s} \quad (6.22)$$

where

$$C_{ox} = \frac{\epsilon_i}{\delta}, \text{ and } C_s = qD_s. \quad (6.23)$$

Here C_d is the capacitance of an ideal Schottky barrier, while C_{ox} is the capacitance due to the interfacial layer with thickness δ and permittivity ϵ_i . C_s can be considered as an extra capacitance due to the charge in the interface states. However, if the capacitance meter test signal frequency is high enough (about 1 MHz), the interface states are not able to follow the test signal any more. Thus, at high frequencies, C_s becomes zero.

The derivation of the above equations assumes a continuous distribution of interface states. Some models predict that interface states should occur in bands. This, together with a general lack of knowledge regarding the exact nature of interface states, means there exists no reliable way in which the capacitance measurements can accurately be corrected for the effect of interface states. (See for instance Rhoderick 1988 for a discussion on the shortcomings of current theories.) Some methods have been suggested (Brews 1973, discusses the case of MOS structures) but in general, they reduce the accuracy of the measurement, or require extra measurements to be made. For this reason it seems the best results are obtained if the sample is prepared properly to reduce the interfacial layer thickness to a minimum, and a test signal frequency of 1 MHz or higher is used during capacitance measurements to minimize the effect of any interface states that may be present.

The effect of an inversion layer

In chapter 4 it was mentioned, that, when a large reverse bias is applied to a Schottky contact, it could happen (in the case of a n -type semiconductor) that the bands bend upwards to such an extent that the part of the valence band closest to the metal is moved above the position of the Fermi level in the bulk of the semiconductor. If it is assumed that the Fermi level remains flat, right up to the interface, it should be possible for a large number of holes to accumulate in the region where the Fermi level lies below the valence band. This layer, which is effectively p -type, is called the inversion layer. In this case the depletion region approximation would no longer be valid.

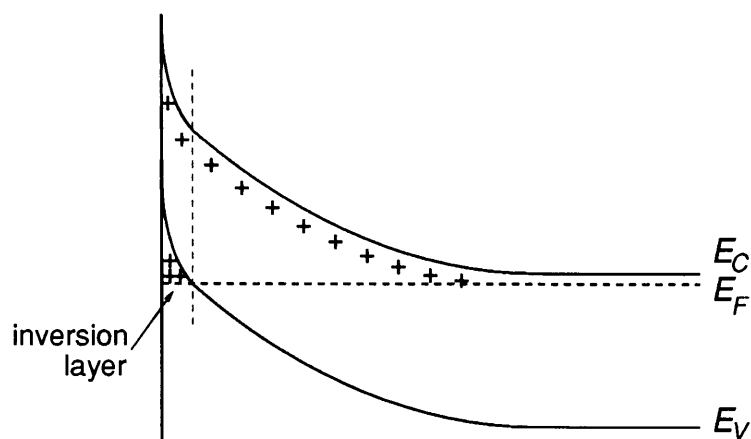


Figure 6.5: The formation of an inversion layer in a Schottky diode. Here it is assumed that the Fermi level remains flat throughout the depletion region.

Rhoderick (1988) gives a qualitative treatment of the phenomenon. In his treatment he assumes that the effect of the holes in the inversion layer on the shape of the barrier will be minimal, unless their concentration is comparable with N_D . This will only happen if the valence band lies higher than the distance ξ below the hole quasi-Fermi level ζ_p . At the interface ζ_p corresponds to the metal Fermi level, which, when reverse bias is applied, lies higher than the Fermi level in the bulk of the semiconductor. Consequently, the concentration of holes in the inversion region is much less than predicted by figure 6.5. Furthermore, because the exponential energy dependence of p , the barrier rises steeply in the inversion region. For this reason, the inversion region is very thin ($< 100 \text{ \AA}$), and should have only a minimal effect on the CV characteristics of the diode. The only cases in which the effect of the inversion region becomes significant, is when the barrier height is close to the size of the band gap of the semiconductor, or when a thick interfacial layer is present.

In many cases it is possible to bias Schottky diodes far (larger than 10 V) into reverse bias, without observing any significant deviations from the depletion region approximation. This was found to be true even in extreme cases investigated by Walpole *et al* (1971), involving Schottky barriers on PbTe and InAs. They found that, despite the fact that the barrier heights of these Schottky diodes were higher than the band gap of the semiconductors on which they were fabricated, they still displayed linear $1/C^2$ versus V characteristics for high reverse bias.

By means of deep level transient spectroscopy (DLTS), Ma *et al* (1988) also found evidence that the Fermi level does not stay flat in the depletion region. They observed that when Schottky diodes with a low barrier height were fabricated on GaAs, certain defects (the EL2 defect) seemed to become unobservable, although it was known that the defects were still present in the semiconductor. Similar results were also obtained by Auret *et al* (1992) when the barrier height of Schottky diodes was lowered by sputtering the substrates with Ar ions before evaporation of the metal. According to Ma *et al*, the disappearance of the EL2 level is due to the bending of the Fermi level in the depletion region. In the case of low barrier height Schottky diodes, the Fermi level in the depletion region was bent so much that it never fell below the level of the EL2 defect, which is roughly in the middle of the band gap.

The bending of the Fermi level is calculated by Ma *et al* by considering the current flow through the Schottky diode under reverse bias, as described by the drift and diffusion of carriers in the diffusion region. For a given bias voltage, the current density can be written as

$$J = \frac{kT\mu N_C \exp[-F(w)/kT] - \exp[-F(0)/kT]}{\int_0^w \exp[-qV(x)/kT] dx}, \quad (6.24)$$

where μ is the electron mobility, N_C is the effective density of states and $F(0)$ and $F(w)$ are the quasi-Fermi energies at the metal-semiconductor interface and the depletion region edge, respectively. If it is assumed that the bands are bent parabolically, as described by equation (4.7), the integral in equation (6.24) can be evaluated as

$$\int_0^w \exp\left(\frac{-qV(x)}{kT}\right) dx = \exp\left(\frac{q\phi_b}{kT}\right) L_D D\left(\frac{W}{L}\right), \quad (6.25)$$

where $L_D = (2\epsilon kT/N_D q^2)^{1/2}$ and the $D(x)$ is the Dawson integral defined as (Abramovitz and Stegun 1972)

$$D(x) = e^{-x^2} \int_0^x e^{t^2} dt. \quad (6.26)$$

By using equation (6.24), it is possible to obtain an expression for the Fermi level in the depletion region. The results indicate that the Fermi level does not drop far below the middle of the band gap, even for Schottky diodes with a barrier height of 0.9 eV. The typical form of the Fermi level as described by Ma *et al*, is shown in figure 6.6. In the light of this finding it seems unlikely to be possible to create an inversion layer in Schottky diodes as easily as suggested by the model developed in chapter 4.

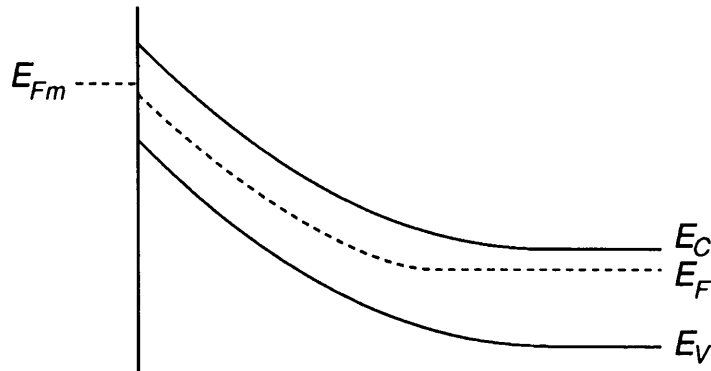


Figure 6.6: Fermi level in the depletion region as calculated by Ma *et al* (1988)

Capacitance under forward bias

Up to now no mention of the capacitance of the Schottky contact under forward bias has been made. Although the mathematical treatment, according to the depletion region approximation, still predicts the presence of a capacitance during forward bias, conduction across the barrier could nevertheless influence the accuracy with which the capacitance can be determined. For instance, in the case of *p-n*-junctions, minority carriers injected during forward bias cause deviations in the capacitance reading. However, in the case of Schottky diodes, minority carrier injection occurs to a much lesser extent, and capacitance measurements made under forward bias can still be used to determine the carrier density. The main factor limiting measurements under forward bias is conduction across the barrier.

Conduction during forward and reverse bias

The capacitance of a Schottky diode is best measured while the diode is under a moderate reverse bias. The main factor determining the region of applied bias over which the capacitance can be measured is conduction across the barrier. For good quality Schottky diodes with moderately high (> 0.7 eV) barrier heights, the reverse bias is limited by avalanche breakdown, while the maximum forward bias that can be applied is limited by forward conduction across the barrier.

In Schottky diodes avalanche breakdown occurs very rapidly, and in many cases damages the Schottky diode to such an extent that a permanent increase in reverse current is observed. Therefore, the maximum allowable reverse bias is well defined. This is not the case in the forward direction and, since it is frequently necessary to know the dopant distribution as close to the surface as possible, it is important to define a parameter that would give an indication of the accuracy of the measurements. In many cases the so-called *dissipation factor* D is used. The dissipation factor for a parallel R - C circuit is the ratio between the reactance of the capacitor and the resistance of the resistor, or $1/\omega RC$, where ω is the angular frequency of the test signal. In general, D may be calculated directly from the phase angle by the relation $D = \cot \theta$. If the reactance of the capacitor is much smaller than the resistance of the resistor, the conduction by the capacitor will dominate over conduction by the resistor. This implies that the phase angle between the applied test signal voltage and the measured current will be close to 90° , and D will be very small. As the parallel conduction increases (i.e. the resistance decreases) D will slowly increase to 1 when $\theta = 45^\circ$. As mentioned previously, the most accurate capacitance measurements are made when phase angle θ is close to 90° . As θ decreases, the measurement error increases. For the HP 4192A LF Impedance analyser, the measurement error doubles for $D > 0.1$. As a general rule, the best measurements are obtained when $D < 0.05$.

Problems due to the numerical differentiation of data

It is well known that an inherent problem of numerical differentiation is that the derivative will always be less accurate than the original data (Press *et al* 1987). In the case of CV profiles this problem becomes more acute since the derivative must be calculated from measured data and not from a mathematical function. To obtain an optimum profile two factors have to be weighed. Firstly, if the carrier density varies rapidly, the capacitance should be measured at closely spaced points to minimize the averaging of the calculated distribution. On the other hand, closely spaced data points lead to greater errors during differentiation, and poor accuracy. Because of this effect some authors have even suggested that carrier density profiles obtained by CV techniques are inherently noisy (Deming *et al* 1985). However, McGillivray (1988) has shown that accurate, noise free profiles can be obtained by choosing suitable intervals for differentiation.

Errors due to the capacitance meter

Amron (1967) and, more recently, Blood (1986) have considered the effect of a constant relative error η that results in a capacitance $C_m = (1+\eta)C$ being measured when the true capacitance is C . However, in most modern capacitance meters the main cause of errors,

during the measurement of carrier density profiles, is the presence of random rounding errors which occur because of the digital nature of the instruments. These random errors seem to have a more significant effect than systematic measurement errors caused by the capacitance meter. The reason being that in most cases systematic errors do not vary between adjacent points, while the random errors, due to rounding and other factors, vary greatly between closely spaced points, thus causing much larger errors during the differentiation process. This effect is in many cases compounded by capacitance meters in which the number of significant digits displayed (and returned to the computer) is determined by the absolute accuracy of the instrument, which is in many cases an order of magnitude lower than the repeatability. This causes the random error, due to rounding, to increase drastically. However, some capacitance meters (eg. the HP 4192A impedance analyser) can be modified to suppress this feature, allowing the maximum number of significant digits to be displayed at all times (see the experimental section for details).

McGillivray (1988) has made a detailed study of the effect of these random errors on the carrier density profiles obtained from *CV* measurements. In his analyses he assumes that the measured capacitance is given by $C_m = C + R$, where R is the sum of the measurement systems rounding and random errors. When the value for C_m is substituted in equation (6.7), and terms of the order R^2 and higher are neglected, it can be shown that the relative error in the calculated carrier density profile is given by

$$\frac{\Delta N(w)}{N(w)} = \frac{3\Delta C/2}{C[1 + (\Delta C/2R)]} - \frac{1}{1 + (\Delta C/2R)}. \quad (6.27)$$

If it is assumed that $R \ll \Delta C$ and $\Delta C \ll C$, the above equation can be simplified to

$$\frac{\Delta N(w)}{N(w)} = \frac{2R}{\Delta C}. \quad (6.28)$$

From this equation it can be seen that, for a 1-percent error, the condition $\Delta C \geq 200R$ must be satisfied. This condition can be satisfied in a number of ways. The first, and probably the most simple method, is to measure the *CV* characteristics with a very small step e.g. 0.01 V. The condition $\Delta C \geq 200R$ is now enforced during the differentiation of the data, by increasing the interval over which the differentiation occurs until the change in capacitance is large enough. This technique has the advantage that it can be applied after the measurement, and that the value of R can be adjusted for optimum results, without having to re-measure the data. The main disadvantage is that a very large number of points have to be measured, while only every fifth point or so is used. This problem can be overcome by dynamically varying the step size during the measurement.

Miller (1972) has suggested an electronic method, which relies on a feedback loop that adjusts the voltage applied to the sample, to ensure constant capacitance intervals. This technique has been used in some commercial instruments.

McGillivray suggested a method by which the voltage step size can be calculated during the measurements. By first rewriting equation (6.7) and substituting finite differences for

derivatives he obtained an expression for ΔV in terms of ΔC

$$\Delta V = \frac{q\epsilon_s N(w) \Delta C}{C^3}. \quad (6.29)$$

When the 1-percent noise criterion is substituted in the above equation it becomes

$$\Delta V = \frac{q\epsilon_s N(w) (200R)}{C^3}. \quad (6.30)$$

This relation can now be used to calculate the voltage step during measurements.

When the above procedure is followed, note that the value of R should be measured for every range of the capacitance meter. On some meters (eg. the HP 4192A LF Impedance Analyser) it is sometimes impossible to determine the range on which the meter is set. In these cases the software should provide its own range-selecting algorithm to replace the autoranging facility on the capacitance meter. Other errors could occur due to scale changes during measurements, when the difference between readings on the two scales could be as large as the absolute accuracy of the instrument. Ideally, after a new range has been selected, the previous point should be re-measured, so that the points over which differentiation is carried out are all measured on the same range.

Determining the carrier distribution right up to the interface

When the carrier concentration of a semiconductor is determined by means of depletion profiling, it is impossible to determine the carrier concentration right up to the surface. However, certain information can be determined from the length of the depletion region at the largest possible forward bias, but this is not sufficient to determine the exact charge distribution. Giacoletto (1957) and later Kim (1988) and Yeo *et al* (1990) have shown that by combining depletion *CV* profiling with etching the carrier density profile can be determined right up to the surface of the semiconductor. This method is involved as it requires the use of etching combined with depletion *CV* profiling. In many cases it is easier to grow a layer of a few μm on top of the structure to be profiled. However, in cases where ion implantation profiles are studied, this technique may be useful.

6.3 Other contact systems suitable for *CV* measurements

In addition to vacuum deposited Schottky diodes, other contact systems are also suitable for *CV* profiling. These include: metal oxide semiconductor (MOS) structures, *p-n* junctions, mercury contacts and electrolyte contacts. Van Gelder *et al* (1971) and McGillivray *et al* (1988) discuss the *CV* characteristics of MOS capacitors. MOS structures are used when the thermal oxide plays an important role in the determination of the doping profiles. Because MOS structures have a thick oxide layer, which reduces conduction across the barrier, an inversion layer is more easily formed in these structures than in a Schottky diode. To overcome this problem, pulsed capacitance measurements are sometimes used. During these

measurements bias is applied for only a couple of microseconds, during which the inversion region does not have time to form, allowing the depletion region to be analysed to a greater depth (van Gelder *et al* 1971). This, however, requires the use of a fast capacitance meter, and reduces the accuracy of the capacitance measurements.

Carrier density profiles can also be obtained from p - n junctions (Hilibrand *et al* 1960). In this case the one side of the junction is usually doped heavily, so that it will not contribute significantly to the capacitance of the device. The capacitance of the junction under reverse bias can then be considered only due to the depletion region on the one side of the barrier. In this case the junction can be analysed in a similar way as was done for a Schottky diode. It should be noted that, because of minority carrier injection under forward bias, the forward capacitance of the junction can not be used to obtain doping information. Therefore, the technique can not be used to analyse the doping profile close to the junction. In general, p - n junctions give less reliable results, which are often more difficult to analyse.

For routine material assessment the cleaning and metal deposition procedures may prove too expensive and time-consuming. Here mercury and electrolyte contacts provide an ideal solution. The mercury contact is formed by mercury in a capillary tube, while the electrolyte contact is generally formed by mounting the sample against a electrolyte bath with a hole in the side. An o-ring is used to define the contact area and eliminate leakage of the electrolyte. The main advantage of these types of contacts is that they provide a reasonably good contact without any extensive sample preparation. Their main disadvantage is that it is difficult to determine the area of the diode accurately, and in many cases these contacts have a high series resistance.

The electrolyte contact has a further advantage. If the contact is made with a suitable electrolyte, this electrolyte can be used to etch the sample at the same time as the CV response is being measured. Due to the high series resistance of the electrolyte, the capacitance is usually measured at a lower frequency of about 3 kHz. The reverse bias is modulated at a rate of about 30 Hz, and the change in the capacitance is then related to the carrier density at the depletion region by using equation (6.7). The depth can be obtained by multiplying the etch rate with time, and adding the depth of the depletion region to this value. Using this technique, it is possible to profile much deeper into the semiconductor than is possible by depletion profiling. The main disadvantages of this technique is that inaccuracies arise due to the high series resistance of the electrolyte, and also due to uncertainties regarding the etch rate and the surface area of the contact. See Blood (1986, 1987) for an excellent discussion on this technique.

6.4 Effect of the Debye-Hückel screening length on CV profiling

In the above section the abrupt depletion region approximation has been assumed. However, as mentioned earlier, the depletion region edge is not abrupt, but there is a transition region over which the charge density drops off more or less exponentially.

Debye and Hückel, who have investigated a similar problem, have derived a formula which describes the screening of a charge in an electrolyte by other, mobile charges. If it is assumed that the charged particles are distributed according to the Boltzmann distribution (which is also valid for electrons at energies about $3kT/q$ above the Fermi level (see chapter 2)), it can be shown (see for example Jackson 1975) that the potential in the electrolyte is spherically symmetric, and given by

$$V(r) = Zq \frac{e^{-r/L_D}}{r}, \quad (6.31)$$

where q is the electron charge and L_D is the so called Debye length, which is equal to $(kT\epsilon/4\pi q^2 n)$ in the case of a single charge in an electrolyte, or a plasma. In the case of a depletion region in a semiconductor, the problem can, because of symmetry, be reduced to one dimension. Here the charge distribution is given by

$$V(r) = Zq e^{-r/L_D}, \quad (6.32)$$

and the Debye length is given by

$$L_D = \sqrt{\frac{kT\epsilon_s}{q^2 N_D}}, \quad (6.33)$$

where k is the Boltzmann constant, T is the absolute temperature, and N_D is the local doping density. This derivation is only valid for small charges, for which the free carriers close to the charge are not completely depleted. For larger charges, such as in the case of the depletion region of a Schottky diode, the potential distribution can be approximated quite well by assuming a normal parabolic potential in the depletion region, up to a depth w' , followed by an exponentially decreasing potential in the transition region, or the so called Debye tail. Thus, the charge in the semiconductor does not reach its equilibrium value before several Debye lengths deeper than the depletion region edge, as shown in figure 6.7.

A similar situation arises at abrupt doping transitions. For example, when there is an abrupt step in the doping profile, the charges do not follow the doping profile exactly, but follow a smooth transition between the two extremes, as indicated in figure 6.9.

For this reason, when the depletion width is increased by increasing the applied voltage by ΔV , the charges are not all depleted from the same depth, but from an area ranging over several Debye lengths, as shown in figure 6.8. Because of this, the measured doping profiles become “smeared out”, and it becomes impossible to distinguish any features smaller than a Debye length. For this reason the measured carrier density profile is often referred to as the *apparent* carrier density profile and indicated by $\hat{n}(x)$. In 10^{15} cm^{-3} doped GaAs, the Debye length at room temperature is about $0.14 \mu\text{m}$, but becomes $0.043 \mu\text{m}$ for 10^{16} cm^{-3} doped material. When relatively large structures in highly doped material are to be profiled, the effect of the Debye length averaging is negligible. However, in the case of semiconductor

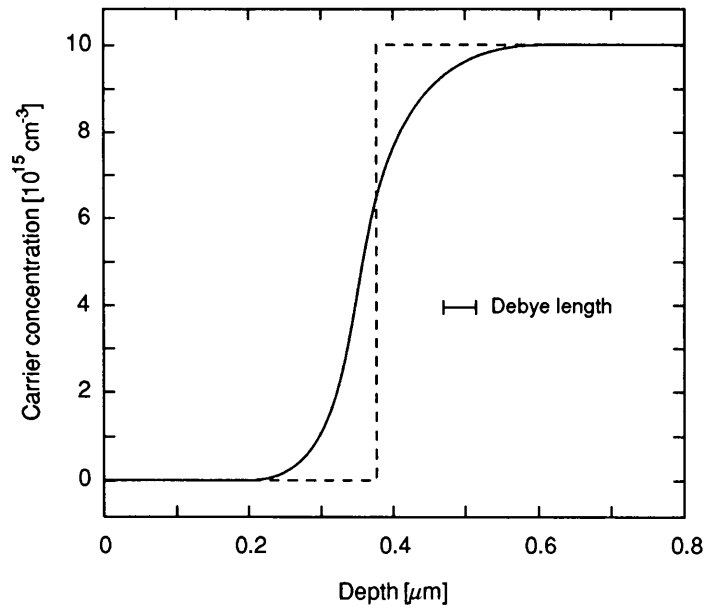


Figure 6.7: a) Majority carrier density at the depletion region edge. The dotted line indicates the carrier density as predicted by the depletion region approximation, while the solid line indicates the exact value as calculated by the simulation program described in section 8.8. This graph was calculated for Schottky diode manufactured on 10^{16} Si-doped GaAs at 300 K, with a total forward bias of 1 V. The Debye length in this material is $0.043 \mu\text{m}$.

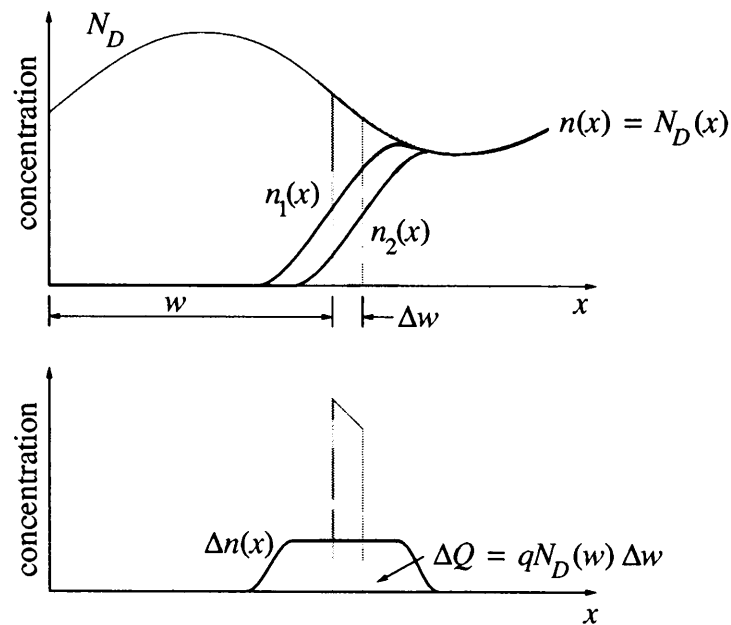


Figure 6.8: Charge distribution in the depletion region when Debye length averaging is taken into account. The grey lines indicate the distribution according to the depletion approximation.

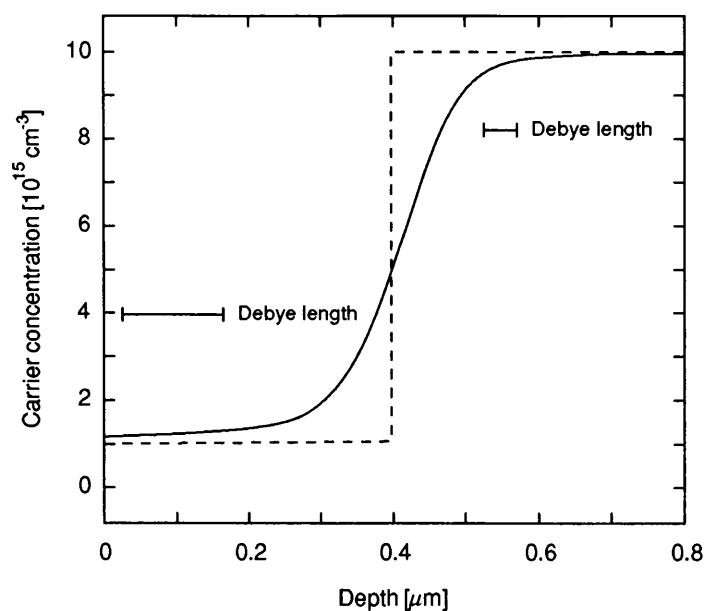


Figure 6.9: Carrier density in a 10:1 doping step in Si-doped GaAs at 300 K, as calculated by the simulation program described in section 8.8. The dashed line indicates the doping profile.

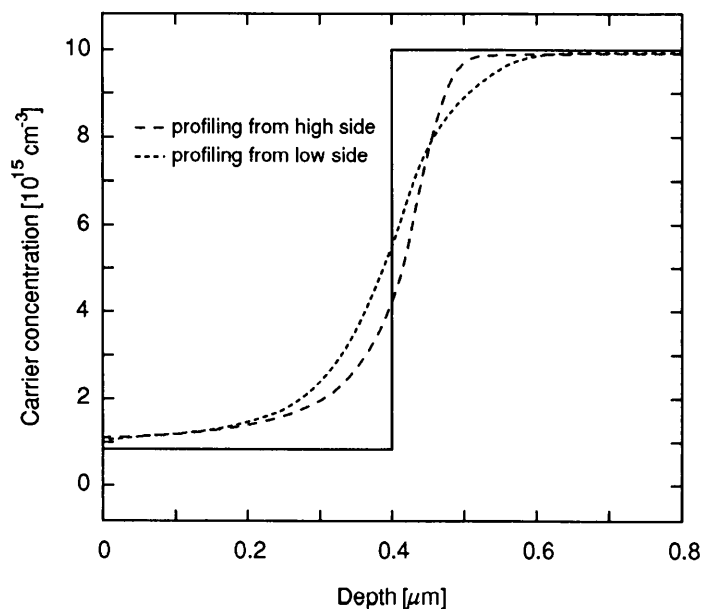


Figure 6.10: a) CV profile of a 10:1 doping step in GaAs as calculated by the simulation program described in chapter 7. The apparent doping profiles as measured by profiling from the high as well as from the low side are shown. The solid line indicates the position of the step.

microstructures, Debye length averaging becomes important. Debye length averaging also causes the form of the measured carrier concentration profile to depend on the direction from which the structure is profiled. This can clearly be seen in figure 6.9, but is even more pronounced in the case of semiconductor heterojunctions (see figure 7.4(a)). This phenomenon is discussed in detail Johnson *et al* (1971).

The shape of $\hat{n}(x)$ for a given profile can be calculated by solving the boundary-value problem mentioned in chapter 4 by numerical methods, using a computer. However, the converse problem, where the doping profile has to be calculated from $\hat{n}(x)$, is intractable. It seems that, according to this classical analysis, it is impossible to increase the resolution of CV profiling to more than the Debye length of the semiconductor.

Nevertheless, Kennedy *et al* (1968, 1969) have proposed a technique by means of which the original doping concentration can be obtained. According to this technique, the doping concentration can be obtained from the measured carrier concentration by applying the formula

$$N(x) = n_o(x) - \frac{kT\epsilon_s}{q^2} \frac{d}{dx} \left[\frac{1}{n_o(x)} \frac{d}{dx} n_o(x) \right]. \quad (6.34)$$

However, in the derivation of this formula, the depletion region approximation has been assumed, and only the Debye averaging occurring at doping steps has been considered. For this reason this correction is of limited use, and it has been shown that in some cases it can even lead to erroneous results. Johnson *et al* (1971) give a complete discussion of the limitations of the above mentioned method.

The Debye length can be successfully reduced by cooling the sample. For instance by reducing the temperature from 300 K to 12 K, the Debye length can be reduced fivefold. This technique is useful for reducing the Debye length in semiconductors like GaAs, where the donor level lies very close to the conduction band. In these semiconductors freeze-out occurs only at extremely low temperatures, and it is still possible to perform CV profiling at temperatures around 10 K.

7

CV measurements on isotype heterostructures and δ -doped layers

Traditionally *CV* measurements have been applied to the determination of shallow-dopant or free-carrier depth profiles in semiconductors. If *CV* measurements measured the true carrier distribution $n(x)$, it would be possible, assuming that the semiconductor is not degenerate, to determine the shape of the conduction band edge in a heterojunction from equation (6.7) and using the relation between the conduction band and the Fermi level derived in chapter 2

$$E_C(x) - E_F = -kT \ln[n(x)/N_C(x)]. \quad (7.1)$$

As explained in the previous chapters, because of the non-zero Debye length in semiconductors, the profile obtained by *CV* measurements does not correspond to the doping concentration $N_D(x)$ or the free carrier density $n(x)$, as suggested in some earlier papers. For this reason the carrier concentration obtained by means of the *CV* technique will be referred to as the *apparent carrier concentration* $\hat{n}(x)$. An example showing both the true and the measured carrier concentrations in a heterojunction is shown in figure 7.2

Kroemer *et al* (1980) demonstrated that heterojunctions may also be investigated by the *CV* technique, giving information on heterojunction band offsets and charged interface states.

7.1 Analysis according to Kroemer *et al*

The relationship between $\hat{n}(x)$ and the properties of the heterojunction can be investigated in a similar fashion as was done in chapter 5. Consider the conduction band edge depicted in figure 7.1. Here a Schottky diode was fabricated on the lower conduction band side of an isotype heterojunction. When the voltage applied across the junction is increased from V to $V + \Delta V$, charges are removed from both the edge of the depletion layer and the notch on the low conduction band side of the heterojunction. As previously, we can define a distribution $\Delta n(x)$ which gives the change in carrier density due to the voltage increment ΔV .

For the capacitance meter the change in charge density is the same as if all the electrons had been depleted from a position $\hat{x}$, called the centroid of the charge change, given by

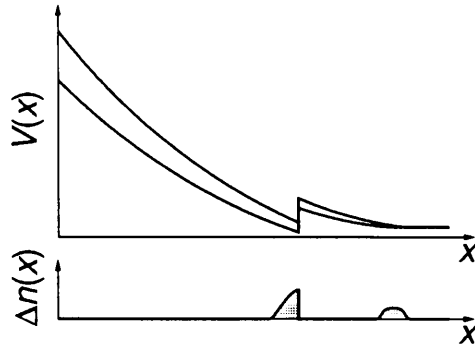


Figure 7.1: Charge distribution in a heterojunction in the depletion region of a Schottky diode. (After Kroemer 1984)

$$\hat{x} = \frac{\int_0^{\infty} \Delta n(x) x \, dx}{\int_0^{\infty} \Delta n(x) \, dx} . \quad (7.2)$$

The equivalence can easily be proven by inserting the two charge distributions in Poisson's equation followed by twofold integration.

From the calculated apparent carrier density profile shown in figure 7.1, it is clear that the apparent profile bears little resemblance to the real carrier concentration. Nevertheless, a number of quantities are conserved during this smearing process. Firstly, because the capacitance meter measures the change in charge in the depletion region, the total number of carriers is conserved:

$$\int_0^{\infty} n(x) \, dx = \int_0^{\infty} \hat{n}(x) \, dx . \quad (7.3)$$

From electrical neutrality it follows that this integral should be equal to the sum of all charges in the region, i.e. the integral of the net donor concentration, plus the density σ_i of any fixed interface charges that may be present. If the donor concentration is known independently, the interface charge may be calculated as

$$\sigma_i = \int_0^{\infty} [N_D(x) - \hat{n}(x)] \, dx . \quad (7.4)$$

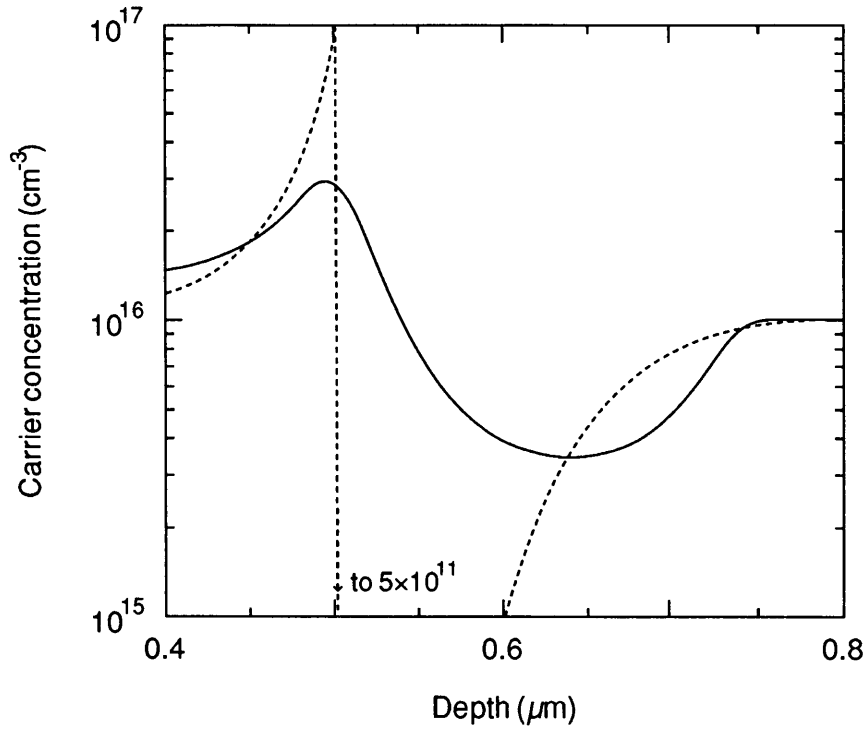


Figure 7.2: The true (dashed line) as well as the apparent (solid line) carrier density profiles in a GaAs-AlGaAs heterojunction, as calculated by a simulation program. The conduction band offset was 0.30 eV, and the doping level was 10^{16} cm^{-3} on both sides of the junction. The effect of interface charge was ignored.

It can be shown that the first moment of the carriers is conserved as well, so that

$$\int_0^{\infty} n(x)x \, dx = \int_0^{\infty} \hat{n}(x)x \, dx. \quad (7.5)$$

Using this relationship (and equation (7.3)), the electrostatic potential difference between the two sides of the heterojunction can be calculated from the apparent carrier concentration

$$\Delta\Phi = \int_0^{\infty} [N_D(x) - \hat{n}(x)](x - x_j) \, dx. \quad (7.6)$$

For a homojunction, $\Delta\Phi$ is the conventional diffusion potential $\phi(\infty) - \phi(0)$. For an abrupt heterojunction with a conduction band discontinuity ΔE_C , the electrostatic potential difference across the barrier is (see chapter 5):

$$\Delta\Phi = \frac{kT}{q} \ln \left[\frac{n(\infty)/N_C(\infty)}{n(0)/N_C(0)} \right] + \frac{\Delta E_C}{q}. \quad (7.7)$$

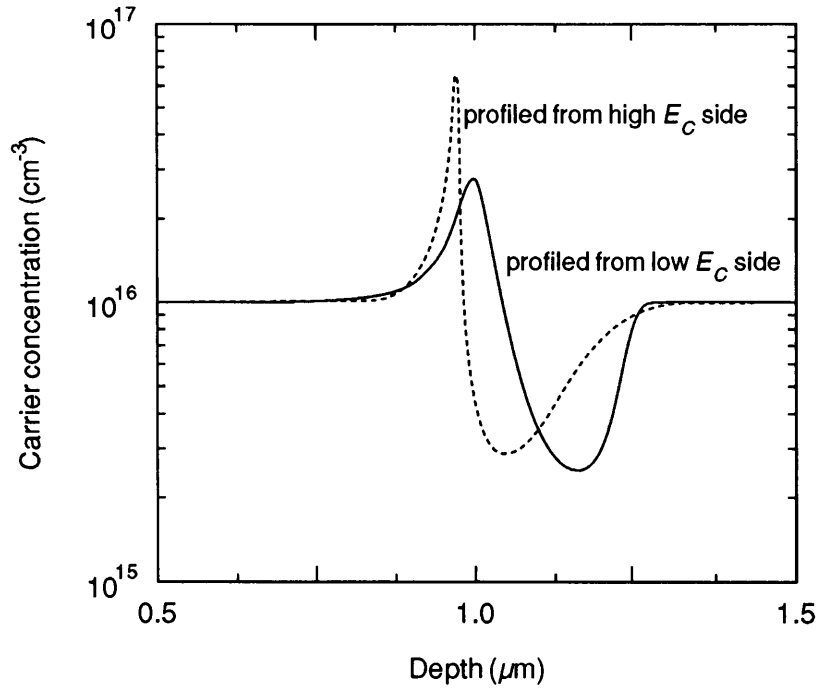
Thus, by using the above two equations, it is possible to determine the conduction band discontinuity ΔE_C from the measured $\hat{n}(x)$ values, provided that $N_D(x)$ and the position of the heterojunction x_i is known independently.

In many cases $N_D(x)$ is not known independently. However, if the doping profile is known to be uniform on both sides of the junction, where it changes abruptly, the carrier density on each side of the junction can be approximated by its value in a region relatively far away from the interface where $N_D = n(x) = \hat{n}(x)$. The position of the heterojunction x_i can be determined by inspection of the $\hat{n}(x)$ profile, using a graph (such as that in figure 7.1) as a guide. Using this method, Kroemer *et al* and others (e.g. Ogura *et al* 1983, see Kroemer 1984 for more references) have obtained reasonably repeatable results. Furthermore, it was established that the ratio $\Delta E_C:\Delta E_V$ is not 85:15 as was previously believed, but closer to 62:38. These results are also verified by other techniques (Kroemer 1984).

A number of comments and elaborations have been made to this theory. The first two important comments were made by Kroemer in 1984. Firstly he proved that, since the potential difference between the two sides of a heterojunction is not changed by grading, the above mentioned technique should also give the same answer in the case of graded heterojunctions. These predictions are confirmed by results quoted in their paper. It should be noted, however, that the compositional grading could also cause a grading in the doping concentration $N_D(x)$ that could cause further uncertainties. Another assumption that has also been made, is that the dielectric constant of the two semiconductors is identical. However, Babic (1984) proved that the dielectric constant “cancels out”, and that equations (7.4) and (7.6) are correct as they stand.

Note that the accuracy of this method is to a large extent determined by the accuracy of the assumed position of the heterojunction. For example, to determine the interface charge accurately to 10^{10} cm^{-2} , it is necessary to know the position of the heterojunction to an accuracy of at least $0.01 \mu\text{m}$, in 10^{16} cm^{-3} doped material. By looking at the simulated graph in figure 7.2, it seems that it may just be possible to determine the position to the desired accuracy. However, if the Schottky diode is manufactured on the high E_C side, or if interfacial charges are present, the depth of the junction can not be determined as easily as in the previous case. Figure 7.3(a) shows the simulated shape of the apparent carrier distribution for a heterojunction as profiled from both the high and the low E_C side, while figure 7.3(b) illustrates the effect of interfacial charge.

a)



b)

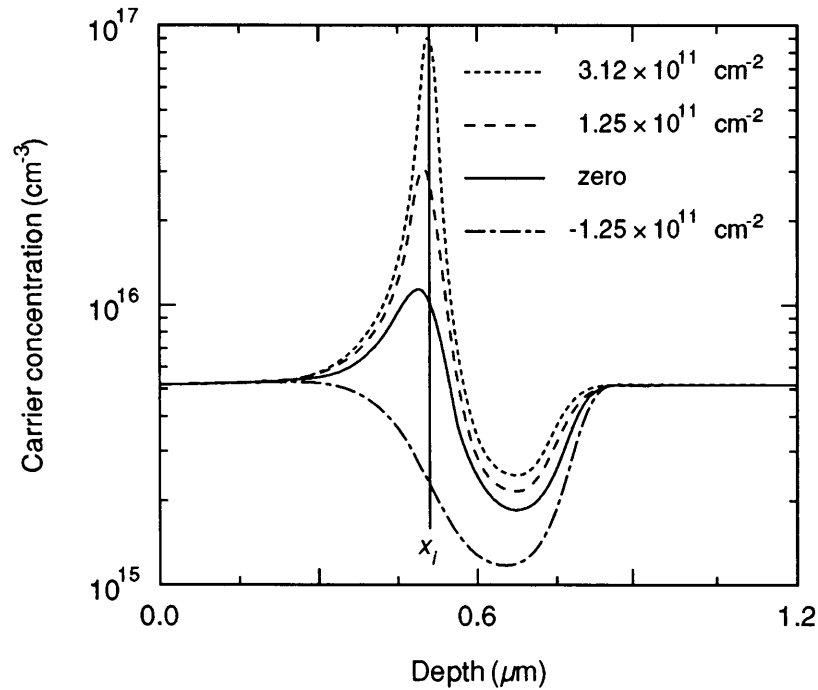


Figure 7.4: (a) Simulated apparent carrier density profiles of a heterojunction profiled from both the low E_C side (solid line) and the high E_C side (dashed line), as simulated by the simulation program described in chapter 8. $\Delta E_C = 0.3$ eV. (b) Simulated apparent carrier density profiles of a heterojunction, profiled from the low E_C side, illustrating the effects of an interfacial charge. $\Delta E_C = 0.2$ eV. (After Rimmer et al 1991)

Other factors have also been found to influence the accuracy of the determined band discontinuity. 't Hooft *et al* (1986) investigated the effect of the donor depth. In their discussion they show that both the donor depth, as well as the presence of compensating acceptors, can influence the value obtained for the conduction band discontinuity. The reason being, if all the donors are not ionized, it follows that equation (7.3) is no longer valid. Furthermore, the position of the Fermi level, relative to the conduction band edge, is also no longer given by a simple relation such as (2.25). This means that expression (7.6) is also not valid. Figure 7.4 shows a graph obtained by computer modelling, showing the measured ΔE_C as a function of donor depth for different doping concentration.

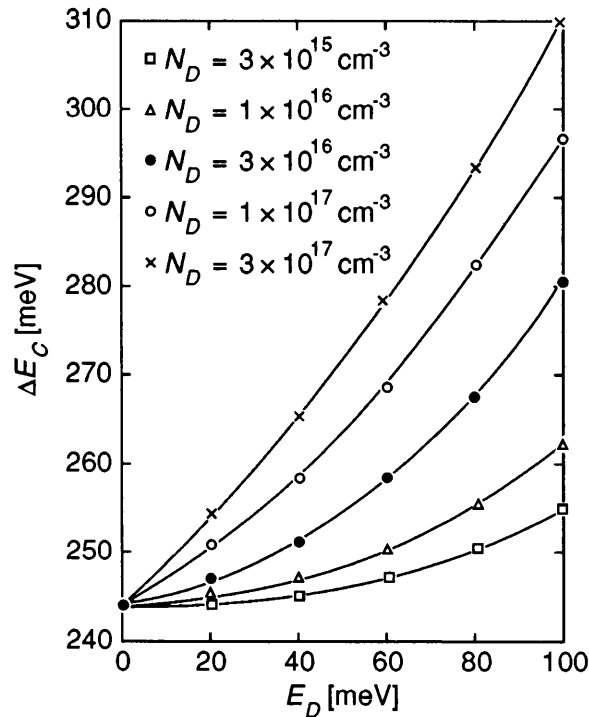


Figure 7.4: Measured ΔE_C as a function of donor depth for different doping concentrations (after 't Hooft *et al* 1986)

The effect of deep levels, and specifically the *DX* centre (Mooney 1991) in AlGaAs on the determination of the GaAs/AlGaAs heterojunction band discontinuity, has been investigated by Subramanian (1988). The *DX* centre is a deep level defect that occurs in $\text{Al}_x\text{Ga}_{1-x}\text{As}$ for $x > 0.2$. At room-temperature this defect has a response time in the order of microseconds, and can thus influence measurements made at a test signal frequency of 1 MHz. However, this effect would probably become negligible at slightly higher frequencies.

Kazmierski *et al* (1987) found that in the case of GaInAs/InP, deep levels severely affect the shape of the *CV* profile. In his paper he describes a very strong frequency and temperature dependence of the measured conduction band discontinuity and interface charge density, as

obtained by the method of Kroemer. Furthermore, he noted that the apparent depth of the heterojunction also depends strongly on the temperature and the frequency used. This is attributed to the high density of deep traps in the material, that can still respond to frequencies of 1 MHz and higher. For this reason it seems that results obtained by the method of Kroemer *et al*, should, when a significant number of deep levels are present in the material, be treated with caution.

7.2 An alternative method for the calculation of the depletion region capacitance, according to Ogawa *et al*

Recently Ogawa *et al* proposed another method according to which the capacitance of the depletion region could be calculated. In the paper (Ogawa *et al* 1991) it is mentioned that one of the great advantages of their technique is that it does not require an assumption of the presence of an interface charge at the heterojunction. This technique will be discussed later in this section.

As explained above, Kroemer *et al* (and all other authors that I am aware of) determined the capacitance of the Schottky diode from the charge distribution by using the relation $C = dQ/dV$. Ogawa *et al* determine the capacitance of the Schottky diode from energy considerations. Although the “extended abstract” spans over three journal pages, the authors do not motivate their choice of method, and why the results obtained should be superior to those obtained by the traditional method. They also fail to give a clear outline of the derivation. In the following pages I shall give, what I consider a more detailed and more correct version of the derivation mentioned in the paper. Consider what happens when an AC current $i(t)$ flows through the junction, as would be the case in a typical CV measurement, when a small AC signal is superimposed on the DC bias applied to the junction. Assuming that all the work done by the applied signal is used to increase the energy of the charge distribution in the junction, it follows that for a small current i_c

$$V i_c = V \frac{dQ_w}{dt} = \frac{dW}{dt} = \frac{d}{dt} \left[\frac{1}{2} \int_0^\infty \epsilon(x) [E(x)]^2 dx \right], \quad (7.8)$$

where V is the potential difference across the junction, W is the energy of the charge distribution in the depletion region (Jackson, 1975), $E(x)$ is the electrostatic potential in the depletion region, and $\epsilon(x)$ is the permittivity of the semiconductor. From this equation, it follows that for a small amount of charge δQ_w flowing through the diode

$$V \delta Q_w = \int_0^\infty V(x) \delta \rho(x) dx = \delta W. \quad (7.9)$$

Thus, the left-hand side of the equation is now equal to the change in electrostatic energy δW due to a change in the space charge density of $\delta \rho$. The capacitance of the diode can now

be calculated by expressing the charge Q_w in terms of the electrostatic energy W as

$$C_w = \frac{dQ_w}{dV} = \frac{1}{V} \frac{dW}{dV}, \quad (7.10)$$

where W is as in equation (7.8). Thus, using this equation, it is possible to calculate the capacitance of the Schottky diode, using only the electric field in the depletion region, and the applied bias.

By substituting the relevant expressions for $E(x)$ and $V(x)$ obtained for the depletion region approximation, it can be shown that equation (7.10) yields the same result as that obtained in chapter 4. However, when a more realistic approximation to the charge distribution in the depletion region is made, the results differ. For instance, an approximation quite often used, is to approximate the decay of the charge in the depletion region by an exponential decay function with a decay constant of L_D . The charge density in the semiconductor ρ can then be expressed as

$$\rho(x) = \begin{cases} qN_D & 0 < x < w \\ qN_D e^{-(w-x)/L_D} & x > w \end{cases}. \quad (7.11)$$

When this charge density is used, and the capacitance is calculated according to the methods prescribed by Kroemer *et al*, the capacitance is found to be

$$C_{sc} = \frac{\epsilon}{w + L_D}, \quad (7.12)$$

while when the capacitance is calculated according to Ogawa *et al* the capacitance is

$$C_w = \frac{\epsilon}{w + L_D} \frac{1}{1 + [L_D/(w + L_D)]^2}. \quad (7.13)$$

Thus the capacitance according to Ogawa *et al* is larger than the conventional depletion region capacitance by a factor of $1/[1 + [L_D/(w + L_D)]^2]$, for this approximation.

Clearly, the reason for this discrepancy lies in the addition of a transition region. Thus, when charge is removed from the depletion region edge, it is not removed from a single point, with a single potential, but from a whole region, in which the electrostatic potential is not constant. Consequently the capacitance can not be determined in the same way as it would be for a parallel plate capacitor.

However, it is not clear whether the method suggested by Ogawa *et al* is preferable. For instance, it is obvious that the AC current flowing through the junction Q_w is not equal to the extra charge accumulating in the depletion region, $Q_{sc} = \int \rho(x) dx$. This contradicts the assumption that no DC current is flowing through the junction.

The problem can also be looked at from another viewpoint. The capacitance meter measures capacitance by applying a small increase in voltage, ΔV , to the junction, and measures the current flow because of this voltage step. Therefore it seems that the conventional method, where the capacitance of the junction is calculated as dQ/dV , is justified.

As for the method dispensing with the existence of an interface charge at the heterojunction, Kroemer's method does not imply the existence of interface charge, but rather offers a method to measure it if certain assumptions are made. Ogawa *et al* do not make these assumptions, accordingly they see the interface charge as part of their doping profile. Furthermore, as interface states in GaAs/Al_xGa_{1-x}As have been observed by other techniques (Mutsumoto 1983, Rimmer *et al* 1992), it seems reasonable to expect a certain amount of charge to be localized at the heterojunction interface.

7.3 CV profiling through semiconductors with quantum confinement

In the previous chapter it was shown that the resolution of the capacitance-voltage profiling technique for classical, non-degenerately doped structures is limited by the Debye length. For very narrow layers, however, quantum effects become important, and the extent of the electron (or hole) wave function can become a limiting factor.

Structures in which the dopant atoms occupy a layer of atomic proportions can readily be manufactured by MBE. In GaAs these so-called delta(δ)-layers are grown by interrupting the Ga shutter, while keeping the As shutter open so as to provide an As-stabilized surface. This reduces Ga-re-evaporation and makes cation sites available. (Most popular dopants such as Si, Be and Zn occupy cation sites.) Using this technique Schubert *et al* (1990c) have manufactured Si-doped delta layers in which most of the dopant atoms occupy a single atomic plane. Similar delta doped layers have been manufactured in Si by doping with Boron (Powell *et al* 1991). Schmidt *et al* (1991) have grown Si spiked doped GaAs by means of atmospheric pressure (AP)-OMVPE.

Many applications of delta layers have been suggested. Some of them are (Wood 1991): delta doped FET, punchthrough stoppers in MOSFETs, and in the emitter structure of gun diodes. The width and the surface charge density of the delta layer can play an important role in the performance of the device. These two parameters are most commonly characterized by means of secondary ion mass spectroscopy (SIMS) and CV profiling. However, both SIMS and CV techniques have difficulty in resolving the Si concentration profiles because of the high resolution needed.

Schubert *et al* (1988a, 1990a-c, see also Wood 1991) have shown that the spatial resolution of the CV technique on semiconductors with quantum-confinement is generally limited by the spatial extent of the quantized free carrier system, i.e. by the spatial extent of the ground-state wave function, and not by the Debye screening length.

Figure 7.6 shows what happens when a δ -doped layer is profiled by means of CV profiling. As previously the notation $\Delta q(x)$ will be used to indicate the change in the charge distribution caused by an increase in bias ΔV . Also, the centroid of charge change $\hat{x}$ will be defined as in equation (7.2). It can be shown that, for small voltage changes dV , the centroid of charge change is identical to the position expectation value $\langle x \rangle$. Thus, according to this interpretation, the capacitance can be written as $C = \epsilon_f \langle x \rangle$.

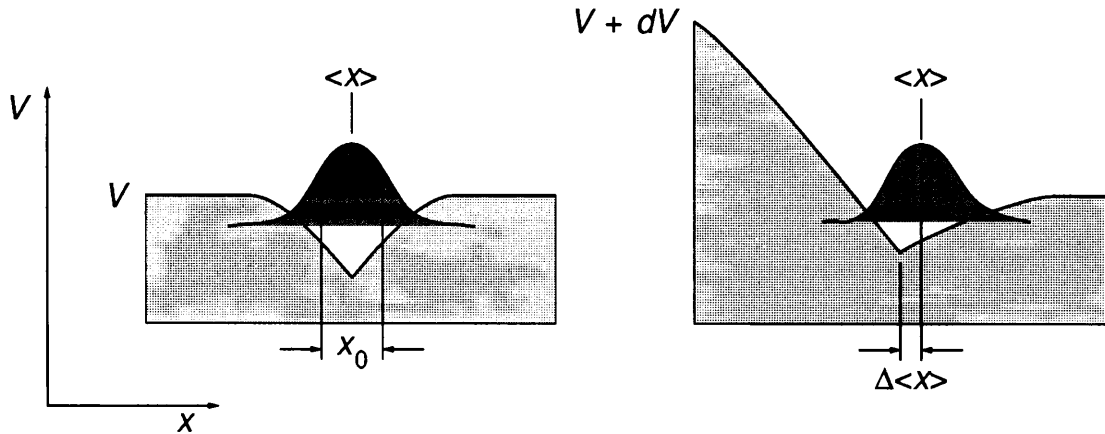


Figure 7.6: Band structure CV profiling through a δ -doped layer. (After Schubert 1990b)

It should be noted that, because of the quantum mechanical nature of the system, there are two additional contributions to the capacitance. For small signals the total capacitance is given by

$$C = \left[\frac{1}{C_{el}} + \frac{1}{C_{qm}} + \frac{1}{C_{Stark}} \right]^{-1}, \quad (7.14)$$

where C_{el} is the capacitance due to the electrostatic potential change, as expected classically, C_{qm} is the quantum mechanical capacitance, and C_{Stark} is the Stark-capacitance. These are briefly discussed in Schubert (1990a). In most cases however, these effects are negligible.

Using the same results as obtained by Kroemer, it is possible to show that the total amount of charge is conserved, and that the centroid of the CV profile coincides approximately with the centroid of the true carrier concentration. The position and concentration of the δ -doped layer can thus be determined directly from the CV profile.

The width of the measured CV profile was determined by considering the perturbation of the ground state wave function by the application of an external electric field E . The ground state wave function was determined by solving the Schrödinger equation for a V-shaped potential well by means of a variational technique. The variational wave function was

$$\psi_0(x) = \sqrt{\frac{2\alpha_0}{5}} (1 + \alpha_0 x) e^{-\alpha_0 x}, \quad (7.15)$$

where α_0 is the variational parameter. The width of the wave function was obtained as

$$x_0 = 2\sqrt{\langle x^2 \rangle - \langle x \rangle^2} = 2\sqrt{\frac{7}{5}} \left(\frac{4\epsilon_s \hbar^2}{9q^2 N^{2D} m^*} \right)^{1/3}. \quad (7.16)$$

The position of the expectation value of the ground state wave function was obtained from second order perturbation theory according to

$$\langle x \rangle_0 = \langle x \rangle_0^0 + \sum_{n \neq 0} \frac{\langle \psi_0 | x | \psi_n \rangle}{E_n - E_0} eE, \quad (7.17)$$

using the wave functions up to the second excited state. When the perturbing field was chosen to be equal to the field produced by the charge distribution, the change in the position expectation value was found to be

$$\langle x \rangle_0 \approx x_0. \quad (7.18)$$

This implies that the resolution of the CV technique in a semiconductor with a size-quantized carrier system is approximately equal to the extent of the ground-state wave function, and not the Debye length. An interesting point to note is that x_0 depends on the effective mass m^* , whereas the Debye length is independent of m^* . This has been observed experimentally by Schubert *et al* (1990a, 1991) in *n*- and *p*-type GaAs, where the carrier profiles for *p*-type GaAs were narrower due to the heavier hole effective mass.

The results obtained by Schubert have been confirmed by Wood *et al* (1991). Wood also demonstrated that the weighted width of all the occupied energy levels in the δ -doped structure should be taken into account when the expected width of the CV profile is calculated. A further interesting result is, that for certain ranges of layer thicknesses, the CV profile underestimates the true width. Figure 7.7 shows the apparent layer width as a function of true layer width for the two lowest energy levels in a Si δ -doped structure. From this figure it can clearly be seen that, at low temperatures, when only the ground state is occupied, the observed CV peak is much narrower than the true dopant distribution.

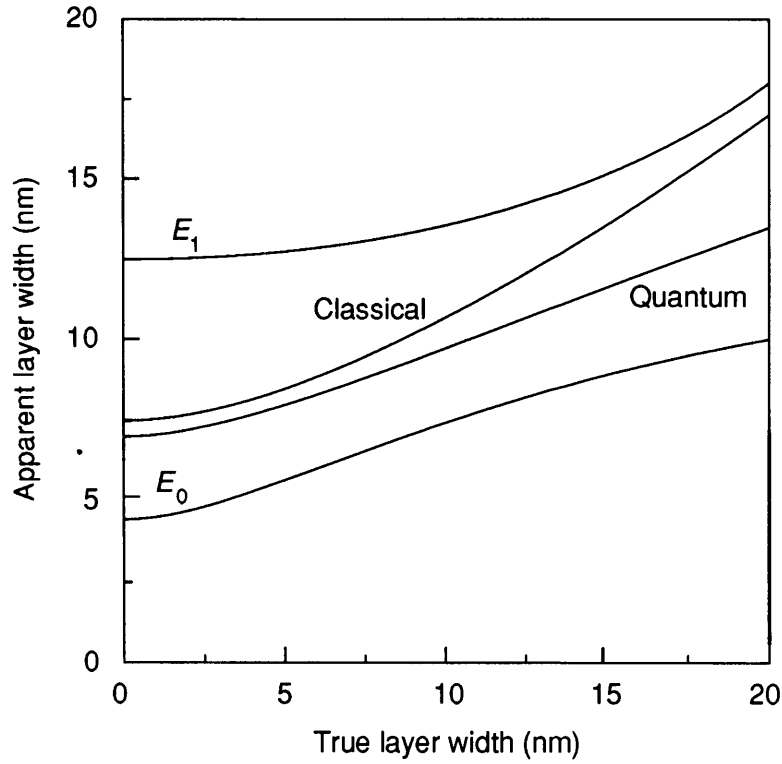


Figure 7.7: Apparent layer width as obtained from the CV FWHM, as a function of true layer width according to classical and quantum mechanical calculations. The simulation was carried out for a $2 \times 10^{12} \text{ cm}^{-2}$ δ -layer in Si, at 300 K. The FWHM of the two lowest energy levels are also shown. (After Wood *et al* 1991)

7.4 CV characterization of quantum well structures

The CV characteristics of a quantum well in the depletion region of a Schottky diode have been discussed by Letatre *et al* (1991). They considered the effect that a single quantum well with width a and distance L below the surface would have on the electrostatic field and potential at the surface. If a constant donor density N_D is assumed over the structure, and the dimensions of the well are much less than the Debye length in the rest of the semiconductor, the potential at the surface of the semiconductor is

$$V = -\frac{eN_D W^2}{2\epsilon_s} + \frac{en_w L}{\epsilon_s} \quad (7.19)$$

where en_w is the charge per unit area located in the well. The charge per unit area in the depletion region is given by

$$Q = e(N_D W - n_w), \quad (7.20)$$

where W is the width of the depletion layer. The number of electrons in the well can be determined by summing over the number of electrons in the quantum well

$$n_w = 2n_{\parallel} kT \sum_i \ln \left[1 + \exp \left(\frac{E_i - E_{FW}}{kT} \right) - \frac{E_i - E_{FW}}{kT} \right], \quad (7.21)$$

where E_{FW} is the Fermi level in the quantum well (which is identical to the Fermi level in the bulk of the semiconductor in a steady state condition), and $n_{\parallel}$ is the two-dimensional density of states given by

$$n_{\parallel} = m_{\parallel}^* / 2\pi\hbar^2. \quad (7.22)$$

The energy of the energy levels E_i relative to the position of the conduction band in the neutral semiconductor can be obtained by assuming a constant charge density in the well, and integrating between Poisson's equation between W and $L + a$

$$E_i = \frac{[W - (L + a)]^2 e^2 N_D}{2\epsilon_s} + \frac{e^2 N_D}{\epsilon_s} [W - (L + a)]a - \frac{e^2}{2\epsilon_s} \left(\frac{n_w}{2a} - N_D \right) a^2 - \Delta E_C + \Delta E_i. \quad (7.23)$$

By using these relations, the capacitance of the junction with the well inside the depletion region can be found as

$$C = \epsilon \frac{1 + \alpha \frac{W - L}{a}}{W + \alpha L \frac{W - L}{a}}, \quad (7.24)$$

where

$$\alpha = \frac{2n_{\parallel} e^2 a \sum_i \frac{1}{1 + \exp[(E_i - E_{FW})/kT]}}{\epsilon - (n_{\parallel} e^2 a / 2) \sum_i \frac{1}{1 + \exp[(E_i - E_{FW})/kT]}}. \quad (7.25)$$

These equations can now be used to obtain the capacitance-voltage characteristics by means of a self-consistent approach. For a given potential V a *a priori* n_w is chosen. Then equation (7.19) is used to determine W . Now it is possible to determine E_i by using equation (7.23). By using equation (7.21), a second estimate for n_w is calculated. This is repeated until the values for n_w converge. From these values the capacitance can be obtained from equations (7.24) and (7.25). Figure 7.8 compares the CV characteristics as obtained by equation (7.24) with experimental results. The step observed at about -1 V is due to the fact that this model

is only valid for $W \geq L + a$, and ignores the space charge regions that form on the sides of the well. The step is not abrupt because of the effects of Debye screening. Despite this shortcoming, the model gives good results. When results obtained by this model were compared to simulated results, there was, according to Letatre *et al*, exact agreement between the analytical and simulated results.

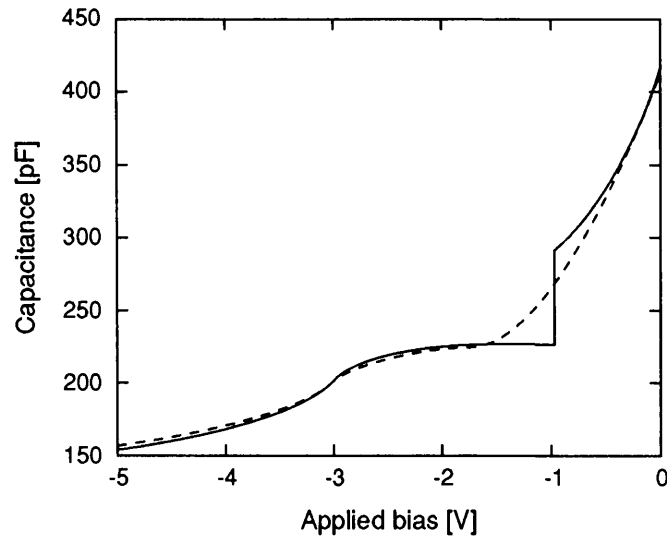


Figure 7.8: CV profile of a GaAs/Ga_{0.75}In_{0.25}As/GaAs quantum well, as measured at 230 K (dotted line), and simulated by using equation (7.24). After Letatre *et al* (1991)

Aleshkin *et al* (1991) have developed a method according to which a number of parameters of the quantum well can be determined. By using their method, the distance from surface, dopant concentration in the well, and the depth of the two-dimensional sub-band can be estimated. In their analysis, Aleshkin *et al* divide the CV characteristics in three areas. Firstly in the area $V < V_1$ the depletion region of the contact is still far away from the QW, the CV characteristics are not affected by the QW. This region is followed by a transition region where the space charge due to the contact, merges with the space charge due to the quantum well. As a result of this, the capacitance decreases rapidly. For a reverse bias between V_1 and V_2 , charges are depleted from the QW and the capacitance changes only slightly. This causes the so-called plateau, also observed by Letatre *et al*. If the reverse bias is increased further, the capacitance decreases rapidly again. For $V > V_2$, the capacitance varies according to the relation derived by Letatre *et al*, until it becomes more or less bulk-like for very high reverse bias.

The position of the QW can be estimated by calculating the capacitance at the plateau, and using the relation $x = \epsilon_s / C$.

The charge in the QW can be estimated by the size of the first step in the capacitance at V_1 ,

by making use of charge neutrality. Here it is assumed that the charge depleted from the sides of the QW is equal to the charge in the QW. Using this assumption, it can be shown that

$$\rho_0 \cong 2N_D \epsilon_s \left\{ \frac{\Delta_1}{2} - \frac{\pi \hbar^2}{m^* e^2} + \left[\frac{\Delta_1^2}{4} + \left(\frac{\pi \hbar^2}{m^* e^2} \right)^2 \right]^{1/2} \right\} \quad (7.26)$$

where $\Delta_1 = 1/C_2 - 1/C_1$, C_1 and C_2 are the capacitances before and after the first transition region. The value ρ_0 includes the effect of interface states.

The surface density of electrons in the QW can be estimated from the extent of the plateau along the voltage axis. If it is assumed that charges are depleted from the quantum well only, and the effect of Debye length averaging is ignored, it can be shown that

$$N_0 \cong \frac{\epsilon_s}{L} \Delta V \quad (7.27)$$

The energy of the first sub-band in the quantum well can be found from the size of the capacitance step at V_2 . Here it is assumed that, before the step, all the electrons are depleted from the QW, i.e. the first sub-band is just above the Fermi level. As the reverse bias is now increased, the capacitance decreases sharply until the end of the second depletion region next to the quantum well is reached. By using these two reference points, and again ignoring the effect of Debye length averaging, an expression for the sub-band energy E_0 can be found.

$$E_0 = -\frac{3}{5}\mu + \frac{e^2 \epsilon_s N_D \Delta_2^2}{8} \left[1 + \left(1 + \frac{4\pi \hbar^2}{m^* e^2 \Delta_2} \right)^{1/2} \right]^2, \quad (7.28)$$

where μ is the chemical potential and $\Delta_2 = 1/C_2 - 1/C_3$.

Using these equations, Aleshkin *et al* obtained results that correspond reasonably well with photoluminescence results and DLTS results. It should however be noted that, because of Debye length averaging, the steps in the CV profile are in many cases not abrupt. This makes it very difficult to make objective estimations of Δ_1 , Δ_2 , and ΔV . Furthermore, a large number of approximations and simplifications have been made during the derivation of these equations. For this reason, results obtained by this method should be interpreted carefully, and preferably checked by means of computer simulation. This method, however, could prove to be useful to determine initial values for a modelling program.

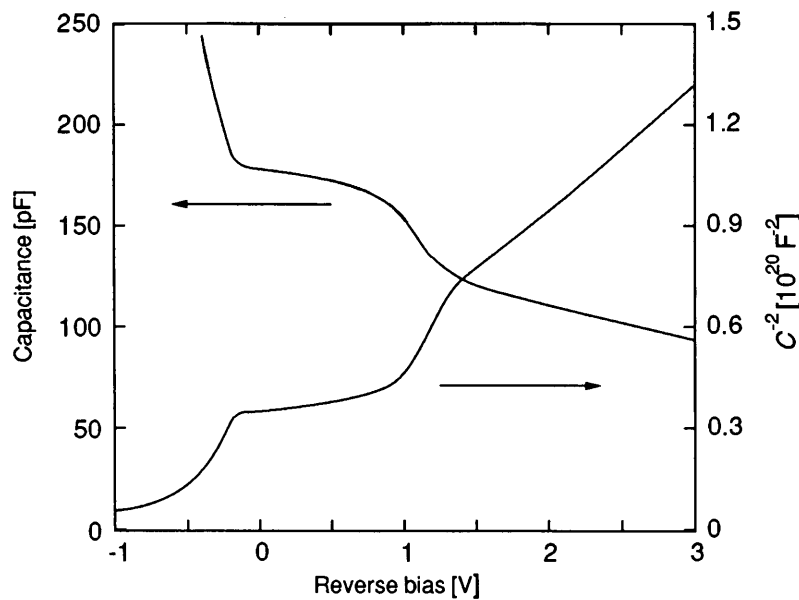


Figure 7.9: CV profile of a quantum well. After Aleshkin *et al* (1991)

7.5 δ -doped heterostructures

Recently a number of authors (Liu *et al* 1990, Shen *et al* 1991 and Notari *et al* 1991) investigated the effect of δ -doped layers in heterojunctions on conduction band discontinuities and the CV profile width. It was found that by δ -doping close to the interface, it is possible to significantly alter the effective band discontinuity at a heterojunction interface. Another phenomenon that was observed is that when a δ -doping spike is placed in a quantum well, the wave function of the electrons is much narrower than it would be in a normal semiconductor. The result is that the electrons are localized very well and that CV profiling through the structure yields an extremely narrow carrier profile with a full width at half maximum of as little as 12 Å.

7.6 CV profiles of semiconductor superlattices

Aleshkin *et al* (1991) investigated the CV profile of a semiconductor superlattice structure which resembles that of a number of quantum wells in succession. This leads to a “staircase” shaped C^{-2} vs V graph, or a depth profile with a number of spikes. See also the simulated results by Whiteaway (1983). These profiles can be analysed in a similar fashion than those for quantum well structures, though the analysis is more involved.

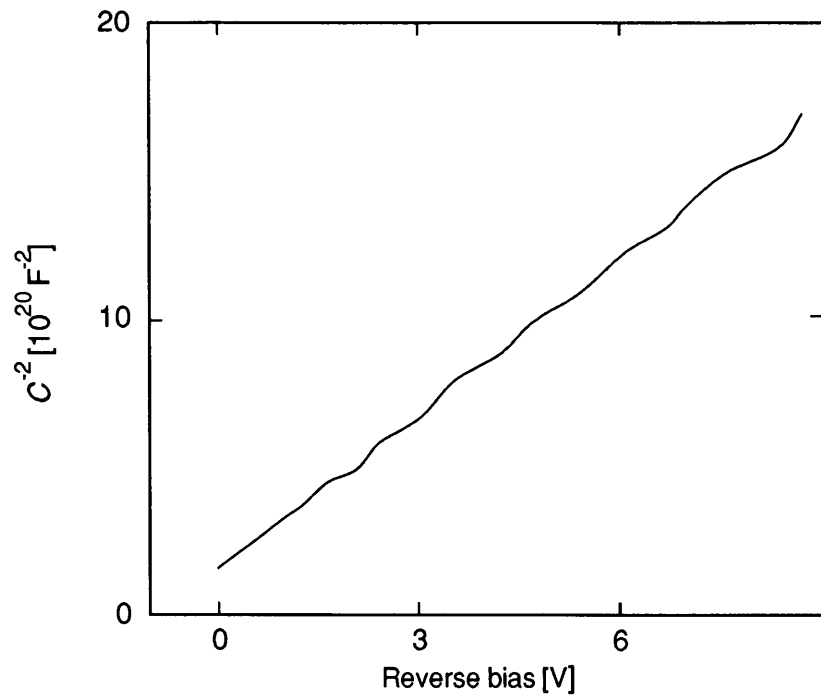


Figure 7.10: C^2 - V characteristics of a superlattice with 30-40 Å $\text{In}_{0.3}\text{Ga}_{0.7}\text{As}$ layer separated by GaAs layers, determined at 77 K. After Aleshkin et al (1991).

7.7 Computer simulation

In many cases it is impossible to obtain an analytical expression for the CV characteristics of a structure. Even when this is possible, it is often preferable to confirm the results obtained by the analytical method, by modelling the CV characteristics of the device and comparing the modelled results to the measured values.

If an analytical expression for the CV characteristics is not known, the device structure can be determined by simulating the assumed device structure, and comparing the simulated profile with the measured profile. At this stage certain parameters of the model can be adjusted until the simulated profile fits the experimental profile. It is then assumed that the modelled structure is representative of the real one. In this way it is possible to extract information from a CV profile even if the analytical CV relationship is not known.

The CV characteristics of a Schottky diode can be obtained by numerical techniques in a similar way as was used for the analytical calculation. This involves the solving of Poisson's equation for different applied voltages, and then calculating the differential capacitance per unit area of the diode by using the relation

$$C = \frac{dQ}{dV} = \epsilon_s \frac{dE}{dV}. \quad (7.29)$$

The boundary value problem can be written as

$$\frac{d^2V}{dx^2} = \frac{1}{\epsilon_s} \rho(x), \quad (7.30)$$

where

$$dV/dx = 0 \text{ as } x \rightarrow \infty, \quad (7.31)$$

and

$$V = V_0 \text{ at } x = 0. \quad (7.32)$$

Here it is assumed that the Fermi level remains flat throughout the structure, i.e. there is no current flow across the junction. In many cases the problems caused by the creation of an inversion region are ignored by not taking the valence band into account. As discussed earlier, this assumption seems reasonable in the case of a Schottky diode without an interfacial layer. It is also usually assumed that the semiconductor is semi-infinite, i.e. that it is never depleted right up to the ohmic contact. This allows the use of the boundary condition (7.31)

The charge density in the semiconductor, $\rho(x) = N_D^- + n + N_A^+ + p$, can be calculated by means of the methods given in chapter 2. This should take all charges into account, including those from interfacial layers, deep levels, and quantum confinement. In the most simple cases, where only changes in doping concentrations are considered, it is assumed that all the dopants are ionized, and that the electrons in the conduction band are distributed according to the Boltzmann distribution, as described in chapter 2,

$$n = N_C \exp\left(-\frac{E_C - E_F}{kT}\right). \quad (2.14)$$

A similar result has been obtained by Johnson *et al* (1971), by assuming the current in the reverse-biased junction to be essentially zero, so that

$$J_z = q\left(D \frac{dn}{dx} - \mu n E\right) = 0. \quad (7.33)$$

By making use of the Einstein relation $D/\mu = kT/q$, and substituting $E = -dV/dx$, it follows that

$$n = n_0 e^{-qV/kT}, \quad (7.34)$$

where n_0 is the value of $n(x)$ at the position where V is taken to be zero.

However, in cases where the Fermi level lies very close to or above the conduction band, equation 2.14 is not a good approximation. In such cases the more exact formulation of equation (2.12) should be used

$$n = N_C \frac{2}{\sqrt{\pi}} F_{1/2} \left(\frac{E_F - E_C}{kT} \right) \quad (2.12)$$

This equation involves the calculation of a Fermi-integral that, in order to be efficient, would require the use of a look-up table. An alternative to calculating the Fermi-integral numerically, is to use an approximation, as suggested by Unger (1967)

$$n \cong N_C A (1 + 0.15A) \quad (7.35)$$

where

$$A = \ln[1 + \exp\{(E_F - E_C)/kT\}]. \quad (7.36)$$

According to Whiteaway (1983), this approximation is accurate to within 1% of the Fermi-Dirac functions for values of $(E_F - E_C)/kT$ smaller than 7.5. In most cases this range should be sufficient to allow most structures to be modelled.

The concentration of ionized donors can be determined by making use of equation (2.21).

$$N_D^+ = N_D \left[1 - \frac{1}{1 + \frac{1}{g} \exp\left(\frac{E_D - E_F}{kT}\right)} \right] \quad (2.21)$$

At an interface the effects of different dielectric constants, a heterojunction band offset, and an interface charge are taken into account by using the relations $\epsilon_2 E_2 = \epsilon_1 E_1 + q\sigma_i$ and $E_{C2} = E_{C1} + \Delta E_C$.

The effect of quantum confinement can only be correctly dealt with by calculating the solutions to the eigenstates in a self-consistent way. However, in many cases the effects of Debye smearing are more important than the perturbation of the carrier distribution due to the electric field. In these cases a good approximation can be obtained by ignoring the effects of the electric field on the energy levels, and by calculating their occupation according to the Fermi-distribution.

The most simple way to solve Poisson's equation is to use an iterative technique. For every value of V_0 an initial value of E_0 is estimated. The differential equation is now solved by means of the "shooting" or "hosepipe" method, according to which the value of the electric field at the interface is guessed. The differential equation is solved numerically up to a point x_2 chosen sufficiently far away from the interface that the semiconductor is never depleted to that depth. If the boundary condition at $x = \infty$ is not satisfied, the initial value of E_0 is modified and the whole process is repeated. This process continues until either the boundary

condition is satisfied or E_0 is determined to the desired accuracy. The disadvantage of using this technique is that the computer has to repeat the shooting procedure up to forty times before a solution that satisfies the boundary conditions is obtained. Despite improvements such as the dynamic mesh concept (Iniewski et al 1992) this technique remains slow and takes about half an hour (5 min processor time) on a mainframe and several hours on a powerful microcomputer. Therefore this technique is unsuitable for inverse modelling on a desk-top computer.

7.8 A faster method for the computer simulation of CV profiles

Rimmer *et al* (1991) have developed a faster method for calculating CV profiles. By this method a *one shot* integration technique is used, instead of the iterative technique discussed above. This method is suitable if the structure can be separated into regions, each with its own shallow-dopant concentration, material composition, etc., with abrupt changes at the interfaces between the regions. These regions correspond to the epitaxial layers of the structure. The layers are numbered consecutively, from the region assumed to contain the ohmic contact, outwards towards the Schottky barrier.

According to this technique Poisson's equation can be integrated analytically to give a relationship between the field and potential at any point. A potential is chosen at the interface between regions 1 and 2, and the corresponding field is calculated. This calculation provides the initial values for *one shot* numerical integration of Poisson's equation through the remaining regions out to the surface.

The following treatment is applied to *n*-type semiconductors. For simplicity, a reduced potential U is defined as

$$U = (E_F - E_i)/kT, \quad (7.37)$$

where E_i is the position of the Fermi level if the semiconductor were intrinsic. Assuming that the electrons are distributed according to Boltzmann statistics, the carrier density in the conduction band can be written as $n = n_i e^U$, where n_i is the intrinsic carrier density of the semiconductor. In this case Poisson's equation can be written as

$$\frac{d^2 U}{dx^2} = \frac{1}{2L_d^2} (e^U - e^{U_b}) \quad (7.38)$$

where $L_d = (\epsilon_s kT / 2q^2 n_i)^{1/2}$ is the intrinsic Debye length. U_b is the flat-band value of U where $n = N_D$. This equation can now be integrated, subject to the boundary conditions that $U \rightarrow U_b$ and $dU/dx \rightarrow 0$ as $x \rightarrow \infty$

$$\left(\frac{dU}{dx}\right)^2 = \frac{1}{L_d^2} [e^U - e^{U_b} - (U - U_b) e^{U_b}] \quad (7.39)$$

This gives an analytical relationship between the electric field $E = kT \, dU/dx$ and the potential at any point, but note that the sign of the field must be determined by inspection.

The electrostatic potential in the structure is now determined by first using equation (7.39) to determine the electric field for a specific electrostatic potential at the interface furthest from the Schottky diode. Using these initial values, equation (7.38) can be integrated numerically towards the surface, to obtain the electric field and potential at the surface. This process is repeated for a slightly different electric field at the initial interface. The capacitance of the Schottky diode can now be determined from the simulated data in the usual way.

The advantage of this technique is that the only iterative process involved, is finding an initial value for the electric field at the $1/2$ interface. After this, the technique requires only a single integration over the semiconductor for each applied bias. This results in a speed increase of at least an order of magnitude.

If the semiconductor is degenerate, or the effects of a finite donor depth become important, and the Boltzmann approximation is no longer valid, this problem can be overcome, as previously, by making use of a suitable approximation for the Fermi-integral. An approximation introduced by Blakemore (1962) is

$$F_{1/2}(\eta) = e^\eta / (1 + ce^\eta) \quad (7.40)$$

where $c = 0.27$ and $\eta = (E_F - E_C)/kT$. According to Missous (1985) the value of $c = 0.22$ is more suitable, and approximates the integral to within $\pm 7\%$. Substituting this approximation into Poisson's equation yields

$$\frac{d^2U}{dx^2} = \frac{q^2}{\epsilon_s kT} \left(\frac{n_i e^U}{1 + b e^U} - \frac{N_D}{1 + G e^U} \right), \quad (7.41)$$

where

$$G = g \frac{n_i}{N_C} \exp\left(\frac{\phi d}{kT}\right), \quad b = cn_i/N_C, \quad (7.42)$$

g is the ground state degeneracy, n_i is the intrinsic carrier concentration and N_C is the effective density of states as defined in the non-degenerate case.

Equation (7.41) can be integrated analytically to give

$$\left[\left(\frac{dU}{dx} \right)^2 \right]_{x_2}^{x_1} = \frac{1}{L_d^2} \left[\frac{1}{b} \ln(1 + b e^U) + \frac{N_D}{n_i} \ln(G + e^U) \right]_{U_2}^{U_1}. \quad (7.43)$$

Equations (7.41) and (7.43) replace equations (7.38) and (7.39) in the case of degeneracy and finite donor depth. The effects of deep levels may be included in a similar fashion.

Rimmer *et al* (1991) applied this method to a number of heterostructures, and found that it agreed with their experimental results. This technique can be used successfully to model multi-layer structures on a desk-top computer within a realistic time scale. The accuracy of the method is acceptable for most purposes.

7.9 Comparison between CV profiling and SIMS.

In the previous sections the limitations of CV profiling for both classical and quantum structures have been discussed. Secondary ion mass spectroscopy (SIMS) is another well-known technique that is used regularly to analyse impurity distributions in semiconductors.

During SIMS analyses, the surface of the sample is bombarded with a beam of ions (O_2^+ , Ar^+ or Cs^+) in the 1 to 20 keV range, which cause the upper atomic layer to be sputtered off in a controlled manner. Most of the sputtered material is removed from the surface as neutral atoms or molecules, but a small fraction is ejected as charged ions. These so-called secondary ions are accelerated into a mass spectrometer, where they are separated by their mass/charge ratio. In this way an analysis of the sample may be obtained. The yield of secondary ions is however, dependent on the element to be detected as well as the matrix. This means that the instrument has to be calibrated using standard samples for each impurity species in the specific matrix.

Depth profiles are obtained by increasing the ion current density to about $100 \mu A/cm^2$ so that the surface material is removed at a significant rate (about $1 \mu m/h$). Hence atomic concentration depth profiles can be recorded. Again, however, the sputtering rate is matrix dependent, and the instrument has to be calibrated by means of standard samples, or by measuring the crater depth after analysis.

The resolution of the SIMS technique is to a large extent limited by the sputtering process. The two major factors reducing the resolution are uneven sputtering and ion mixing. Uneven sputtering is caused by small deviations in the sputtering beam. The resolution is reduced because all the ions are not sputtered from the same layer. The effect of uneven sputtering is cumulative, causing the resolution to reduce as profiling is done deeper into the sample. This effect can be reduced by sputtering an area that is much larger than the area to be analyzed. Ion mixing is caused by the sputtering ions knocking some of the surface ions deeper into the substrate, thus “mixing” the upper layers of the semiconductor. Another problem that could occur during sputtering is that the primary ions are incorporated into the matrix, thus causing the matrix to expand and reducing the yield of secondary ions (Vandervorst and Clarysse 1992). For a good discussion of the SIMS technique applied to compound semiconductors, see Grattapain and Huber (1991).

The most advanced second generation SIMS instruments are very close to achieving the

ideal specifications for layer profiling:

- 1) Probing depth from near surface (10 nm) to several microns
- 2) Depth resolution of 5 nm, lateral resolution of 1 μm
- 3) Analytical sensitivity down to 1 part in 10^9 ($4 \times 10^{13} / \text{cm}^3$) for all electrically active elements
- 4) Ability to accurately measure concentration depth profiles over a dynamic range of six orders of magnitude

However, in order to obtain these ideal specifications, the apparatus has to be set up very carefully, and even then it is not always possible to achieve all of the above specifications at the same time. Furthermore, SIMS is a very expensive technique, and requires highly skilled operators and intricate instrumentation. The required calibration makes use of expensive standard samples, which are sometimes hard to obtain. Also, since SIMS is a destructive technique, these samples can be used a limited number of times only, after which they have to be replaced.

In comparison with SIMS, *CV* profiling is an inexpensive technique, and can be performed using inexpensive apparatus which requires little, if any, calibration. Furthermore the calibration of this apparatus is independent of the elements being analysed. Since the equipment for measuring *CV* profiles is relatively simple, and well established technology is used, the measurements do not have to be performed by a highly trained operator, and the whole process can be easily automated. The main disadvantage of the *CV* technique compared to SIMS is that, as mentioned previously, the depth range and resolution of the *CV* technique may be limited in some cases.

Schubert (1991) investigated the resolution of the SIMS technique. After he determined optimum measurement conditions for SIMS, he measured the depth profiles of a number of MBE grown δ -doped epitaxial layers by means of both SIMS and *CV* depth profiling. From the SIMS depth profile he obtained peaks with a full width at half maximum of 29 Å, which were the narrowest SIMS depth profiles yet obtained. For *CV* measurements, the peak widths were 20 and 49 Å for $4 \times 10^{12} \text{ cm}^{-2}$ δ -doped *p*- and *n*-type samples, respectively. The difference in width of the C-V profiles is due to the difference in spatial extent of the electron and hole wave functions. The heavy hole wave functions are spatially more confined than electron wave functions. As explained previously, the spatial width scales with carrier mass according to $m^*-1/3$. The ratio $(m_e/m_{hh})^{-1/3}$ for GaAs is 1.9, which agrees reasonably with the experimental ratio of profile widths of 2.4. Note that according to the classical analysis, the profiles in both the *n*-type and the *p*-type material should have the same widths.

8

Experimental procedure, results and discussion

All capacitance measurements performed during this study were done on vacuum deposited Schottky contacts, fabricated on chemically cleaned semiconductor substrates. As the material was obtained from different sources, the exact growth conditions were not always known. However, the layers investigated were always grown epitaxially on n^+ substrates, so that ohmic contacts could easily be grown on the back surface, while Schottky contacts were grown on the front surface.

8.1 Sample preparation

Chemical cleaning was performed before evaporation of the ohmic, as well as the Schottky contacts. The procedures used in both cases were similar, except that cleaning before the evaporation of Schottky diodes, included etching. Myburg *et al* (1992a) describe the chemical cleaning procedure in detail. It involves degreasing in boiling trichloroethene, followed by rinsing once in iso-propanol and then twice in de-ionized water ($\rho > 10^{18} \Omega\text{cm}$). Hereafter the sample is etched, for about 30 s, in a solution of 3 parts NH_3 (15 mol dm^{-3}), 1 part H_2O_2 (30%) in 150 parts de-ionized water, at 25 °C. It was found that this solution etches at a rate of about 2 000 Å/min. If carrier density profiles close to the surface were required, etching was shortened to as low as 5 s. However, if these samples were recently grown and were clean, etching was omitted. Etching was followed by another rinse in de-ionized water, followed by oxide removal in 6 mol dm^{-3} HCl (2 min) and a final rinse in de-ionized water. The samples were dried under a stream of high purity nitrogen, and immediately transferred to the evaporator.

Ohmic contacts were formed by the deposition of Ni (50 Å), AuGe (2 000 Å) and Au (2 500 Å) on the n^+ back surfaces of the samples, before the fabrication of the Schottky contacts. The contacts were annealed at 450 °C for 2 min in a quartz tube, filled with a high purity mixture of 15% H_2 and 85% N_2 , at a pressure of 100 mbar. After the fabrication of ohmic contacts, the sample was cleaved in rectangles of about 3 by 5 mm, on which Schottky contacts were evaporated. After cleaning, the samples were transferred, by means of a fast introduction system, to the high vacuum evaporation chamber, where the pressure recovered to the 10^{-8} mbar range within a few minutes. Here the contact metals were evaporated onto the semiconductor through a mechanical mask to create contacts with a diameter of about 0.73 mm.

The Schottky contact metals that were used, were Pd, Ru (see Myburg *et al* 1993) and, for lower barrier heights on *n*-GaAs, Mg. Ru was evaporated by electron beam evaporation, while Pd, Mg and Au contacts were evaporated from alumina crucibles by resistive evaporation. A metal shield (Myburg *et al* 1992a) was used during electron beam evaporation to protect the semiconductor from damage by stray electrons emitted from the evaporator (see figure 8.1).

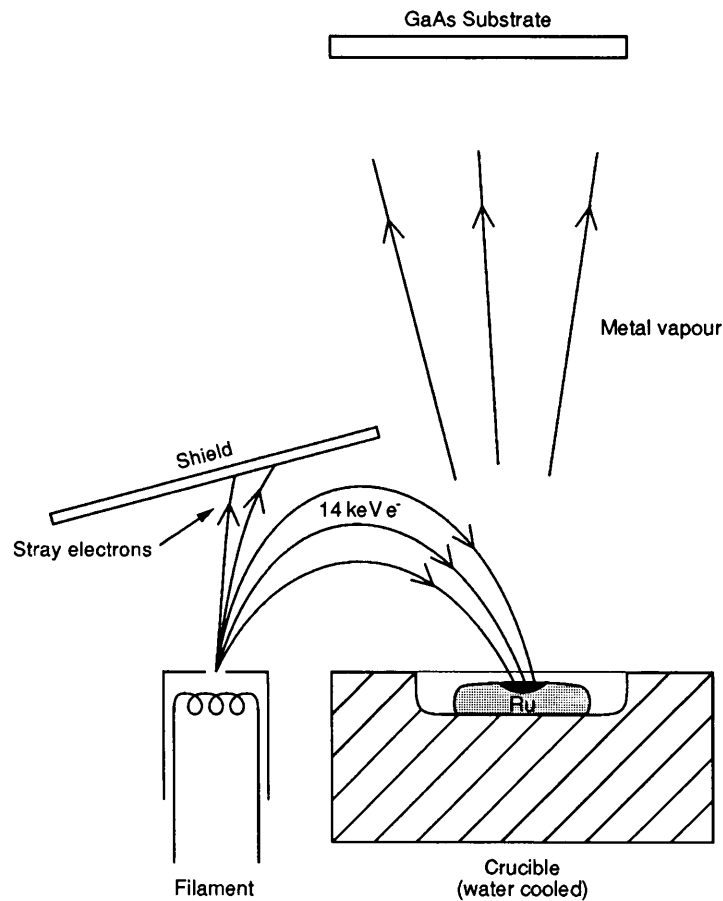


Figure 8.1: Schematic diagram of an electron beam evaporator fitted with a shield to minimize substrate damage by stray electrons.

8.2 *IV* measurements

Before any *CV* profiles were measured, the quality of the contacts was evaluated by means of *IV* measurements. The measurements were made by an HP 4148A pA meter/voltage source, capable of measuring currents as low as 10^{-14} A. The sample was screened from light and electrical noise by enclosing it in a light-tight metal box during measurements. The most important characteristics obtained from the *IV* graph were: the series resistance R_s , the barrier height $\phi_b^{(IV)}$, the ideality factor n , and the leakage current at 1 V reverse bias $I(-1)$.

Since the contacts were easily damaged when lowering the probe, and also by movement of the probe during the cooling process, IV measurements were performed after the samples had been mounted in the cryostat. Damage caused in this way often resulted in an increase by more than an order of magnitude in the reverse leakage current, rendering the CV measurements less accurate.

A typical IV curve, obtained from the OMVPE spike-doped sample, is shown in figure 8.2. For most samples series resistance was less than $10\ \Omega$ and the leakage current at 1 V reverse bias was less than 10^{-9} A. The ideality factor was always less than 1.1. The only exception that did not conform to the previous specifications, was the δ -doped quantum well sample, discussed in section 8.7. This sample was grown by means of MBE and had indium contacts that degenerated due to diffusion of the indium into the semiconductor. Attempts were made to remove the old contacts and evaporate new contacts onto the sample, but these contacts were only marginally better. The IV characteristics of the In contacts are shown in figure 8.3.

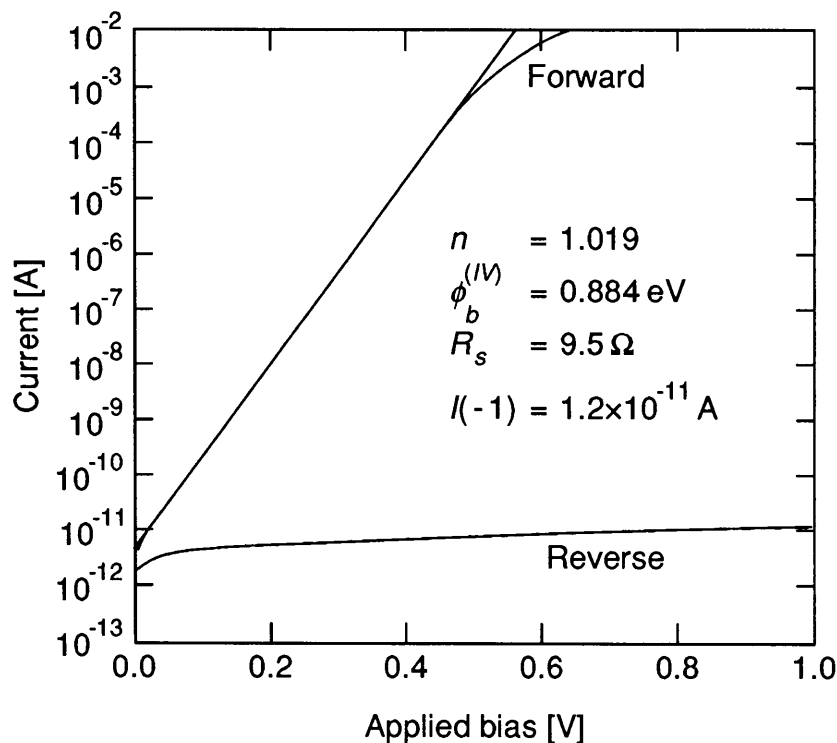


Figure 8.2: A typical IV graph obtained during this study. This graph was obtained from a contact on the Si spike-doped sample, described in section 8.6.

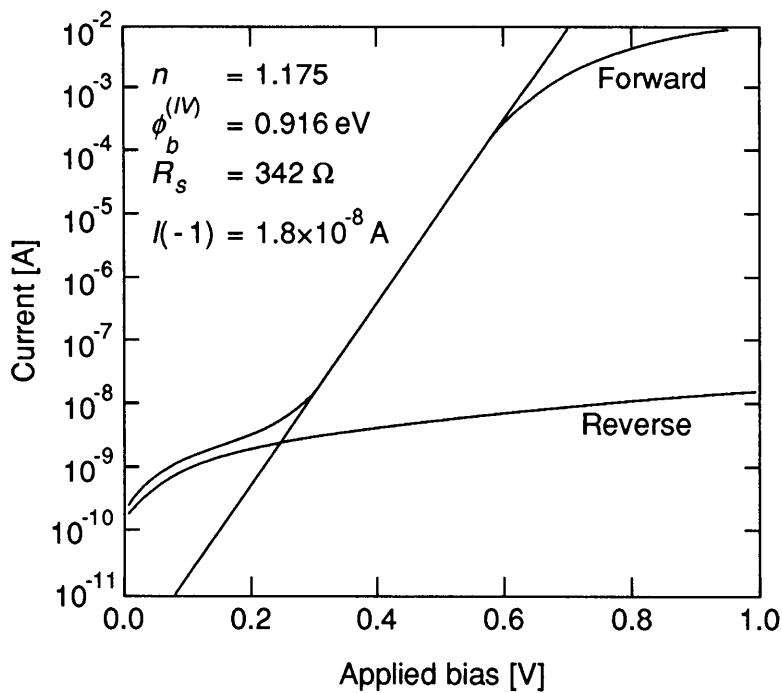


Figure 8.3: *IV characteristics of the In contacts on the δ -doped quantum well sample. Note the large series resistance and the high leakage current (probably due to recombination).*

8.3 CV measurements

The CV data was measured by an HP 4192A Impedance Analyzer, controlled by a computer via an IEEE interface. For room temperature measurements the samples were mounted on a vacuum chuck, which at the same time served as the “low” contact terminal. The Schottky contacts were probed from above. The wiring from the measurement terminals of the Impedance Analyzer was as specified in the users manual (Hewlett-Packard 1986). To minimize interference from light and electronic noise, the measurements were performed using four-wire, floating-ground techniques, and the sample was kept in a light-tight, earthed metal enclosure.

Except where noted otherwise, the measurements were made at an oscillator level of 5 mV, and a test frequency of 1 MHz, while the capacitance meter was set to its “parallel conductance” and “average” settings. The capacitance meter was calibrated to “open circuit” before measurements, and a warm-up time of 30 min was allowed after switch-on.

Problems due to the HP 4192A Impedance Analyzer

While doing the measurements, a number of problems due to the Impedance Analyzer were discovered. The first problem regards the number of significant digits that were displayed and returned to the computer. As described earlier in section 6.2, the amount of noise on a CV profile is to a large extent determined by the number of digits returned by the capacitance meter. The standard HP 4192A Impedance Analyzer displays only a limited number of

significant digits. The number of digits displayed is determined by the absolute accuracy of the instrument. However, in many cases the repeatability of the instrument is much higher. For *CV* measurements the repeatability and resolution of the capacitance measurement is more important than the absolute accuracy. Therefore an increase in the number of significant digits displayed by the capacitance meter, would decrease the amount of noise in the depth profile. The number of significant digits displayed was increased by performing the modification described in the users manual (Hewlett-Packard 1986) p.3-86, allowing the capacitance meter to display the maximum number of significant figures, regardless of the current measurement accuracy. In spite of this modification, there was one situation in which the capacitance meter did not display the full number of significant digits. Sometimes when the scale was changed to a more sensitive range, the Impedance Analyzer continued to display the same significant figures as in the less sensitive range (i.e. the resolution did not change). This problem can be solved by first selecting a more sensitive scale than desired, before selecting the desired scale. In this study, however, the problem was avoided by starting the *CV* measurements at the largest reverse bias, where the sample had the lowest capacitance. Since the capacitance increased monotonically with decreasing reverse bias, the ranges were selected in order of decreasing sensitivity.

The second problem was that the DC source of the capacitance meter had a very high impedance, especially on the low capacitance ranges. In the 2 and 20 pF ranges it was as high as 20 k Ω . Consequently, the voltage supplied by the internal voltage regulator of the HP 4192A was not applied directly to the sample and a significant voltage drop occurred across the internal circuits of the HP 4192A. Although the DAC (digital to analogue converter) and the associated voltage regulator are very accurate (± 2 mV in our case), there is no feedback mechanism allowing it to compensate for a voltage drop in the rest of the DC biasing circuit. Consequently, as the forward bias is increased, the size of the voltage steps across the sample decrease, and the measured carrier profile curves upwards close to the interface (see figure 8.5). Because the impedance of the internal DC bias source depends on the measurement scale, scale changes caused large “jumps” in the applied bias. The problem was corrected by measuring the voltage applied to the diode with an HP 34401A Multimeter. Any effect the multimeter could have, was minimized by placing a 10 M Ω high-voltage (low capacitance) resistor in series with each measuring lead. These resistors did not influence the multimeter, since, on the low voltage ranges, the multimeter has an input impedance higher than 10 G Ω . The effect of electrical noise pick-up and the test oscillator was minimized by setting the multimeter to average over 2 s (100 power line cycles). Since the random error in the voltage reading was small, one voltage reading only was taken for each bias step. The effect of scale changes was reduced by monitoring the voltage step during the scale change. If the voltage step after a scale change was larger than 1.5 times the set value, the applied bias was reduced to eliminate the discontinuity.

Measurement procedure

To improve the repeatability of the measurements, the sample was kept under reverse bias, until the capacitance reading remained stable. This procedure took approximately one minute. Hereafter the *CV* characteristics of the sample were measured, starting at the maximum reverse bias. After setting the bias, the first capacitance reading was ignored, thus

allowing the biasing and measuring circuits to settle. Subsequently ten capacitance measurements were taken at the applied bias, and the average was calculated. Theoretically, this procedure reduces the random measurement error by a factor three. Usually this reduction is sufficient to reduce the measurement error to the same size as the rounding error.

Low temperature CV measurements

For low temperature measurements the sample was mounted in an Air Products APD HC-2 cryostat, on a special sample holder that isolated the sample electrically, but ensured excellent thermal contact with the tip of the cold finger. Myburg *et al* (1992b) describe the construction and performance of this sample holder (illustrated in figure 8.4). Contact to the back ohmic contact was established by putting the sample on a piece of indium foil. Both the Schottky contact and the indium foil were connected to the measurement circuit by beryllium copper probes. To minimize damage to the Schottky contact, the tips of the probes were rounded by sanding with very fine sanding paper. Also, care was taken not to scratch the contact when lowering the probe. To ensure that the ohmic contact made good electrical and thermal contact with the indium foil, an additional probe was used, when necessary, to apply pressure to the sample next to the Schottky contact.

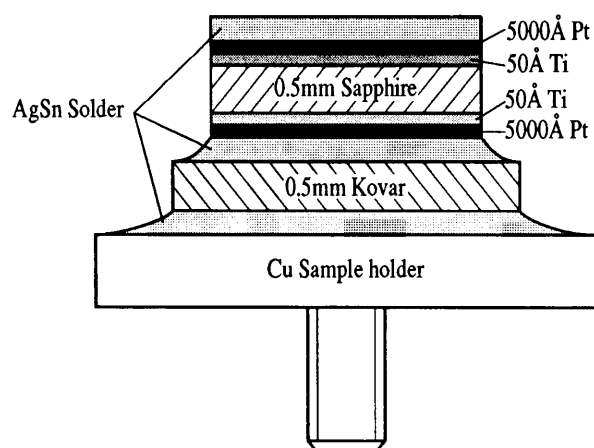


Figure 8.4: Schematic diagram of the sample holder that was used during low temperature measurements.

Calculation of carrier density depth profiles

In most cases the capacitance measurements were made at 0.01 V intervals. This was the smallest amount by which the internal bias of the HP 4192A could be increased. The small spacing of the measurements made it possible to choose the differentiation steps independently, after the measurement. The data was analysed according to the method described by McGillivray (1988). The value of ΔC was chosen to optimize the results for minimum noise and maximum resolution. The material parameters given in chapter 3 were used in all calculations.

8.4 General experiments to evaluate the measurement setup

The measurement setup was evaluated by performing several measurements on homogeneously doped samples. First, the size of the random error in the measurements made by the Impedance Analyzer was determined by measuring the capacitance of a sample at a fixed bias. The standard deviation of these measurements was obtained as an estimation of the random error in the capacitance measurement. All the measurements were performed using the standard measurement parameters as described in section 8.2. The results are shown in table 8.1. Only samples with a dissipation factor of less than 0.01 at the stated conditions were used, since damaged samples could cause the random error to increase up to tenfold. The discrepancy between ranges was found to be about the same as the random error of the less sensitive range.

Range	Resolution		Random error	Absolute error ²
	standard	modified ¹		
2 pF	1 fF	0.1 fF	± 1.0 fF	40 fF
20 pF	10 fF	1 fF	± 1.3 fF	200 fF
200 pF	100 fF	10 fF	± 11 fF	2 pF
2 nF	1 pF	100 fF	± 30 fF ³	20 pF

¹The modification referred to is described in section 8.3.

²The absolute error was calculated according to the manual, assuming an oscillator level of 5 mV. In the case of a 50 mV oscillator level, the absolute error decreases fourfold.

³On the 2 nF and higher ranges, the displayed value did not show any random changes. In these cases the random error was calculated by assuming that the error is distributed according to a uniform distribution, ± 0.5 times the resolution.

Table 8.1: Absolute and random errors in the capacitance measurements for different measurement ranges.

The results (table 8.1) show that on most ranges the random error is much smaller than both the absolute error and the number of digits displayed by the unmodified instrument. Thus, by increasing the number of displayed digits, the amount of noise in the CV profile is reduced, as described in section 6.2. According to the calculations of McGillivray, this modification should reduce the amount of noise tenfold.

The effectiveness of the technique of McGillivray was determined by producing a number of depth profiles from the same set of CV data, but using different capacitance intervals for differentiation. The amount of noise was estimated by calculating the standard deviation of the points over a small region. These results, along with those predicted by McGillivray are shown in table 8.2. Clearly the amount of noise in the CV depth profile is correctly predicted by the method of McGillivray. The change in the depletion region depth Δx , which corresponds to the increase in capacitance, is also shown. This value can be used as an estimate of the reduction in resolution due to the size of the differentiation steps. Since the

Debye length in 10^{17} cm^{-3} material is about 14 nm at 300 K, averaging, due to the size of the capacitance step, is negligible in all the cases considered in table 8.2. However, if the sample were cooled to 10 K, the Debye length would be reduced by a factor of 5 to about 2.5 nm. In this case a careful compromise between noise and resolution should be found. Note that the capacitance is inversely proportional to the width of the depletion region, hence, for a fixed ΔC , the value of Δx will depend on the depletion region depth.

ΔC	Δx	$\Delta N_D/N_D$ (predicted)	$\Delta N_D/N_D$ (measured)
0.05 pF	0.1 nm	13.9%	8.7%
0.1 pF	0.3 nm	7.0%	4.4%
0.2 pF	0.6 nm	3.5%	2.2%
0.5 pF	1.3 nm	1.4%	1.0%

Table 8.2: Amount of noise in CV profiles for different capacitance steps, as obtained for a $1 \times 10^{17} \text{ cm}^{-3}$ doped sample. The capacitance of the sample was measured on the 200 pF range, and the average of ten measurements were taken, thus reducing the random error to a third of its normal value. Also shown is the increase in the depletion region width Δx which corresponds to ΔC when the depletion region capacitance is approximately 120 pF.

The effect of the high impedance of the DC voltage source of the HP 4192A Impedance Analyzer is shown in figure 8.5. The “bending” of the carrier density graph close to the interface can be seen (solid line). The discontinuity in the graph is due to a scale change. The change in the impedance of the DC voltage source during a scale change causes a change in the applied voltage. Also shown is the “corrected” profile (dotted line), where the HP 34401A Multimeter was used to measure the applied bias. Since the applied bias is now measured directly across the sample, the scale change does not cause a discontinuity in the measured carrier concentration profile. The slight bending in this graph is due to the series resistance of the sample becoming significant as the conduction across the barrier increases as the forward bias increases.

The values obtained for the dissipation factor, D , at a number of bias voltages is shown in table 8.3. For voltages smaller than 0.10 V, D remains smaller than 0.02, which is an indication of the excellent quality of the Schottky diodes. In the region 0.10 to 0.25 V, the dissipation factor increases to 0.1. Here the capacitance readings are still fairly accurate. In the region 0.25 to 0.30 V, D increases to 0.5, which means that some of the accuracy is lost (both the absolute and random errors increase by a factor two), but the readings are still usable. However, at 0.32 V applied bias, the dissipation factor suddenly increases to 1.0, clearly indicating that the capacitive component of the impedance of the sample is no longer dominant.

By comparing the graph in figure 8.5 to the dissipation factor values in table 8.3, it is evident that when using a multimeter to monitor the applied voltage, the capacitance meter readings are usable for $D < 0.5$.

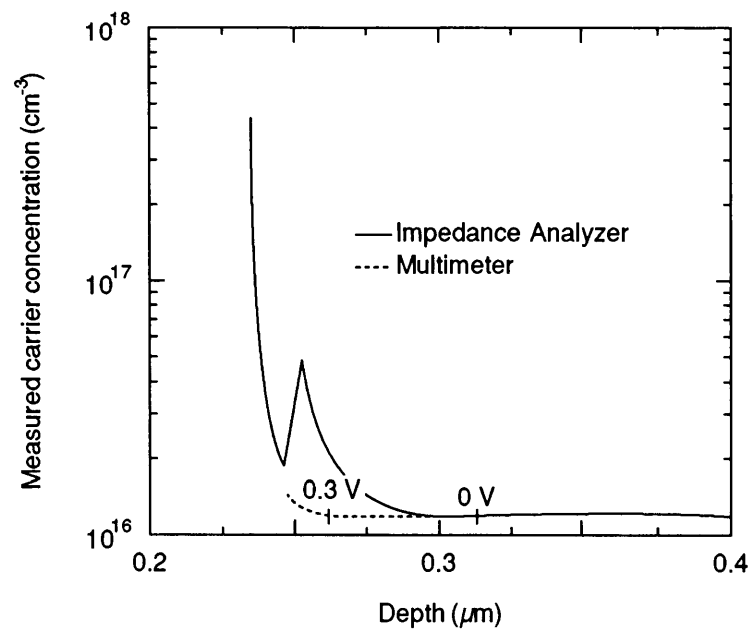


Figure 8.5: CV profiles of a homogeneously doped sample, measured with (dotted line) and without (solid line) the use of a multimeter to measure the applied bias. The applied bias is also indicated.

Applied bias [V]	Dissipation factor (D)
< 0.00	< 0.01
0.10	0.02
0.25	0.10
0.30	0.50
0.32	> 1.00

Table 8.3: Measured dissipation factors at different applied bias, obtained from the same sample as was measured for figure 8.5.

8.5 Measurement of an OMVPE GaAs-AlGaAs heterojunction

The GaAs-Al_{0.3}Ga_{0.7}As heterojunction was grown by the Department of Physics, UPE, by means of OMVPE. CV profiles of this structure were measured, and the heterojunction parameters were calculated according to the method of Kroemer *et al* (1984) (see section 7.1). These results were used to calculate a simulated CV depth profile that was compared to the measured profile. The heterojunction parameters were then varied slightly to obtain an optimum fit.

According to the method of Kroemer, the conduction band offset was $\Delta E_C = 0.28 \pm 0.03$ eV, while the interfacial charge was calculated as $\sigma_i = 1.6 \pm 0.7 \times 10^{11} \text{ cm}^{-2}$. After comparing the simulated CV profile with the measured CV profile, a conduction band offset of 0.27 ± 0.01 eV seemed to provide a better fit. Small variations in the interface charge did not seem to improve the fit significantly. These results are compared by those obtained by Kroemer *et al* (1981) and Okomura *et al* (1985) in table 8.4. The standard deviations indicated here, take into account the inaccuracies when determining the position of the heterojunction and determining the carrier densities. Grading in the doping profile at the interface, is not taken into account.

	Interface charge σ_i	Conduction band offset ΔE_C
This study (Kroemer's technique)	$1.6 \pm 0.7 \times 10^{11} \text{ cm}^{-2}$	$0.28 \pm 0.03 \text{ eV}$
This study (computer simulation)	—	$0.27 \pm 0.01 \text{ eV}$
Kroemer <i>et al</i> (1981)	$2.74 \times 10^{10} \text{ cm}^{-2}$	0.248 eV
Okumura <i>et al</i> (1985)	$< 1 \times 10^{10} \text{ cm}^{-2}$	$0.25 \pm 0.01 \text{ eV}$

Table 8.4: Comparison between the results obtained in this study and those obtained by Kroemer *et al* (1981).

When comparing the results in table 8.4, it should be kept in mind that in this study, the molar fraction of the AlGaAs was not determined accurately. Furthermore, the high interface charge could also influence the accuracy of the of the determined conduction band offset (see chapter 7).

Both the measured and the optimum simulated depth profiles are shown in figure 8.6. The correspondence between the simulated and the measured CV depth profiles indicate that the results obtained by the method of Kroemer are consistent with the measured carrier profile. Figure 8.7 shows the effect of a small increase in ΔE_C in the conduction band offset, on the carrier density profile.

The measured and simulated CV profiles of another heterojunction grown under different conditions are shown in figure 8.8. Here the fit is not as good as in the previous case. The discrepancies are most likely due to grading effects. For this heterojunction the conduction band discontinuity was $0.22 \pm 0.3 \text{ eV}$, while the interfacial charge was $1.8 \pm 0.7 \times 10^{10} \text{ cm}^{-2}$.

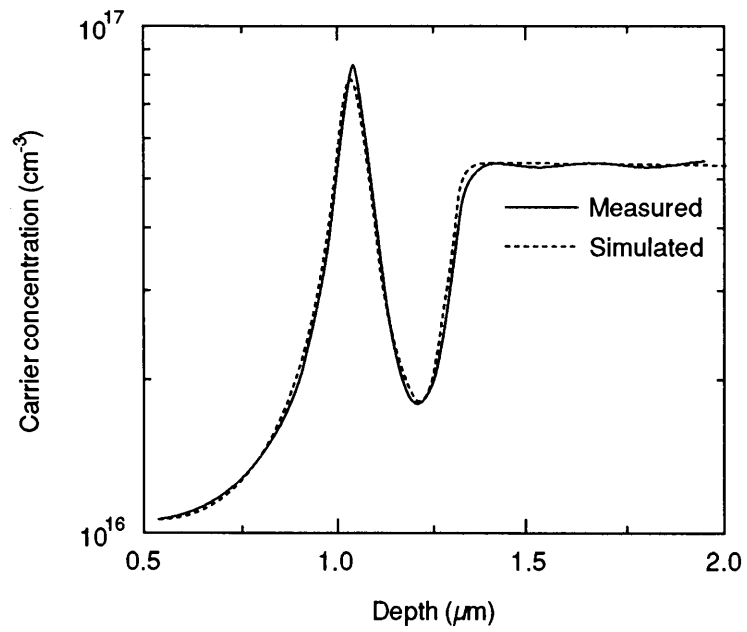


Figure 8.6: Measured (solid line) and simulated (dashed line) CV profile of a GaAs- $Al_{0.3}Ga_{0.7}As$ heterojunction.

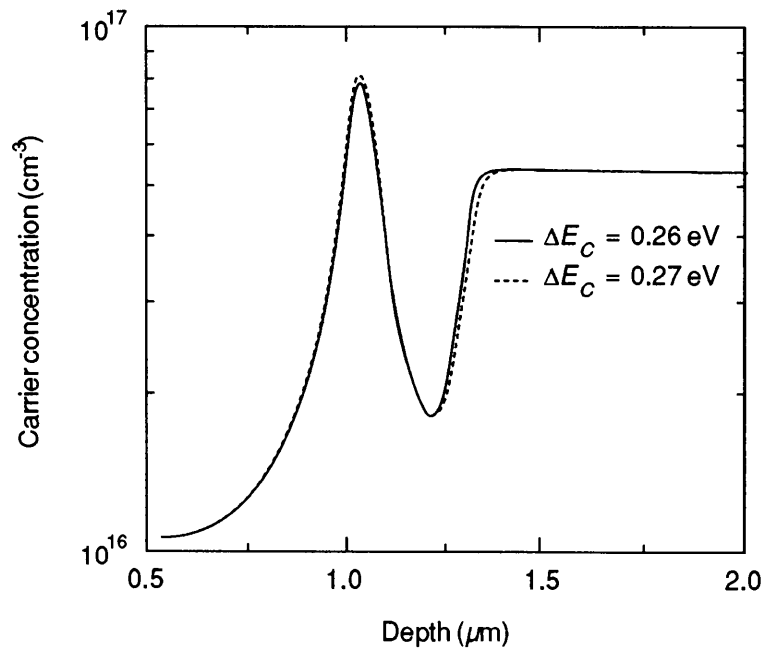


Figure 8.7: Simulated profiles of heterojunctions with conduction band offsets of 0.26 eV (solid line) and 0.27 eV (dotted line).

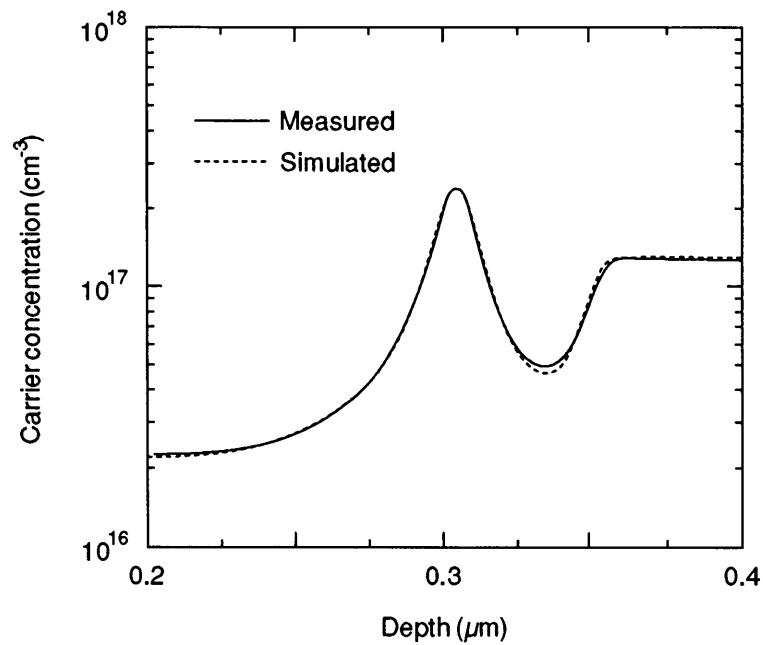


Figure 8.8: Measured (solid line) and simulated (dashed line) CV profiles of a GaAs- $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$ heterojunction.

The low-temperature CV characteristics of a heterojunction were also measured (see figure 8.9). Because of the large number of defects in AlGaAs, the Fermi level moves to the middle of the band gap at low temperatures. This causes the size of the depletion region in

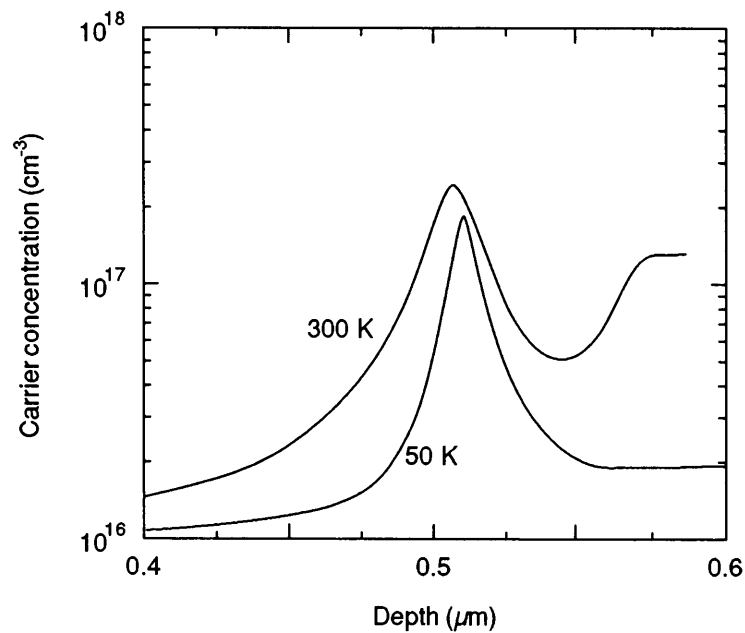


Figure 8.9: Measured CV profiles of a heterojunction at 50 K and 300 K.

the AlGaAs to decrease. Thus, at low temperatures the “trough” becomes smaller or even disappears. Because the position of the Fermi level is no longer given by equation 2.21, the method of Kroemer can no longer be used. The room temperature and low temperature *CV* profiles of a heterojunction are shown in figure 8.9.

In this section it has been shown that, when applied carefully, the method of Kroemer gives reasonably accurate results for the heterojunction band offset and interfacial charge. When a simulated *CV* profile of the assumed structure is calculated, the correspondence between the simulated and the measured profile is quite good. However, in most cases the fit can be improved even further by varying the parameters slightly. The values obtained in this study for the conduction band offset corresponded well with those obtained by other authors using the same technique. Although the measured interface charge was higher than found by other authors it was still within acceptable limits.

8.6 OMVPE Spike-doped GaAs sample

A Si spike-doped sample was grown by Mikomtek in an OMVPE reactor at the CSIR. The sample was designed to have six $5 \times 10^{17} \text{ cm}^{-3}$ doping spikes, ranging from 50 Å to 200 Å (see figure 8.10). The sample served as a test structure for the hot electron injector of a millimetre wave Gunn diode. The room temperature as well as the low temperature (12 K) CV characteristics of the sample were measured and compared to simulated CV profiles. The sample was also analysed by SIMS. The peak widths and the dopant concentrations as measured by the two techniques were compared.

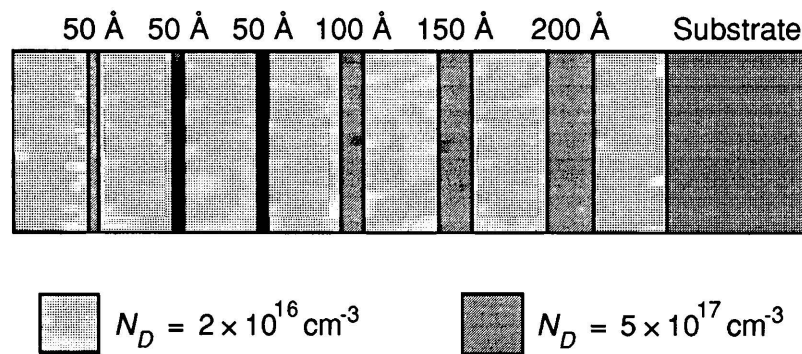


Figure 8.10: Structure of the Si spike-doped sample

Growth

The Si spike-doped GaAs sample was grown by Mikomtek in a low pressure, horizontal III-V OMVPE reactor at the CSIR. The layers were grown on a 10^{18} cm^{-3} Si-doped GaAs substrate oriented (100), 2° off towards $\langle 110 \rangle$. The sources were trimethylgallium, trimethylaluminium, arsine and silane, in a hydrogen ambient. The growth temperature was 700°C (which varied about 50°C across the 2 inch wafer) and the growth pressure was 100 mbar, while the group V to group III reagent molar ratio was 150. The growth rate was $2.0 \mu\text{m/h}$.

Doping increases significantly at higher temperatures, hence doping on the 2 inch wafer varied significantly. To minimize the effect of doping variations, the samples used in this experiment were taken from the central region of the wafer.

To minimize sputtering time during SIMS analysis, only a thin capping layer (500 Å) was grown on top of the structure. After growth, the wafer was cleaved in two, and one half was returned to the reactor, where a 10^{16} cm^{-3} Si-doped capping layer of $0.5 \mu\text{m}$ was grown on top of the structure. This made it possible to profile the structure right up to the original "surface".

SIMS analysis

The SIMS analysis was done by Loughborough Consultants, UK, on a Cameca IMS4F. Cs^+ and O_2^+ primary ion bombardment was used. The Cs^+ beam increases the sensitivity to Si, and allows the Si to be determined in concentrations as low as 10^{16} cm^{-3} . The Cs^+ ion beam was accelerated through 15 kV. A depth profile was also measured using a 10 kV O_2^+ ion beam, which allows for higher resolution in the Si profile. According to Loughborough Consultants, the Si doping level was quantified to an accuracy of $\pm 10\%$, and the depth scale to an accuracy of $\pm 4\%$. The beam was rastered over an area of $250 \times 250 \mu\text{m}^2$, while ions were collected from a circle of $60 \mu\text{m}$ diameter in the middle of the sputtered area.

The SIMS profile, measured using a 15 kV Cs^+ primary ion beam, is shown in figure 8.11. Due to the high energy of the ions, the peak broadening due to ion beam mixing is more pronounced in the Cs^+ profile than in the lower energy O_2^+ SIMS profile (see figure 8.12). Although the broadening of the peaks can partially be ascribed to ion beam mixing, most of the broadening in the O_2^+ profile is probably sample related. Due to this broadening, it is difficult to quantify the peak widths. However, the area under each peak can be used as an indication of the sheet doping density in each peak (see table 8.5). According to the SIMS profiles, the background doping density was $2 \times 10^{16} \text{ cm}^{-3}$ which agreed with the designed value. However, the designed peak doping density of $5 \times 10^{17} \text{ cm}^{-3}$ was not attained.

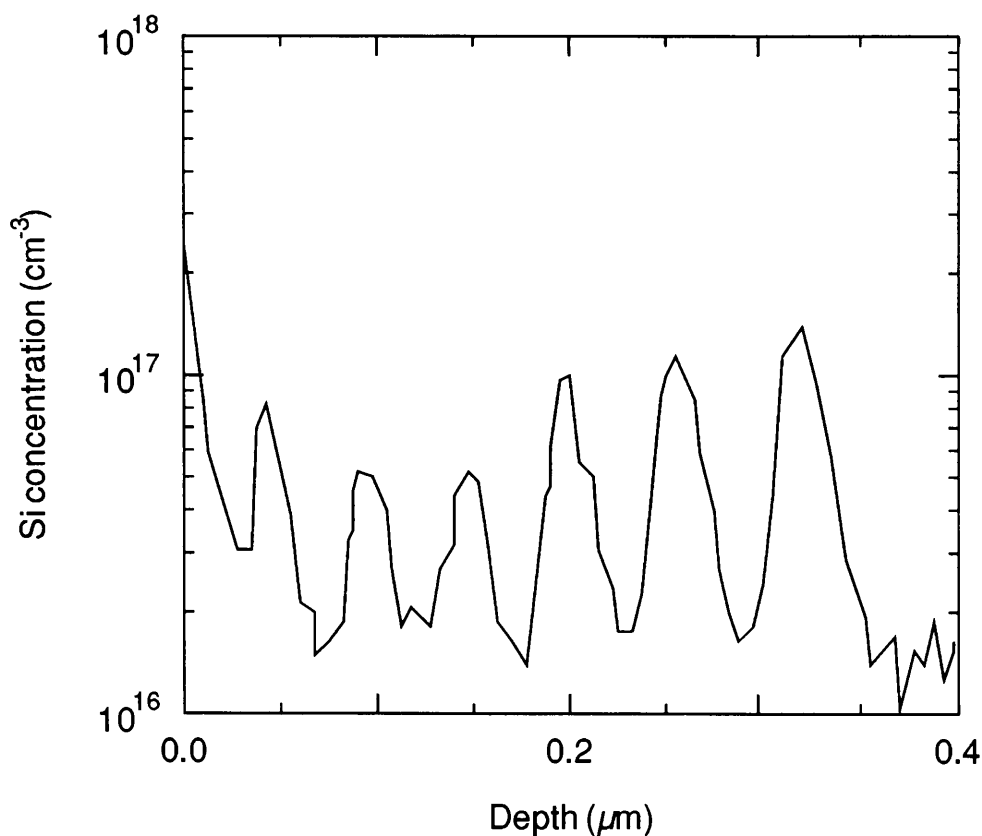


Figure 8.11: Cs^+ SIMS profile of the Si spike-doped sample.

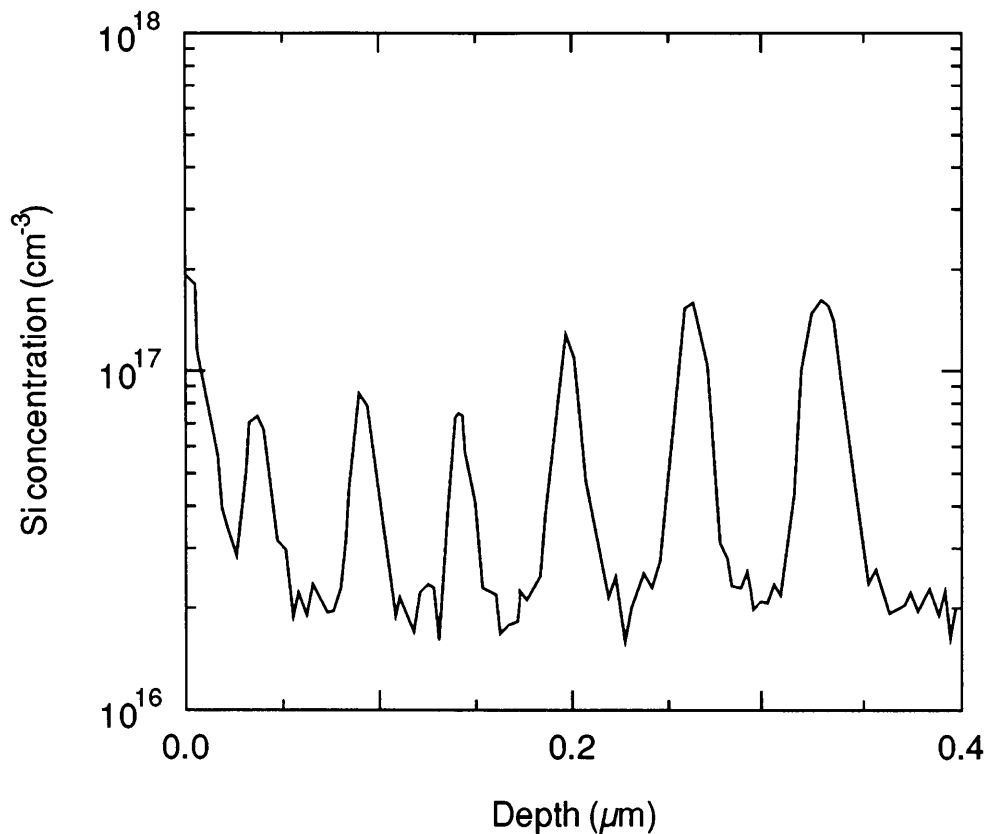


Figure 8.12: O_2^+ SIMS profile of the Si spike-doped sample.

CV analysis

For the purpose of CV analysis, ohmic and Pd Schottky contacts were deposited as described in section 8.1. Both samples, with and without the capping layer, were analysed. However, in order to measure as close to the surface as possible, the sample without the capping layer was not etched during cleaning. As the sample was recently grown and still clean, this was not expected to influence the *IV* and *CV* characteristics seriously. Room temperature *CV* measurements were performed at 300 K, using the standard measurement setup, while the low temperature *CV* measurements were performed at 12 K in a cryostat, using the setup as described in section 8.3. The room temperature as well as the low temperature *CV* characteristics of the uncapped sample are shown in figure 8.13. The resolution of the *CV* technique is increased significantly when the sample is measured at low temperatures (see section 6.4). In Si doped GaAs, low temperature measurements are possible, since the Si donor level lies close to the conduction band, causing freeze-out to occur at very low temperatures only.

In figure 8.14 the 12 K *CV* depth profile of the spike-doped sample is compared to a simulated depth profile. The simulated depth profile was calculated by a simulation program (see section 8.8). The peaks in the measured profile are significantly broader than those in

the simulated profile, indicating that the interfaces were not abrupt, and that significant grading had occurred during growth.

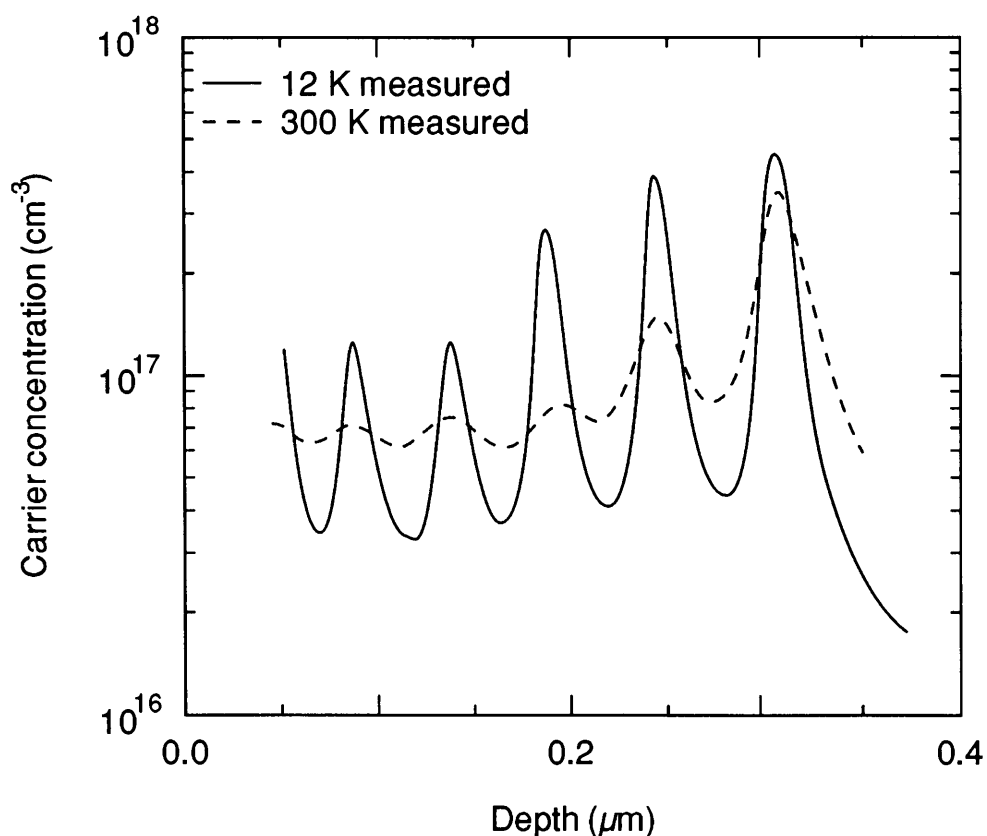


Figure 8.13: CV depth profile of the uncapped Si spike-doped sample measured at 300 and 12 K. Due to forward conduction, the first peak is obscured.

The CV profile of the structure with the extra capping layer is shown in figure 8.15. The addition of the extra capping layer enabled the first peak to be visible, but the last peak is now obscured due to reverse breakdown of the Schottky diode.

As with the SIMS analysis, the broadening of the peaks make it difficult to quantify their width. In CV profiles, broadening due to Debye length averaging depends strongly on the carrier concentration. Accordingly, the broadening is much less at the top than at the base of the peak. Due to this broadening at the base, the background doping density between the peaks can not be determined from the carrier profile. However, the carrier concentration in the region after the last peak can be used as an indication of the background carrier concentration. The background doping density was measured as approximately $1.7 \times 10^{16} \text{ cm}^{-3}$, which is similar to the SIMS results.

The CV peak doping densities range from 1 to $5 \times 10^{17} \text{ cm}^{-3}$, and are much higher than those of the SIMS profile, and closer to the designed value of $5 \times 10^{17} \text{ cm}^{-3}$. The variation in peak

height is also much larger than in the case of the SIMS profile. Since the variation in peak height in the measured CV profile is much less than in the simulated CV profile, this variation can be ascribed to broadening of the peaks during growth. The reason for the approximately constant peak heights in the SIMS profile is not known.

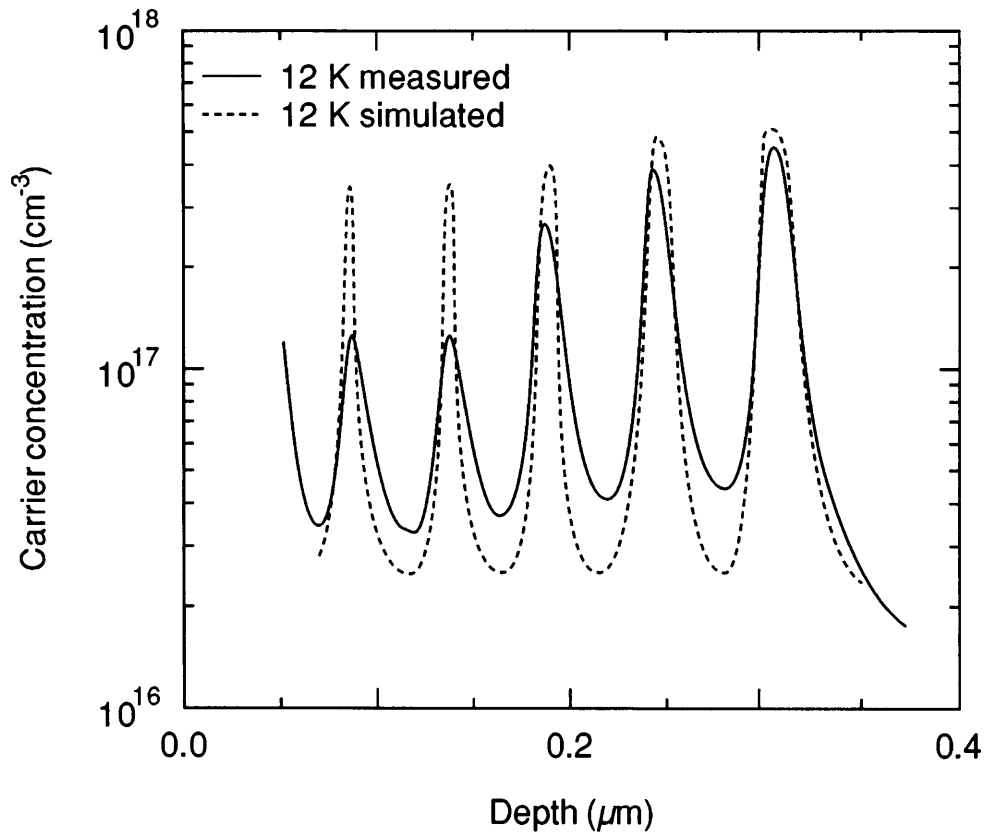


Figure 8.14: Simulated and measured CV depth profiles of the uncapped Si spike-doped sample at 12 K.

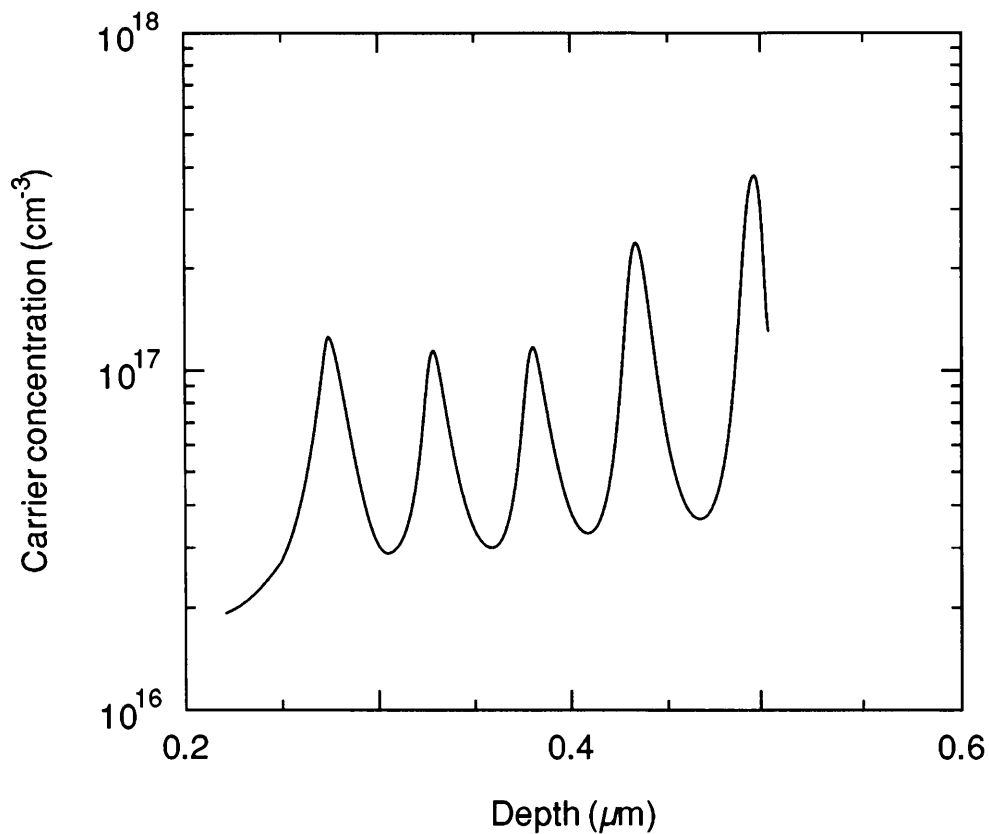


Figure 8.15: CV depth profile of the capped Si spike-doped sample measured at 12 K. Due to reverse breakdown of the Schottky diode, the last peak is obscured.

Comparison between CV and SIMS results

A comparison between the CV and the SIMS results is given in tables 8.5 and 8.6. Since the number of carriers is conserved during the Debye averaging process, the peak areas, as calculated from the CV depth profiles, are assumed to be more accurate than the SIMS results. These results indicate that the carrier concentration in the peaks was constantly underestimated by the SIMS measurements. This can probably be ascribed to lack of proper calibration of the instrument.

The separation between the layers as calculated by CV and SIMS is shown in table 8.6. Although the layer thickness measured by CV is consistently lower than that measured by SIMS, the values are in good agreement.

Parameter	Peak number			
	1-3 (average)	4	5	6
Designed:				
Sheet carrier concentration (10^{11} cm^{-2})	2.5	5.0	7.5	10.0
Ratio (normalised: peak 1 = 1)	1.00	2.00	3.00	4.00
Width ($\text{\AA}$)	50	100	150	200
CV (Simulated):				
Sheet carrier concentration (10^{11} cm^{-2})	2.50	5.01	7.48	10.0
Ratio (normalised: peak 1 = 1)	1.00	2.00	3.00	4.00
CV (Measured):				
Sheet carrier concentration (10^{11} cm^{-2})	1.90	4.05	5.86	7.75
Ratio (normalised: peak 1 = 1)	1.00	2.13	3.08	4.08
O₂⁺ SIMS:				
Sheet carrier concentration (10^{11} cm^{-2})	0.73	1.47	2.2	3.0
Ratio (normalised: peak 1 = 1)	1	2.0	3.0	4.1

Table 8.5: Comparison between the areas under the peak as measured by CV and SIMS. The peaks are numbered from the front surface of the semiconductor.

Peak numbers	Layer separation in $\text{\AA}$		
	Designed	O ₂ ⁺ SIMS	CV
2 to 3	550	510	549
3 to 4	575	550	520
4 to 5	625	600	550
5 to 6	675	640	610

Table 8.6: Comparison between the distance between peaks as measured by CV and SIMS. As previously the peaks are numbered from the front surface of the semiconductor.

8.7 Delta-doped quantum well structures

The delta doped quantum well structure consists of a strained InGaAs layer, sandwiched between two GaAs layers. The layers were undoped except for a Si δ -doping spike in the middle of the quantum well. The structures were grown by Prof D G Liu at the Institute of Electronics of the National Chiao Tung University, Taiwan, and described in the paper Liu *et al* (1990). They were grown on (001) GaAs substrates in a Varian GEN II MBE system. The growth temperature was 580 °C for the GaAs layers, and 480 °C for the InGaAs layer. The structures consisted of a 6 000 Å buffer layer of GaAs, as 20 Å InGaAs layer, and finally a second GaAs layer of 450 Å. The samples were analysed using CV measurements.

The CV depth profile is shown in figure 8.16. The quantum well confines the electron wave function of the δ -doped layer to a very narrow region, producing a very sharp profile, with a full width at half maximum (FWHM) of only 14 Å. Using similar samples, Liu *et al* (1990) have obtained FWHM peak widths as low as 12 Å.

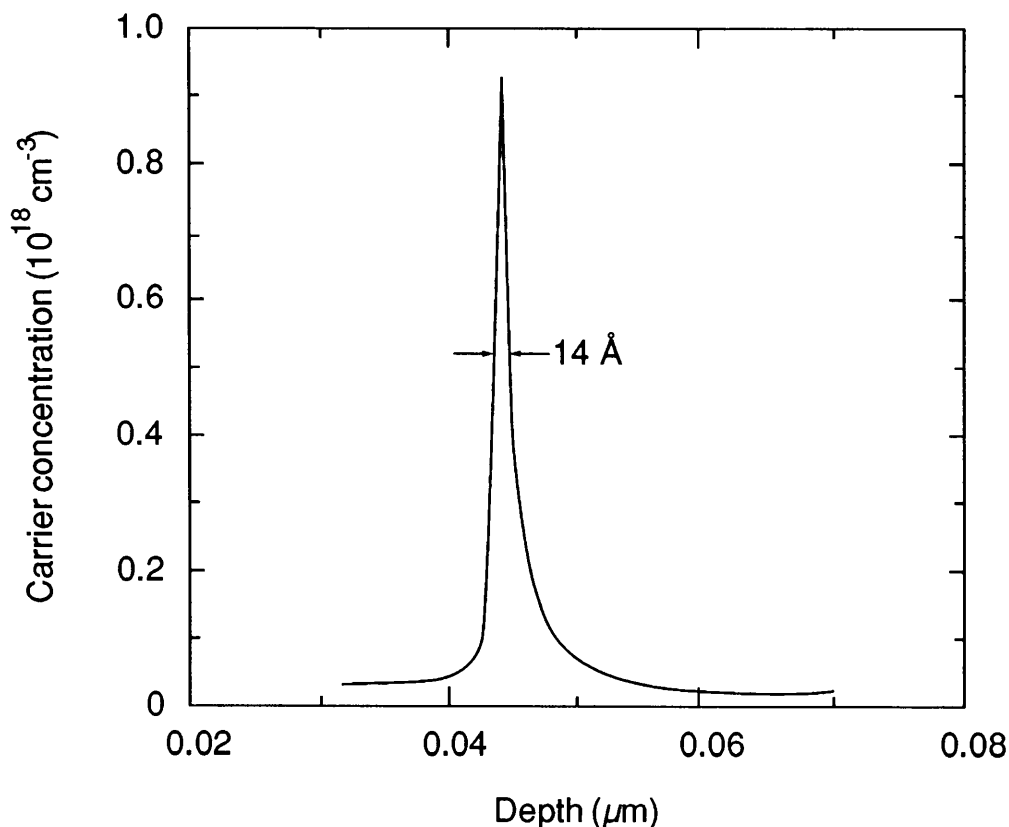


Figure 8.16: CV depth profile of the δ -doped quantum well. Here the FWHM was 14 Å.

8.8 Computer simulation of CV depth profiles

CV depth profiles were simulated on a computer, using the shooting algorithm described in section 7.7. The differential equation was solved using the 4th order Runge-Kutta method (Press *et al* 1986). The occupancy of states in the conduction band was calculated using the approximation devised by Unger (1967) (see equations 7.35 and 7.36). It was assumed that the Fermi level remains flat throughout the depletion region. The ionization of donors was calculated according to equation (2.22), while charge contributed by the valence band and the acceptors was ignored. The bisection method was used to determine a value for the electric field at the interface $E(0)$ that satisfied the boundary condition $E(\infty) = 0$.

The program was written in FORTRAN-77, and compiled to run on a Pernetel PS/90 mainframe. Another version written in interpreted BBC BASIC VI, to run on an Acorn ARM3 processor. In order to improve the calculation speed, this version was later adapted to use different stepsizes for different regions.

Since the simulation of CV depth profiles requires a large amount of computer time, only a limited number of capacitance points could be measured. To improve the appearance of the simulated graphs, a four point differentiation formula (Abramovitz and Stegun 1972) was used to calculate the carrier density profiles. This technique produces smoother, more symmetric graphs. Examples of simulated depth profiles calculated by these programs are shown in figures 8.6 to 8.8 and 8.14. Other examples are shown in the theoretical part of this dissertation. For the sake of convenience, these have been repeated on the following pages.

To evaluate the relative performance of the programs on the different computers, the programs were used to calculate the CV profile of the spike-doped sample described in section 8.6. The program, running on the mainframe, took approximately 15 min processor time, while it took about 12 hours on the microcomputer. With stepsize control the execution time was reduced by more than half, to 5 hours.

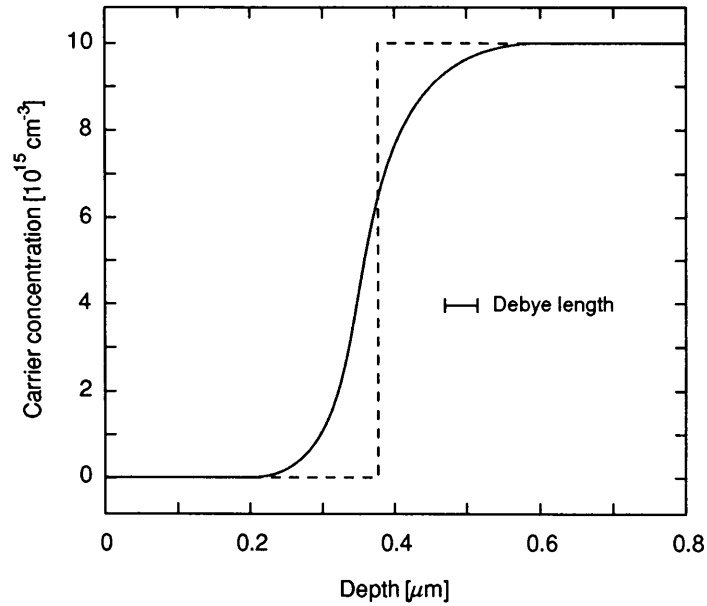


Figure 8.17: Majority carrier density at the depletion region edge. The dotted line indicates the carrier density as predicted by the depletion region approximation, while the solid line indicates the exact value as calculated by the simulation program. This graph was calculated for a Schottky diode manufactured on 10^{16} Si-doped GaAs at 300 K, with a total forward bias of 1 V. The Debye length in this material is $0.043 \mu\text{m}$.

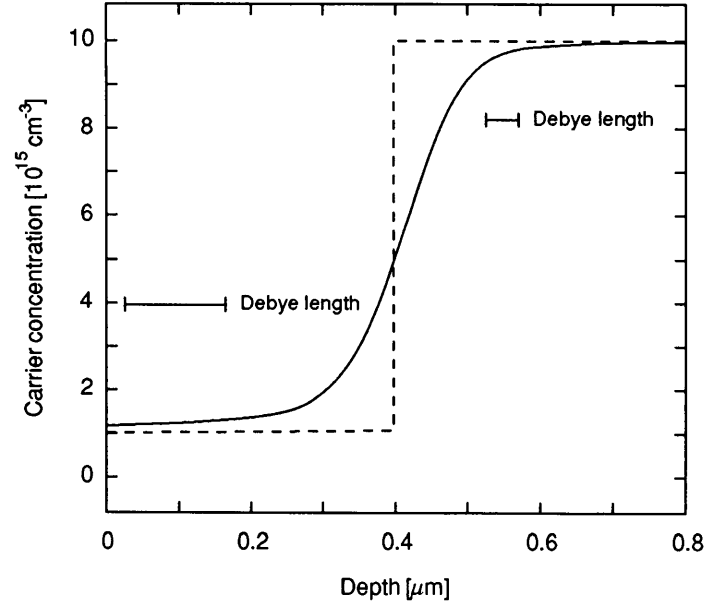


Figure 8.18: Carrier density in a 10:1 doping step in Si-doped GaAs at 300 K, as calculated by the simulation program. The dashed line indicates the doping profile.

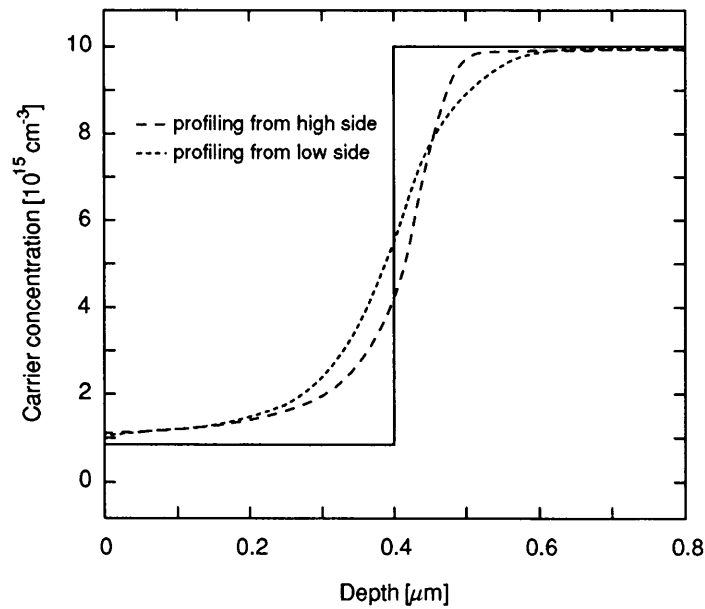


Figure 8.19: Simulated CV profile of a 10:1 doping step in GaAs. The apparent doping profiles as measured by profiling from the high as well as from the low side are shown. The solid line indicates the position of the step.

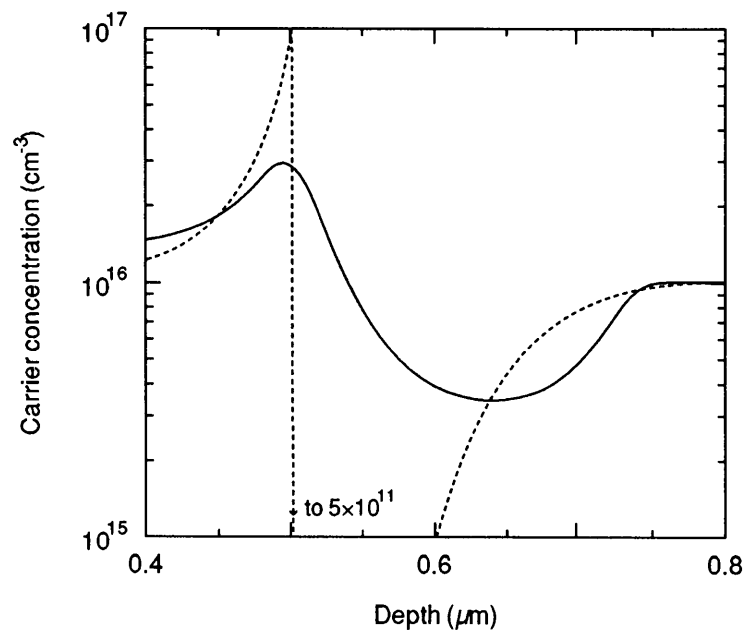


Figure 8.20: Simulated CV profile of a heterojunction (solid line) and the actual carrier concentration (dotted line). The dopant concentration was 10^{16} cm^{-3} on both sides. This graph illustrates the effect of Debye length averaging on the CV profile of a heterojunction.

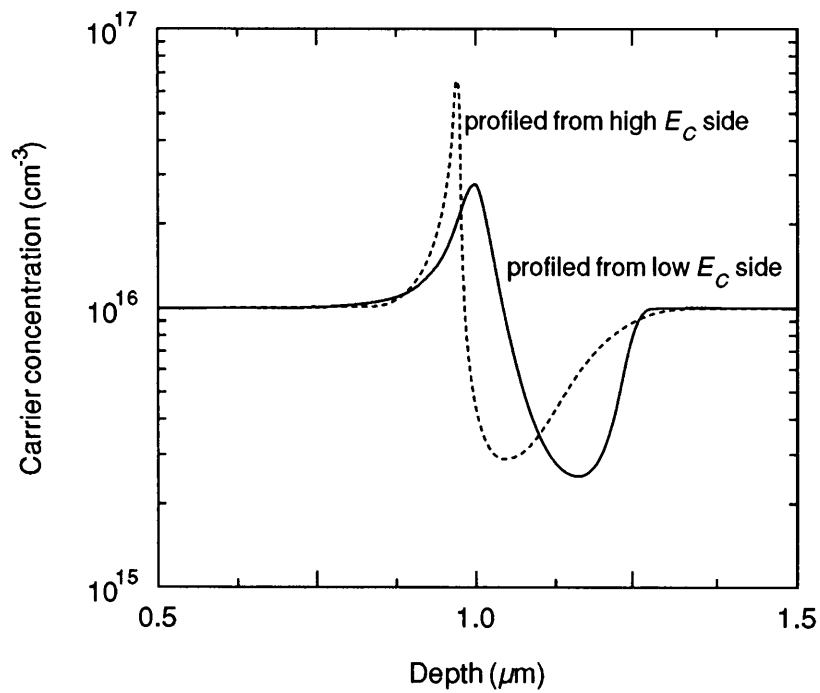


Figure 8.21: Simulated CV profile of a heterojunction as profiled from the low E_C side (solid line) and from the high E_C side (dashed line). The junction is at $x = 1 \mu\text{m}$. Although it is easy to determine the position of the heterojunction from the profile performed from the low E_C side, it is extremely difficult to determine the position of the heterojunction when profiling from the high E_C side.

8.9 Error analysis

In this section a short description of the origin of a number of errors which could influence the accuracy of the measured doping profile will be discussed. Only measurement errors will be discussed. Effects due to Debye length averaging, deep levels and other effects have been discussed in detail in chapters 6 and 7. The reduction of noise has also been discussed previously.

The absolute errors in the determination of CV carrier density profiles can be ascribed to a number of sources. The two most important sources of error in this case were the capacitance meter and the uncertainty in the material constants of the semiconductors.

Depth scale

Since the depth scale is calculated directly from the capacitance measurements, the error in the capacitance measurements should directly influence the error in the depth scale. For the capacitance measurements at low oscillator levels, the absolute error of the capacitance meter, under the standard measurement conditions described in section 8.3, was about $\pm(1\% \text{ of the reading} + 3 \text{ digits})$. Since the measurements were always performed at the most sensitive scale, the 1% error is much larger than 3 digits, accordingly the error in the capacitance can be assumed to be 1%. The error in the determination of the contact area was estimated to be about 2%.

There is some controversy regarding the dielectric constant of GaAs. In many cases the low frequency dielectric constant of GaAs is quoted as 12.8, but a number of publications state a value of 13.1. There has also been some speculation regarding the frequency and doping dependence of the dielectric constant (see Blakemore 1982). For this reason it seems safe to assume an error of approximately 3% in the dielectric constant.

As a result, the total error in the depth scale is approximately 5%, which is in the same order as the depth scale accuracy in other depth profiling techniques such as SIMS.

Concentration scale

For a single point the error in the concentration is to a large extent determined by the random error in the capacitance measurements. In this case the error can be determined according to the method of McGillivray described in section 6.2. If the average of a number of points is taken or the area under a peak is integrated, the effect of noise in the profile becomes negligible. In this case the error in the concentration is determined in a similar way as that of the depth scale. An error of approximately 6% can be assumed.

Determining of heterojunction band offsets and interface charge

The technique developed by Kroemer is very elegant. However, even if the assumptions are valid, large errors can occur. The most important factors that could contribute to errors are inaccuracies in the determination of the dopant concentrations on either side of the heterojunction and the inaccuracy in the determination of the position of the heterojunction. For instance, in the sample measured in section 8.7, a $1 \times 10^{16} \text{ cm}^{-3}$ error in the carrier

concentration on either side of the junction would cause an $2 \times 10^{11} \text{ cm}^{-2}$ error in the measured interface charge, and an error of 0.02 eV in the conduction band discontinuity. In the same situation an error of $0.001 \text{ } \mu\text{m}$ in the position of the heterojunction would cause an error of 0.01 eV in the calculated conduction band discontinuity. The effect of a number of factors on the calculated heterojunction parameters is shown in table 8.7. Because relatively small measurement errors can cause large errors in the calculated results, it is advisable that the simulated CV depth profile of the assumed structure is compared to the measured CV depth profile, in order to ensure consistency of the results. The heterojunction parameters can now be varied until a good fit is obtained. Since this procedure also takes the shape of the CV depth profile into account, it can be used to reduce the uncertainty in the calculated values significantly.

Measurement error	Error in ΔE_c	Error in σ_i
$\pm 0.001 \text{ } \mu\text{m}$ error in x	$\pm 0.01 \text{ eV}$	0
$\pm 0.5 \times 10^{16} \text{ cm}^{-3}$ error in N_D	$\pm 0.01 \text{ eV}$	$\pm 2 \times 10^{11} \text{ cm}^{-2}$
Integration range limited to $\pm 0.5 \text{ } \mu\text{m}$ from HJ interface	$\pm 0.02 \text{ eV}$	$\pm 5 \times 10^{10} \text{ cm}^{-2}$

Table 8.7: The effect of various errors on the determined conduction band offset and interface charge, when the method of Kroemer et al (1981) is used.

9

Conclusions

The CV profiling technique can be used for the characterization of semiconductors in general. In particular it can be applied to isotype semiconductor heterostructures. The main advantages of this technique is the low cost and that it can be applied routinely to a large number of samples, as necessary in a process control environment. Another advantage is that, for a known semiconductor, this technique requires no calibration for either the depth or the concentration scales. The calibration is independent of the dopant species. Furthermore, CV profiling relies on the electrical properties of the sample, therefore measuring the electrical effects that affect the device operation. Using the method of McGillivray *et al* (1988), it is possible to eliminate most of the noise on the profile, without reducing the resolution of the technique significantly.

CV profiling can be successfully employed to determine both the width of delta-doped layers, and the band-offsets of isotype heterojunctions. Because of Debye length averaging, the resulting data may, however, be very difficult to interpret. This problem can be overcome by making use of a device simulator to construct the carrier concentration profile of a trial structure. The trial structure is then modified, either by hand or automatically, until the CV profile of the trial structure matches that of the real structure. In most cases it can then safely be assumed that the trial structure matches the real structure.

If only limited information is necessary, or if certain assumptions are made, some quantities are conserved during the averaging process. Using these quantities, parameters such as the band offset and interface charge of a heterojunction, can be measured. However, as most of these techniques are very sensitive to small errors, it is recommended that these values be verified by comparing the simulated CV depth profile with the measured depth profile.

In some cases, when the donor levels of atoms lie close to the conduction band edge, as with Si doped GaAs, the resolution of the technique can be enhanced by lowering the temperature of the sample. This also decreases forward conduction in the Schottky diode, allowing measurements to be made closer to the surface. However, in the presence of deep levels, this technique fails.

9.1 Possible future work

Measuring of *CV* profiles when both series resistance and parallel conductance are significant

To my knowledge, none of the current models, is able to compensate for the effect of series resistance when parallel conductance across the barrier is significant. If this problem could be solved it would be possible to measure *CV* profiles closer to the surface than currently. It will most probably be a numerical method, that would make use of data e.g. dynamic resistance, obtained during a previous *IV* measurement.

Simulation

Although the simulation program described in section 8.8 gives good results that agree with the experiment, a large amount of computer time is used, and manual input is needed when fitting simulated *CV* depth profiles to experimental profiles. The use of the program could be further simplified by fitting the simulated profile to the measured profile, using a least squares procedure such as Marquardt-Levenberg. However, before these suggestions can be implemented, the simulation algorithm should be rendered more efficient, by using more sophisticated procedures to select step-size during integration.

Another limitation of the current simulator is that the effects of quantum confinement are not taken into account. This could be done in two stages. As a first approximation, the zero-bias solutions to the Schrödinger equation could be used to determine the quantized energy levels. Later, this program could be developed to solve the Schrödinger equation for each applied bias. However, if such a program is not carefully written, it would use a large amount of computer time.

9.2 Summary

The aim of this study was to investigate conditions in which optimum depletion *CV* depth profiles of heterostructures can be calculated, and to investigate techniques by which semiconductor parameters can be obtained from these *CV* profiles. These parameters were verified by using them to calculate simulated *CV* depth profiles, and comparing these simulated profiles to the measured *CV* profiles. These objectives were successfully realised.

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