Chapter 1

Two dimensional semiconductor and carbon structures – basic properties

1.1 Introduction

Semiconductors which form the heart of modern technology have revolutionized communication industry, optoelectronics industry, and made computer technology possible. Advances in semiconductor material technology have resulted in the development of device structures with dimensions of the order of nanometers. With advent of the growth techniques like molecular beam epitaxy (MBE) and metal-organic chemical vapor deposition (MOCVD), and coupled with development of lithographic processes capable of submicron definition, not only the realization of many layered structures but also the interest in charge and heat transport in layered structures has opened up wide variety of investigations. These layered systems exhibit novel physical properties that are different from those of their bulk-counterparts. These systems are usually referred to as low-dimensional semiconductor structures or semiconductor nanostructures [1.1, 1.2].

The low-dimensional semiconductor structures have ushered in an era of reduced-dimensionality physics. The significant feature, which has made these nanostructured
systems important, is the quantum mechanical restriction of the degrees of freedom of carriers (electrons and phonons) to two, one or even zero dimensions. When the confinement of carriers occurs in one direction, a two dimensional electron gas (2DEG) is realized. A 2DEG may be realized in inversion layers, at heterojunctions and in quantum wells. Confinement in two directions, with the free motion along the third direction, gives a one dimensional electron gas called quantum well wire. The confinement in all the three directions results in a zero dimensional electron gas and the system is referred as quantum dot. The two-dimensional electron gas with a typical thickness of 10 nm realized in quantum wells and inversion layers has, in particular, been extensively studied because of its importance in the development of high performance nanoelectronic devices [1.1-1.4]. The favourite material system used in devices to realize a 2DEG has been GaAs/AlGaAs.

1.2 Bulk Semiconductors

In bulk semiconductor materials, the carriers are free to move in all the directions and the de Broglie wavelength of the carriers is small in comparison with the dimensions of the material. The band structure or the energy $(E)$ versus wavevector $(K)$ relation for the electrons is given by the solution of the time-independent Schrödinger equation:

$$\frac{\hbar^2}{2m_e} \nabla^2 \psi + (E - V(R))\psi = 0$$  \hspace{1cm} (1.1)

where $V(R)$ is the periodic potential produced by the nuclei of the atoms and other electrons, $R$ being the three dimensional position vector of an electron with mass $m_e$. The general solution of equation (1.1) is the Bloch function [1.5, 1.6]

$$\psi(R) = u_K(R) \exp(i \mathbf{K} \cdot \mathbf{R})$$  \hspace{1cm} (1.2)

where $u_K(R)$ is a periodic function having the same periodicity as the crystal lattice. For a
free electron having only kinetic energy, the dependence of \( E \) on \( K \) assumes the form

\[
E = \frac{\hbar^2 K^2}{2m_e}.
\]  

(1.3)

For electrons in semiconductors, mass of electron, \( m_e \) is replaced by the effective mass, \( m^* \).

Figure 1.1 shows the band structure of InN semiconductor. The effective mass of electron, \( m^* \) in InN is obtained assuming the derivative, \( dE_k/dk \), to be parabolic band [1.7].

![Wave vector diagram](image)  

**Wave vector**

**Figure 1.1:** Band structure of InN (from [1.7]).

Many transport properties of a semiconductor are sensitive to the density of states (DOS), i.e. the number of quantum states per unit energy. In other words, the density of states, denoted by \( g(E) \), indicates how densely packed are the quantum states in a particular system. The DOS per spin, per unit volume of a 3D electron gas in a bulk semiconductor for the dispersion relation (1.3) is given by [1.2]

\[
g(E) = \frac{1}{2\pi^2} \left( \frac{2m^*}{\hbar^2} \right)^{3/2} E^{1/2}
\]  

(1.4)
1.3 Semiconductor quasi-2D nanostructures

Quantum confinement of carriers in one direction results in an essentially two-dimensional carrier transport. The width of the 2DEG confinement being very small (~ few nm) yet finite, the confined carriers behave as quasi-two-dimensional (Q2D) systems. Wavefunctions of such systems have a finite spatial extent in one (i.e. the restricted) dimension. The quasi two-dimensional semiconductor structures in which a Q2D carrier (electron or hole) gas can be realized include inversion layers, heterojunctions and quantum wells [1.1-1.4]. Here, we describe the potential profile, density of states, eigen functions and energy eigen values for heterojunctions and quantum wells which are used in the study of 2D physics and its applications.

1.3.1 Heterojunction

A Q2D carrier gas can be realised in a semiconductor heterojunction (HJ) when two different semiconducting materials with different band gaps are joined together at a junction [1.8, 1.9]. It is now possible to make such heterojunctions extremely abrupt through modern materials growth processes; in fact, heterojunctions with interfacial thickness on a dimensional scale approaching only one atomic monolayer may be fabricated. The most well known and applicable examples are SiO₂/Si, GaSb/AlSb, GaInAs/InP and GaAs/AlGaAs heterojunctions with high quality interfaces. Among the III-nitride heterostructures GaN/AlGaN and InN/AlN, have recently received great importance due to their technological applications[1.9 - 1.11].

A schematic diagram of a typical GaAs/AlGaAs HJ is shown in figure 1.2. Doping the wide-band gap side of GaAs/AlGaAs HJ with n-dopants say Si, some electrons are transferred to the (lower lying Γ-point of conduction band of) GaAs layer until an
equilibrium is reached. At equilibrium, charge transfer occurs across the HJ to equalize chemical potential on both sides. As the Fermi level is constant across the interface, the conduction band of Si doped AlGaAs is bent upwards. The doping is done selectively so that the region near the interface does not contain donors; the undoped AlGaAs is called spacer. The spacer is used to reduce the impurity scattering of 2DEG and achieve high mobility. The conduction band in the pure GaAs side of the junction is bent downward and crosses below the Fermi level, pinned by the Si dopants. The Q2D electron gas is formed at

![Figure 1.2: The energy scheme of modulation doped AlGaAs/GaAs HJ.](image)
the interface where the $E_F$ crosses the potential minimum of the conduction band [1.2, 1.3].

The perpendicular effective potential well at the interface is nearly triangular in shape, and the electrons occupy quantum bound states in the triangular well. The spatial extent of the Q2D electron gas is typically 5-10 nm.

The wavefunction and the energy eigenvalues of the Q2D electrons can be described in the effective mass approximation. For heterojunctions, the triangular potential well approximation can be used to represent the potential energy of electrons [1.1]

$$V(z) = \begin{cases} eFz & z > 0 \\ \infty & z \leq 0 \end{cases}$$

(1.5)

where

$$F = 4\pi \left( N_{depl} + f \, n_s \right) \frac{e}{\kappa_s}$$

(1.6)

is the effective field felt by the electrons. In (1.6), $\kappa_s$ is the static dielectric constant, $N_{depl}$ the depletion charge concentration, and $f$ is numerical coefficient. Choosing $f = 1$ gives the field at interface and $f = 0.5$ gives the average field in the active layer. Since the potential energy is taken to be a function of $z$ only, the electron wave function, $\psi_{nk}(r,z)$, can be written as the product of Bloch function, $u_k(r,z)$, a $z$-dependent factor, $\xi_n(z)$, and a plane wave factor representing free motion in the $x$-$y$ plane:

$$\psi_{nk}(r,z) = u_k(r,z) \exp(i \, k \cdot r) \xi_n(z)$$

(1.7)

Here $r$ and $k$ are the position vector and wavevector in the $x$-$y$ plane, respectively, with $r \equiv (x, y)$ and $\xi_n(z)$, is the solution of the Schrodinger equation

$$\frac{\hbar^2}{2m_x} \frac{d^2}{dz^2} \xi_n(z) + \left( E - V(z) \right) \xi_n(z) = 0$$

(1.8)

With the approximation of triangular potential, the solutions are Airy functions [1.1],
\[ \xi_n(z) = A_l \left[ \left( \frac{2 m_z e F}{\hbar^2} \right)^{1/3} \left( Z - \frac{E_n}{e F} \right) \right] \]  

(1.9)

In (1.8) and (1.9), \( m_z \) is the electron effective mass perpendicular to the interface and \( E_n \) are the eigenvalues given asymptotically, for large \( n \), by [1.1]

\[ E_n \sim \left( \frac{\hbar^2}{2 m_z} \right)^{1/3} \left[ \frac{3 \pi e F}{2} \left( n + \frac{3}{4} \right) \right]^{2/3}, \text{ } n = 0, 1, 2 \ldots \]  

(1.10)

In order to make calculations of the properties of the inversion layers much more convenient, approximate solutions have been widely used. The simplest of these is the Fang-Howard one-parameter variational wave function, when only the lowest subband (\( n=0 \)) is occupied [1.8]:

\[ \xi_o(z) = \left( \frac{b^3}{2} \right)^{1/2} z \exp(-bz/2) \]  

(1.11)

The variational parameter \( b \) appearing in (1.11) is given by

\[ b = \left[ \frac{48 \pi m_z e^2}{\kappa_s h^2} \left( N_{depl} + \frac{11}{32} n_s \right) \right]^{1/3} \]  

(1.12)

For the wavefunction (1.11), the average penetration length of the charge into the semiconductor, is

\[ z_o = \frac{3}{b} \]  

(1.13)

and the eigen value in lowest state, \( E_0 \), can be obtained [1.9]

\[ E_o = \left( \frac{36 \pi e^2}{12 b \kappa_s} \right) \left( N_{depl} + \frac{55 n_s}{96} \right) \]  

(1.14)

The energy eigenvalues associated with the wave function of (1.9) are given by

\[ E_{nk} = E_k + E_n = \frac{k_x^2 + k_y^2}{2 m'} + E_n \]  

(1.15)

where \( m' \) is the effective mass along the x-y plane, and \( k^2 = k_x^2 + k_y^2 \).

The DOS function per unit area, per spin for a pure 2DEG system with energy-wavevector dispersion relation
\[ E_k = \frac{\hbar^2 k^2}{2 m^*} \]

can be expressed as
\[ g_{2D}(E) = \frac{g_s g_v m^*}{2 \pi \hbar^2} \]  \hspace{1cm} (1.16)

where, \( g_s \) and \( g_v \) are spin and valley degeneracies, respectively. The DOS is constant and independent of energy. For Q2D systems DOS per unit area per spin for the dispersion relation of the (1.15) is written as \([1.2,1.3]\)
\[ g_{Q2D}(E) = \sum_{n,k} \delta \left( E - E_{n,k} \right) = \frac{m^*}{2 \pi \hbar^2} \sum_n \theta (E - E_n) \]  \hspace{1cm} (1.17)

where the summation extends over the bound states \( n \), and \( \theta(x) \) is the step function.
\[ \theta(x) = \begin{cases} 0 & x < 0 \\ 1 & x \leq 0 \end{cases} \]  \hspace{1cm} (1.18)

The DOS for a Q2D along with that for a 3D electron gas is shown in figure 1.3. The DOS is finite at the bottom of the Q2D level whereas it tends to zero in the bulk case. A Q2D system is truly two-dimensional when one deals with only one electric subband.

**Figure 1.3:** Q2D density of states and comparison with pure 2D DOS (dotted-curve) and 3D DOS (dashed-curve).
1.3.2 Quantum Wells

A quantum well (QW) is one of the quantum heterostructures, in which a Q2D carrier gas can be realized by sandwiching a thin layer (well) of smaller band-gap material between two layers (barriers) of larger band-gap material causing the energy bands of composite material to form a minimum (maximum) in conduction (valence) band of sandwiched layer. Consequently, electrons and holes in the thin well layer are confined in such manner that they behave quantum mechanically as particle-in-a-box with discrete, bound energy states. These structures can be grown using MBE and physical vapor deposition with control of the layer thickness down to monolayers.

In QW heterostructures, with finite/thin the confining barriers, the wavefunctions penetrate into the barrier layers. This penetration affects the transport of electrons in planes parallel to the interfaces as the electron spends part of the time in the barrier layers [1.12]. For a 2DEG confined to move along plane of square symmetric quantum well of width \( L \) the effective potential, \( V(z) \) experienced by electrons is

\[
V(z) = \begin{cases} 
V & \text{for } z < -L/2 \\
0 & \text{for } -L/2 < z < L/2 \\
V & \text{for } z > L/2 
\end{cases} \quad (1.19)
\]

The wavefunction and the energy eigenvalues of the Q2D electrons can be described in the effective mass approximation. For a 2DEG to be confined to move along plane of square symmetric quantum well of width, \( L \) and of barrier height, \( V \), the electron wave functions and energy eigenvalues are given by [1.7]

\[
\psi_{nk}(r,z) = u_k(r)\xi_n(z)\exp(i \mathbf{k} \cdot \mathbf{r}) \quad (1.20)
\]

and

\[
E_n(k) = E_n + \frac{\hbar^2 k^2}{2m} \quad (1.21)
\]
where \( r = (x, y) \) and \( k = (k_x, k_y) \) are, respectively, the 2D position and wave vectors of the electrons with effective mass \( m^* \). \( \xi_n(z) \) is the normalized wave function of the \( n^{th} \) electric subband with energy \( E_n \). Due to the finite barrier confinement of electrons, say in the \( z \) direction, some part of the electron wave function penetrates into the barriers and decays exponentially (see figure 1.4b). The electron wave functions in the well (w) and barrier (b) regions are given by [1.12]

\[
\xi_n(z) = \begin{cases} 
B_{b1} \exp(i k_b z) & z \leq -L/2 \\
A_w \sin \left( k_w \left( z + \frac{n\pi}{2} \right) \right) & -L/2 \leq z \leq L/2 \\
B_{b2} \exp(-i k_b z) & z \geq L/2 
\end{cases}
\]  

(1.22)

where \( k_w = 2\alpha / L \), \( k_b = 2\beta / L \), and the normalization constants \( A_w \) and \( B_{b1} \) and \( B_{b2} \), are expressed as: \( A_w = (2A_o/L)^{1/2} \) and \( B_{b1} = B_{b2} = A_w \cos(\alpha) \exp(\beta) \), with,

\[
A_b = 1 + \frac{\sin(2\alpha)}{2\alpha} \left( \frac{(\cos(\alpha))^2}{\beta^2} \right)^{-1} \quad \text{for } n = 1, 3, 5, ...
\]
and

\[ A_w = (2A_e/L)^{1/2}, \quad B_{b1} = -B_{b2} = -A_w \sin(\alpha) \exp(\beta), \]

\[ A_e = \left( 1 - \frac{\sin(2\alpha)}{2\alpha} + \frac{(\sin(\alpha))^2}{\beta} \right)^{-1}, \text{ for } n = 2, 4, 6... \]

The energy eigen values, expressed as

\[ E_n = \frac{2\hbar^2\alpha^2}{l^2 m_w}, \quad (1.23) \]

are determined for \( \pi(n - 1)/2 < \alpha \leq n\pi/2 \) from the transcendental equation:

\[ (m_b/m_w)^{1/2}(C - \alpha)^{1/2} = \begin{cases} 
  \alpha \tan \alpha & \text{for } n = 1, 3, 5... \\
  -\alpha/\tan \alpha & \text{for } n = 2, 4, 6... 
\end{cases} \quad (1.24) \]

where, \( C = (m_w l^2 V/2 \hbar^2) \).

The wavefunction penetration into barrier, characterized by \( \beta \), is given by

\[ \beta = (m_b/m_w) \left\{ \begin{aligned} 
  \alpha \tan \alpha & \text{ for } n = 1, 3, 5... \\
  -\alpha/\tan \alpha & \text{ for } n = 2, 4, 6... 
\end{aligned} \right. \quad (1.25) \]

where \( m_w \) and \( m_b \) denote the masses of electron in well and barrier regions, respectively.

For quantum wells with infinite barriers (figure 1.4a) \( \alpha = n\pi/2 \) and \( 1/\beta = 0 \).

1.4 Carbon nanostructures

Of recent interest has been another class of quantum structures, namely, carbon nanostructures. Ever since the carbon nanostructures, including graphene, carbon nanotubes and fullerenes have been discovered, there is a high hope that, they can be applied to high performance electronic devices. The advent of 2D carbon nanostructure – graphene, marked the beginning of availability of test-vehicle for understanding of electronic properties in perfectly two dimensional carbon nanostructures. Due to its unique band structure, graphene exhibits several peculiar electronic properties which are absent in conventional 2DEGs. The continuing progress in understanding of electronic properties of
graphene shows promise for the fabrication of devices with enhanced functionalities [1.13]. Therefore, Graphene is interesting not only in view of possible applications but also from the fundamental stand point, due to its unique electronic properties [1.13 - 1.17].

Graphene systems, which include single layer graphene (SLG), bilayer graphene, and graphene ribbon are usually grown on a substrate. The flexibility of bonding in carbon-based systems allows the different structures to show large of number of variety of physical and electronic properties. These electronic properties are, in great part, the result of the dimensionality of these structures. Among systems with only carbon atoms, graphene – a 2D allotrope of carbon – plays important role since it is the basis for understanding the electronic properties of other allotropes. The most straightforward way to obtain graphene is to use the exfoliation technique, which can be performed either mechanically or chemically. Graphene can also be grown using both physical and chemical synthesis techniques such as chemical vapor deposition, epitaxial growth and reduction from graphite oxides [1.14].

1.4.1 **Electronic structure of graphene**

Graphene is a single layer of carbon atoms arranged in a hexagonal honeycomb lattice. It is characterized by mass-less Dirac fermions as charge carriers and a linear dispersion with zero band gap. Graphene lattice is as shown in figure 1.5. The Bravais lattice is triangular, with lattice vectors [1.17]

\[ a_1 = \frac{a}{2} \left( 3, \sqrt{3} \right), \quad a_2 = \frac{a}{2} \left( 3, -\sqrt{3} \right), \]  

(1.26)

where \( a \approx 1.42 \ \text{Å} \) is the carbon bond length.
The honeycomb lattice contains two atoms per elementary cell. They belong to two sublattices, A and B, each atom from sublattice A surrounded by three atoms of sublattice B and vice-versa. The nearest neighbor vectors are

\[ \mathbf{\delta}_1 = \frac{a}{2} (1, \sqrt{3}), \quad \mathbf{\delta}_2 = \frac{a}{2} (1, -\sqrt{3}), \quad \mathbf{\delta}_3 = a (1, 0). \] (1.27)

The reciprocal lattice is also triangular lattice, with lattice vectors

\[ \mathbf{b}_1 = \frac{2\pi}{3a} (1, \sqrt{3}) \quad \quad \mathbf{b}_2 = \frac{2\pi}{3a} (1, -\sqrt{3}) \] (1.28)

The special high-symmetry points \( \mathbf{K}, \mathbf{K}' \) and \( \mathbf{M} \) are shown in figure 1.5 b. The wavevectors at corresponding to these points are given by

\[ \mathbf{K}' = \left( \frac{2\pi}{3a}, \frac{2\pi}{3\sqrt{3} a} \right), \quad \mathbf{K} = \left( \frac{2\pi}{3a}, -\frac{2\pi}{3\sqrt{3} a} \right), \quad \mathbf{M} = \left( \frac{2\pi}{\sqrt{3} a}, 0 \right). \] (1.29)

The tight-binding Hamiltonian is described by 2 x 2 matrix

\[ H(\mathbf{k}) = \hbar v_F \begin{pmatrix} 0 & k_x - ik_y \\ k_x + ik_y & 0 \end{pmatrix}, \] (1.30)

where, \( \mathbf{k}(\equiv k_x, k_y) \) is the wavevector and \( v_F \) is Fermi velocity.
The electron wavefunctions and energy eigen values around the $K$ and $K'$ points at the corners of graphene Brillouin zone are given by [1.13]

$$\psi_{\pm \mathbf{k}}(\mathbf{k}) = \frac{1}{\sqrt{2}} \left( e^{-i\theta_k/2} \pm e^{i\theta_k/2} \right)$$

$$\psi_{\pm \mathbf{k}'}(\mathbf{k}) = \frac{1}{\sqrt{2}} \left( e^{i\theta_k/2} \pm e^{-i\theta_k/2} \right)$$

and

$$E(\mathbf{k}) = \hbar v_F |\mathbf{k}|$$

where, $\mathbf{k} \equiv (k_x, k_y)$ is the 2D electron wave vector and $v_F$ is the Fermi velocity, with $\theta_k = \tan^{-1}(k_x/k_y)$ and ± signs correspond to the $\pi^*$ and $\pi$ bands, respectively. The band structure of graphene is shown fig 1.6a, 1.6b and 1.6c.

It is important to mention that graphene has charge neutrality point (CNP), i.e, the Dirac point, where its character changes from being electronlike to being holelike. In graphene, the carriers are introduced into conduction or valence band by tuning an external gate voltage. The transport properties of graphene can be controlled by gating graphene device using an external gate. This external gate voltage allows controlling of the 2D carrier density in graphene and their nature as well. The 2D carrier density, $n_s$ and external gate voltage, $V_g$ are connected by the relation, $n_s \approx C V_g$, where $C$ depends on the substrate. The carrier concentration in graphene on different substrates of varying thickness and dielectric constant can be obtained by following the scaling

$$n_s[10^{10} \text{ cm}^{-2}] = 7.2 \times \frac{t[\text{nm}]}{300} \frac{3.9}{\kappa_s} V_g[V],$$

where, $t$ and $\kappa_s$ are thickness and dielectric constant of substrate [1.14], respectively. For a SiO$_2$ substrate of thickness 300nm, $C \approx 7.2 \times 10^{10} \text{ cm}^{-2}/V$ and $n_s=10^{10} \text{ cm}^{-2}$ for $V_g = 1V$. 

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Density of States

The unique band structure of SLG near the K point is also accompanied by a unique energy-dependence of density of states (see figure 1.6d). The low-energy density of states of graphene per unit area is given by

$$g_{SLG}(E) = \frac{g_s g_v |E|}{2\pi (\hbar v_F)^2}$$  \hspace{1cm} (1.33)

The linear energy dependence of density of states in (1.33) holds up to $E \approx 0.3t$, beyond which the density of states increases sharply[1.18].
1.4.2 Suspended graphene

Graphene structures, which are usually grown on SiO\textsubscript{2} substrate, undergo degradation in mobility. Since the substrate affects the both the morphology of graphene and provides a source of impurities, one needs to find a way to have electrically contacted graphene without the presence of underlying substrate. Despite tremendous interest and concerted experimental efforts, the presence of strong impurity scattering - which limits the electron mean free path to less than a micron - has been a major barrier to progress [1.17].

One of the strategies adopted to achieve higher mobility graphene samples is to eliminate the substrate altogether by suspending the graphene layer [1.19]. The making of suspended graphene (SG) was an important experimental milestone where after exfoliating graphene and making electrical contact, one then etches away the substrate underneath the graphene so that the graphene is suspended [1.14]. Schematic representation of SG is shown in figure 1.7.

![Schematic representation of suspended graphene](image)

**Figure 1.7:** Sketch of suspended graphene membrane with clamped edges. In figure, \(h_0\), is deflection in out-of-plane direction and \(L\), is the length of membrane [1.19].
In a suspended graphene sample, carbon atoms can oscillate in the direction perpendicular to layer also, which leads to new class of low energy phonons in the flexural branch. The two types of phonons – in-plane and out-of-plane phonons – influence electronic transport of graphene. The out-of-plane phonons have quadratic dispersion relation which leads to high number of low energy phonon population in graphene membrane [1.19].

**Strain in suspended graphene**

SG layers can be under strain either due to the electrostatic force arising from the gate or as a result of micro fabrication to get suspended samples. Strain in graphene is of great importance for both applications and fundamental study. Unexpected strain can affect the performance of the device. On the other hand intentionally induced strain may improve the carrier mobility. Recent studies have suggested that strain can be used to engineer graphene electronic states and hence the transport properties [1.20]. Theoretical and experimental investigations of electron and phonon transport in SG indicate that in the free standing case (absence of strain) the major contribution to electron and thermal transport is from acoustic flexural phonons, and this intrinsic limitation can be reduced by the effect of strain.

**REFERENCES**


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