STUDY OF BASIC THEORY OF SEMICONDUCTORS

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Abstract - *Semiconductors are widely used in our daily life. They are essential in modern electrical devices such as personal computers, digital cameras, and mobile phones. The main reason that makes semiconductor materials so important in modern industrial technology are their unique electrical and optical properties. A semiconductor has electrical conductivity in between that of a conductor and an insulator, which can be easily controlled over a wide range. These are essential advantages for such a wide range of applications. The energy band structure of the semiconductor is the origin of these magic physical properties. The energy band structure of electrons in a semiconductor crystal reflects the periodic potential of the crystal. In the following sections of this chapter, we will present a brief description of the crystal structure, the energy band structure, the effective mass approximation, and the density of states of electrons, to describe the motion of electrons in semiconductors and to study their optical and electrical properties.*

Key Words: the effective mass approximation, periodic potential, motion of electrons, Semiconductors, electrical and optical properties.

INTRODUCTION
1.1 Crystal structure of semiconductors

Solid state physics is mainly related to crystals and the movements of electrons in crystals. The structure of all crystals can be described in terms of lattice sites, and of atom located at these lattice sites. Because of the periodicity of crystals, any two lattice sites R, R′ in a crystal are correlated

R′ = R + m1R1 + m3R3 + m3R3

where m1, m2, m3 are integers, and a1, a2, and a3 are three independent primitive vectors. In the three-dimensional space, there are totally 14 different lattice types, among which face-centered cubic (fcc) is the most common crystal structure of semiconductors. An fcc lattice can be obtained by adding an atom at the centre of each face of a simple cubic lattice, where the simple cubic system consists of one lattice point

at each corner of the cube. The fcc crystal structure is shown in Fig. 2.1(a).

The primitive vectors are: a1 = a(x0 + y0)/2, a2 = a(z0 + y0)/2, a3 = a(x0 + z0)/2,

where a is normally referred to as the lattice constant. x0, y0, and z0 are the unit vectors along the x, y, and z directions.

To study the periodic properties of a crystal, the definition of a reciprocal lattice is introduced as

$e_{iG}r = 1$

where r characterizes the lattice point in the real space,

G = n1b1 + n3b3 + n3b3

describes the reciprocal space, and n1, n2, n3 are integers. For a three dimensional lattice, the reciprocal lattice is determined by

$$b_1 = 2\pi \frac{a_2 \times a_3}{a_1 \cdot (a_2 \times a_3)}, \quad b_2 = 2\pi \frac{a_3 \times a_1}{a_2 \cdot (a_3 \times a_1)}, \quad b_3 = 2\pi \frac{a_1 \times a_2}{a_3 \cdot (a_1 \times a_2)}$$

The Wigner-Seitz cell in the reciprocal lattice contains all points which are nearer to one considered lattice point than to any other, which is also denoted as the first Brillouin zone. The first Brillouin zone of an fcc lattice is presented in Fig.1(b) together with labels of high symmetry lines and points.

1.2 Energy band structures

Periodic lattice structures create a special situation for the electrons. If one denotes the periodic electronic potential V (r) of the lattice by
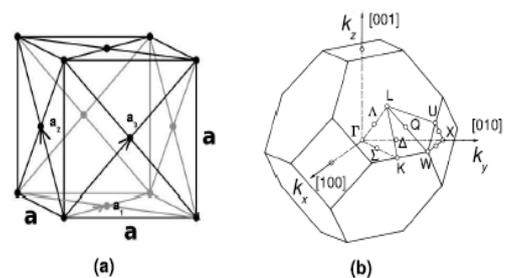
V (r + R) = V (r),

Figure 1: (a) Schematic structure of an fcc lattice, a is the lattice constant. (b) The first Brillouin zone of an fcc lattice.

where R is an arbitrary lattice vector, one can write the Schrodinger equation for the electrons in a periodic potential as

$$\left[-\frac{\hbar^2}{2m_0} \nabla^2 + V(\boldsymbol{r}) \right] \Psi(\boldsymbol{r}) = E \Psi(\boldsymbol{r})$$

where m0 is the mass of the free electron. Because of the periodicity of V (r), the electron wave function has the following form

$$\Psi_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{n\mathbf{k}}(\mathbf{r})$$
$$u_{n\mathbf{k}}(\mathbf{r}) = u_{n\mathbf{k}}(\mathbf{r} + \boldsymbol{R})$$

which is the Bloch theorem. Here k is called the electron wave vector and unk is a periodic function (periodic Bloch function). It is normally difficult to characterize, both experimentally and theoretically, the band structure in the whole Brillouin zone. Many theoretical methods adopt some assumptions and approximations and have to be calibrated together with the experiments. One method to calculate the band structure is called the linear combination of atomic orbitals (LCAO) method, which is also the basis for the so-called as the

tight-binding method [5, 14]. In the tight-binding method, one assumes that the wave functions of the electrons of the crystal atoms are very similar to the ones of the isolated atom in free space, and consider only the interaction between atoms to those of the nearest neighbours. We choose the wave functions of the electrons (orbitals) of 'free' atoms as basis states. Most compound semiconductor materials, have zincblende structures, which is a structure based on an fcc lattice with a cation-anion pair occupying each lattice site. In the sp3-type tight-binding method of , the electron wavefunctions of outer-most shell are described by four atomic orbitals s, px, py, and pz. Each of the atomic orbitals can occur for each of the two sites in the unit cell. Thus the Bloch wave function is

$$\Psi(\boldsymbol{r}) = \sum_m \sum_{j=1}^2 C_{mj}(\boldsymbol{k})\Psi_{mj}(\boldsymbol{r} - \boldsymbol{r}_j)e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$$

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where j = 1, 2 correspond to the different atoms in the unit cell and m refers to the 4 different atom orbitals. By solving the secular equation

$$|\langle \Psi_{m'j'}|H - E|\Psi(\boldsymbol{k}, \boldsymbol{r})\rangle| = 0$$

the band structure can be calculated for different values of k, which is normally referred to as the energy dispersion E = E(k). In general, empirical input parameters are used to evaluate the Hamiltonian matrix. One of the well-known methods was developed by Koringa, Kohn and Rostoker [15, 16] based on the Green's function technique and muffin-tin potential (KKR Green-function method). Another one is called the pseudopotential method [8, 9], where an empirical pseudo potential is introduced in order to obtain good agreement of electronic band structures with experiments. The pseudo-potential method gives surprisingly accurate results with respect to the computation time and resource requirements. Another widely used method is the k τ p theory which was introduced by Kane in 1956 to analyse the energy band structures of III-V compound semiconductors Fig. 2 shows a schematic diagram of the band structure of crystal 4H-SiC. τ 15v is the energy of the valence band top at the centre of the Brillouin zone [000]. The conduction band minimum is on the M valleys, while τ 1c is the conduction band energy at the centre of the Brillouin zone [000]. The energy values of these points determine whether we have a direct or an indirect band gap. If the minimum of the conduction band lies vertically above the maximum of the valence band in the k space, it is called a direct bandgap material, otherwise it refers to an indirect bandgap material. In the particular case of this figure under investigation, 4H-SiC is an indirect semiconductor.
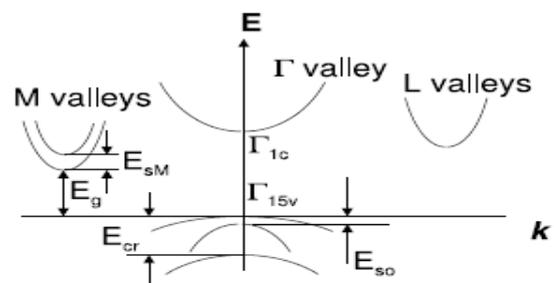

Figure 2.: 4H-SiC band structure.

1.3 Effective mass approximation

An electron in a lattice is under the influence of the periodic lattice potential. To describe the movement of electrons inside the solid material, we introduce the concept of an effective mass. By the Bloch theorem, a definite Block state k in a periodic lattice is described by its energy dispersion relationship, E = E(k), its crystal momentum ¯hk, and a group velocity

$$v = \frac{1}{\hbar} \frac{dE(\boldsymbol{k})}{d\boldsymbol{k}}$$

To describe approximately the electron motion in the crystal, we consider an external force F and Newton's second law of motion that

$$\boldsymbol{F} = \frac{d(\hbar\boldsymbol{k})}{dt}$$

Now we introduce a quantity called "effective mass" such that

$$\frac{dv_i}{dt} = \sum_j \left(\frac{1}{m^*}\right)_{ij} F_j$$

Since

$$\frac{dv_i}{dt} = \frac{d}{dt}\left(\frac{1}{\hbar}\frac{\partial E}{\partial k_i}\right) = \sum_j \frac{1}{\hbar}\frac{\partial^2 E}{\partial k_i \partial k_j}\frac{dk_j}{dt}$$

where i, j = x, y, z. The effective mass therefore is given

$$\left(\frac{1}{m^*}\right)_{ij} = \frac{1}{\hbar^2}\frac{\partial^2 E}{\partial k_i \partial k_j}$$

The effective mass can be negative or positive due to different dispersion relations. Notice that the effective mass is in general a tensor, which means that it can depend strongly on the crystal direction. Many properties of semiconductors can be described by using the effective mass approximation.

2. Density of states and dimensions of materials

To calculate various optical properties such as the rate of absorption or emission and how electrons and holes distribute within the energy band structure of the solid, we need to know the electron density of states (DOS). In semiconductors, the density of states is a property that quantifies how closely energy levels are packed. It is defined as the number of available states per unit volume per unit energy. In a three dimensional bulk system, the number of states between k and k + dk is

$$dN_{3D} = 2\left(\frac{L}{2\pi}\right)^3 4\pi k^2 dk$$

where we assume that the semiconductor is a cube with side L. By using the dispersion relation E(k) = h2k2/2m∗ we can obtain the density of states in terms of energy as

$$g_{3D}(E) = \frac{dN_{3D}}{dE} = \frac{1}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\sqrt{E}$$

For E ≥ 0. For a two-dimensional semiconductor such as a quantum well, in which electrons are confined to a plane, we can get the density of states

$$g_{2D}(E) = \frac{m}{\pi\hbar^2}$$

for E ≥ 0. In one dimension, the density of states becomes

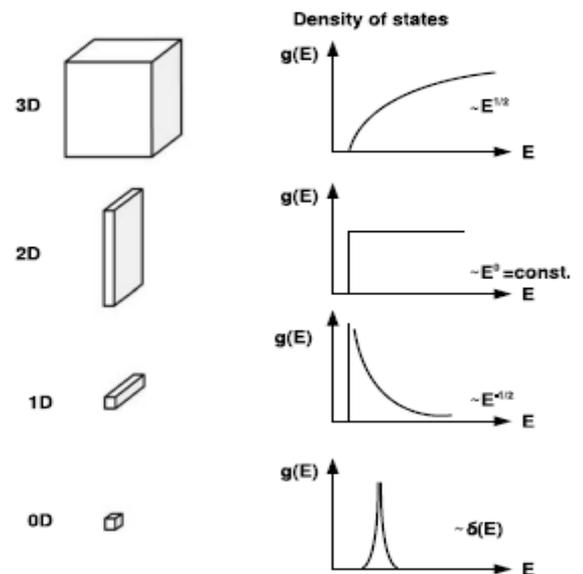$$g_{1D}(E) = \frac{1}{\pi}\left(\frac{m}{\hbar^2}\right)^{1/2}\frac{1}{\sqrt{E}}$$

Figure 3: The relationship between the density of states and the system dimension.

for E ≥ 0. And finally, for a zero dimensional system, e.g. a quantum dot, the energy states are quantised in all directions, and the density of states consists of only δ functions. Fig.2.3 shows the density of states for a bulk material, a quantum well with infinite barriers, a quantum wire with infinite barriers, and a quantum dot. The relationship between density of states and the system dimension is clearly shown in this figure. The DOS in 3D system is a function of E1/2, For a 2D system, the DOS is a step function with steps occurring at the energies of quantized levels. The DOS in a 1D system has an E−1/2 relation with energy. For a 0D system, it is a δ function of E Indirect optical transitions .The conduction band lies directly above the maximum of the valence band in the k space. In contrast, an indirect semiconductor refers to a

semiconductor with a bandgap in which the minimum energy in the conduction band is shifted by a k vector relative to the top of the valence band. Because of the small momentum associated with photons, optical transitions in which both initial and final states are band states are allowed only if the crystal momentum is conserved. Such processes are depicted by vertical lines in the E(k) diagram and are termed vertical transitions. For non-vertical transitions to occur the momentum has to be supplied from other sources including impurities and phonons. Transitions involving a photon state and a phonon or impurity state are termed indirect. Two important examples of indirect radiative transitions are the interband transition from the top of the valence band to a conduction band valley at or near the zone boundary, and intra-valley transitions responsible for free-carrier absorption. Fig. 3 shows the optical transition (emission in this case) processes in semiconductors with a direct bandgap and an indirect bandgap. Basic theory about indirect optical transitions. Whereas here we limit ourselves to describing the rate of phonon-assisted optical transitions.
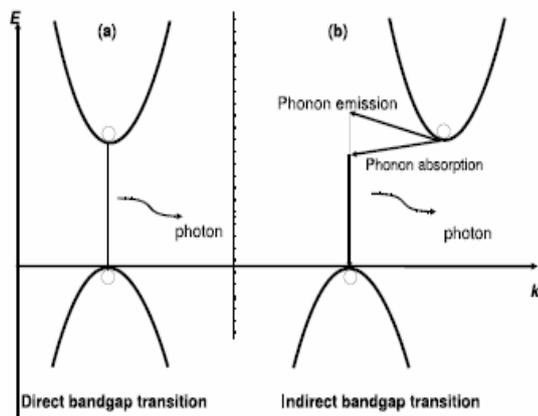

Figure 3: Scheme of optical transition in semiconductor with a direct bandgap and (b) indirect bandgap.

The transition rate from an initial state |i| to a final state |f| is given as by the second-order perturbation theory, where H = H⁻hω + Hep, Ei and Ef are the energies of the initial state and final states, respectively, and tau is the relaxation energy. One route of the transition is that H⁻hω, the optical perturbation, first induces an direct optical transition from the initial state |ii to an intermediate state |αi, requiring conservation of momentum. The phonon perturbation Hep completes the transition by taking the system from |αi to the final state |fi by contributing the phonon momentum in order to conserve the overall momentum and energy conservation. Alternatively, the first step can be accomplished by the phonon perturbation and the second step by the optical perturbation. Here we do not consider the less possible two-phonon (Hep active in both steps) or two-photon processes (H⁻hω active in both steps).

Let the initial state be a Bloch state of the valence band v denoted by |vki and the final state be a Bloch state of the conduction band c denoted by |ck′i. Consider the absorption of a photon of energy ⁻hω, of a phonon of energy ⁻hωq and crystal momentum ⁻hq. The total energies of the initial and final states are then

Ei = Evk + ⁻hω + ⁻hωq

Ef = Eck+q

Here we have already used the relationship of k′ = k + q due to the momentum conservation. If the phonon is absorbed first, the intermediate energy is given by

(a) Eα = Evk+q + ⁻hω

(b) Eα = Eck+q + ⁻hω

When the photon is absorbed first

(a) Eα = Eck + ⁻hωq

(b) Eα = Evk+q + ⁻hωq

(neglecting the photon momentum). Processes (a) and (b) are mutually distinct only when the initial and final states are in different bands. When this is the case the optical transitions for processes (b) are forbidden since they depend upon a matrix element of the form hvk|vki or hck+q|ck+qi, whereas processes (a) entail allowed transitions, therefore we do not need to consider processes (b) further. The sum S over the intermediate states is therefore

$$S = \frac{\langle ck+q|H_{\hbar\omega}|vk+q\rangle\langle vk+q|H_{ep}|vk\rangle}{E_{vk} + \hbar\omega_q - E_{vk+q} + i\Gamma_i} + \frac{\langle ck+q|H_{ep}|ck\rangle\langle ck|H_{\hbar\omega}|vk\rangle}{E_{vk} + \hbar\omega - E_{ck} + i\Gamma_i}$$

If Egk = Eck – Evk is the direct energy gap between bands v and c at k we can use Eq. in the first denominator to write the sum thus

$$S = \frac{\langle ck+q|H_{\hbar\omega}|vk+q\rangle\langle vk+q|H_{ep}|vk\rangle}{E_{gk+q} - \hbar\omega + i\Gamma_i} - \frac{\langle ck+q|H_{ep}|ck\rangle\langle ck|H_{\hbar\omega}|vk\rangle}{E_{gk} - \hbar\omega + i\Gamma_i}$$

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To obtain the total rate associated with the absorption of a photon we must add two further terms to the sum, similar in form to those in Eq. (3.6) which describe the emission of a phonon. If the two terms in Eq. (3.6) are labelled, respectively, S1+ and S2+, the similar terms associated with phonon emission S1– and S2–, the sum over intermediate states is given by S1+ + S2+ + S1– + S2–. In silicon the optical absorption edge is associated with a transition between the top of the valence band and one of the six valleys, and in germanium between the top of the valence band and one of the four L valleys in the conduction band. All of them are indirect transitions. The full calculation of the transition rate

is rather complicated since it involves eight matrix elements (two for each S). Here we only consider a calculation of the partial rate arising from important contributions which we assume to be embodied in the terms S2+ and S2−, because of their small denominators. Since the cross terms between S2− and S2+ do not contribute to the rate, we can write

$$w_{f \leftarrow i} = \frac{\Gamma_i/\hbar}{(E_f - E_i)^2 + \Gamma_i^2}(|S_{2+}|^2 + |S_{2-}|^2)$$

$$|S_{2\pm}|^2 = \frac{|\langle ck \pm q|H_{ep}|ck\rangle|^2 |\langle ck|H_{\hbar\omega}|vk\rangle|^2}{(E_{gk} - \hbar\omega)^2 + \Gamma_i^2}$$

The optical matrix element is identical to that for a direct transition. The square of the phonon matrix element for a given q has the following general form

$$|\langle ck \pm q|H_{ep}|ck\rangle|^2 = \frac{\hbar}{2N_{cell}M'} \frac{C_q^2 I(k, k+q)}{\omega_q} \begin{bmatrix} N(\omega_q) \\ N(\omega_q) + 1 \end{bmatrix}$$

where Ncell is the number of unit cells in the periodic crystal, M′ is the appropriate mass of the oscillator, e.g., the total mass of the unit cell in the case of acoustic modes, M1 +M2, or in the case of long-wavelength optical modes the reduced mass of 1/(1/M1 + 1/M2). Here M1 and M2 are the masses of the two atoms in the unit cell. N(ωq)/V is the phonon density

$$\frac{N(\omega_q)}{V} = n(\omega_q) = \frac{1}{e^{(\hbar\omega_q/k_B R)} - 1}$$

In the case of scattering between valley i and j (inter-valley) involving a phonon of frequency ωq with an inter-valley deformation potential constant Dij

$$\frac{C_q^2 I(k, k+q)}{M'} = \frac{D_{ij}^2}{M_1 + M_2}$$

where M1 +M2 is the total mass of the unit cell. Thus

$$|\langle ck \pm q|H_{ep}|ck\rangle|^2 = \frac{\hbar D_{ij}^2}{2\rho V \omega_q} \begin{bmatrix} N(\omega_q) \\ N(\omega_q) + 1 \end{bmatrix}$$

where ρ is the mass density, V the volume of the crystal within which the photon, electron and photon waves are normalized. We assume that inter-valley scattering is isotropic and independent of q.

3. INDIRECT OPTICAL TRANSITIONS

Finally, the optical transition between a valence band |vki and a conduction band state becomes

$$w_{f \leftarrow vk}(\hbar\omega) = \frac{|\langle f|H_{\hbar\omega}|vk\rangle|^2}{(E_{gk} - \hbar\omega)^2 + \Gamma_k^2} \frac{\hbar D_{ij}^2 N_{val}}{2\rho V \omega_q} \times$$

$$\left\{ \frac{N(\omega_q)\Gamma_k/\hbar}{(E_f - E_{vk} - \hbar\omega_q - \hbar\omega)^2 + \Gamma_k^2} + \frac{[N(\omega_q) + 1]\Gamma_k/\hbar}{(E_f - E_{vk} + \hbar\omega_q - \hbar\omega)^2 + \Gamma_k^2} \right\}$$

when the transition takes place between valley i and j (inter-valley) involving a phonon of frequency ωq with an inter-valley deformation potential constant Dij . Nval is the number of equivalent conduction band valleys containing final states. In Eq. (3.13), the first term headed by N(ωq) corresponds to the phonon absorption, while the other term is the phonon emission. Only one final state is coupled to a given initial state by k conservation for direct inter-band transitions. For indirect transitions the situation is different. Corresponding to a given initial state |vki there is a spread of final states in the conduction band brought about by phonon scattering, and hence the transition rate is given by

$$w_{vk}(\hbar\omega) = \sum_f w_{f-vk}(\hbar\omega) = \frac{|\langle f|H_{\hbar\omega}|vk\rangle|^2}{(E_{gk} - \hbar\omega)^2 + \Gamma_k^2} \frac{\hbar D_{ij}^2 N_{val}}{2\rho V \omega_q}$$

$$\left\{ N(\omega_q)N_c(E_{vk} + \hbar\omega + \hbar\omega_q) + [N(\omega_q) + 1]N_c(E_{vk} + \hbar\omega - \hbar\omega_q) \right\}$$

where Nc(E) is the density of states in a given conduction band valley. To obtain the total transition rate induced by a given photon energy which determines the photoluminescence intensity, we have to sum over all wvk(¯hω) which correspond to allowed processes, keeping ¯hω constant. This means summing over all possible initial states from Ek = 0 to Ekmax, where

$$E_{k_{max}} = \hbar\omega - E_g + \hbar\omega_q \quad \text{phonon absorption}$$
$$E_{k_{max}} = \hbar\omega - E_g - \hbar\omega_q \quad \text{phonon emission}$$

where Eg is the indirect band gap between two bands under investigation (between which the optical transitions occur). We multiply wvk by Nv(Ek)dEk, where Nv€ is the density of states in the valence band. In the case of parabolic bands

$$\int_0^{E_{k_{max}}} \sqrt{E_k(E_{k_{max}} - E_k)} \, dE_k = \frac{\pi E_{k_{max}}^2}{8}$$

and hence we obtain

$$w(\hbar\omega) = \frac{|\langle c\Gamma|H_{\hbar\omega}|v\Gamma\rangle|^2 D_{ij}^2 N_{val}(m_c^* m_v^*)^{3/2}}{(E_{g\Gamma} - \hbar\omega)^2 8\pi^2 \hbar^6 \rho \omega_q V}$$

$$\left\{ N(\omega_q)(\hbar\omega - E_g + \hbar\omega_q)^2 + [N(\omega_q) + 1](\hbar\omega - E_g - \hbar\omega_q)^2 \right\}$$

where the optical matrix element is approximated by the one at the Γ point. At room temperature N(ωq) ≫ 1, so that

$$w(\hbar\omega) = \frac{|\langle c\Gamma|H_{\hbar\omega}|v\Gamma\rangle|^2 D_{ij}^2 N_{val}(m_c^* m_v^*)^{3/2} n(\omega_q)}{(E_{g\Gamma} - \hbar\omega)^2 8\pi^2 \hbar^6 \rho\omega_q}$$
$$\left[(\hbar\omega - E_g + \hbar\omega_q)^2 + (\hbar\omega - E_g - \hbar\omega_q)^2\right]$$

Each type of allowed phonons contributes to the rate expressed by the above equation with Dij and ωq characterizing the mode. Furthermore, indirect inter-band optical transitions differ significantly from direct inter-band transitions in their dependence on photon energy. Near the threshold energy, Eth = Eg∓ħωq for indirect transitions,

while Eth = Eg for direct transitions, the former varies as (¯hω−Eth)2 while the latter varies as (¯hω − Eth)1/2.

4. OVERVIEW OF SIC MATERIALS

SiC is a wide band gap semiconductor with band gaps of 3.28 eV (4H) and 3.03 eV (6H), respectively. Due to the outstanding properties including high electron mobility, high breakdown electric field strength, and high thermal conductivity, SiC has an enormous potential for high-temperature and high-speed-power-device applications, which can work under extreme environments. SiC has also the strong tolerance to radiation damage, making it a good candidate material for defence and aerospace applications. Because of the convenience of combining the well developed Si process technology, SiC-based devices are easier to manufacture compared with other competitors. Starting from 1893, when the properties of SiC were first described, the research on SiC has received growing attention. Continuous progress in the crystal-growth technology of SiC has resulted in large size wafers. Of the large number of its possible poly types, 4H- and 6H- SiC have now been commercially produced in a quality considered appropriate for device applications.
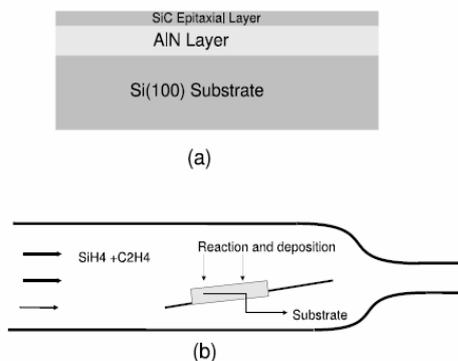
EXPERIMENT AND RESULTS ANALYSIS

(a)

(b)

Figure 3.2: Scheme of (a) 4H-SiC growth on AlN/Si(100) substrate by (b) CVD system. low

Some studies have shown that porous SiC exhibits intense visible luminescence at room temperature. Room temperature photo luminescence spectroscopy of SiC wafers has been reported recently with a peak below 2.0 eV.which is far away from the wide band gap of SiC. A photo luminescence peak at 3.18 eV from 4H-SiC attributed to the band edge emission.

EXPERIMENT AND RESULTS ANALYSIS

In our work, 4H-SiC films were grown on AlN/Si(100) substrates using the chemical vapour deposition (CVD) method. In a typical CVD growth process, the wafer (substrate) is exposed to one or more volatile precursors, which react and or decompose on the substrate surface to produce the desired deposit.In this work, the substrate is Si(100) with a AlN thin film as a buffer layer. AlN was chosen as the buffer layer here because of the small lattice mismatch between AlN and SiC.SiH4 and C_2H_4 were the reaction precursors,shown in Fig. 3.2(a). The deposition temperature was in the range of 1030-1130∘C. The sample cross section structure is schematically shown in Fig. 3.2(b). The AlN layer has a thickness of 200–300 nm. The PL measurements were carried out at room temperature by a325-nmHe-Cd
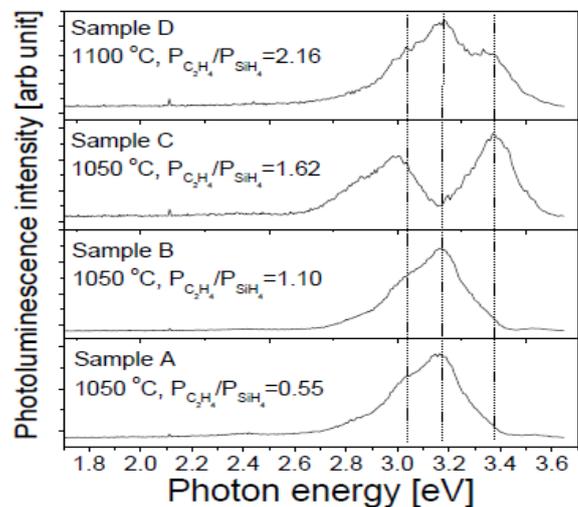
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