Optical and Transport properties of semiconductors heterostructures

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In this paper we review the optical and transport properties of semiconductors heterostructures. Transport properties as the drift-diffusion equation, the diffusion current, the thermionic emission current, and tunelling current. Optical properties of the complex refractive index, the absorption coefficient, the phenomena of reflection, transmission, and the different absorption processes.

1. INTRODUCTION

The junctions formed between two semiconductors(Fig 1a) with different energy gaps are referred to as heterojunction. In general, heterostructures offer a wide range of design choices for novel semiconductor devices (e.g., diodes, transistors, and optoelectronic devices). In an ideal heterojunction, the interface is atomically abrupt (In practical cases, such an ideal structure is nearly realized in $Al_xGa_{1-x}As/GaAs$ heterojunctions). The main advantages are related to the control of the charge carrier transport by controlling the energy barriers and potential variations (on a quantum level, Fig.1b) and to the ability of heterostructures to confine the optical radiation (which is especially essential in optoelectronic devices). Heterostructures are normaly grown by either metal-organic chemical vapor deposition (MOCVD) or molecular beam epitaxy (MBE) epitaxial techniques [2].
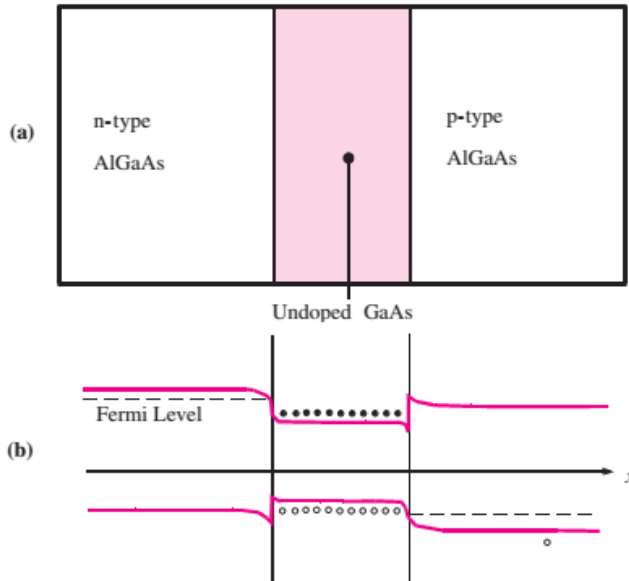

FIG. 1. (a) Structure of a double heterojunction. (b) Dependence of the band edge energies along the growth direction x [1].

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2. TRANSPORT PROPERTIES

A good understanding of charge carrier transport and electrical conduction is essential for selecting or developing electronic materials for device applications.

2.1. Drift-Diffusion Equation

The drift-diffusion model may be obtained by taking zeroth order moments of the Boltzmann Transport Equation and adjoining the Poisson equation. Thus, one obtains the system for N carriers with concentration n_i, carrier recombination R_i, current density J_i , (signed) charge e_i, i = 1,..., N:

$$e_i\frac{\partial n_i}{\partial t} + \nabla \cdot J_i = -e_i R_i \tag{1}$$

$$E = -\nabla\phi \tag{2}$$

$$\nabla \cdot (\varepsilon\nabla\phi) = -\sum e_i n_i - k_1 \tag{3}$$

Here the dielectric constant is denoted by ε, k_1 is the net impurity concentration, and ϕ is the electrostatic potential. There still remains the issue of determining the constitutive current relations. Classical drift-diffusion theory gives, for N = 2, $n_l = n$ (the electron density) , and $n_2 = p$ (the hole density),

$$J_n = -e\mu_n nE + eD_n\frac{dn}{dx} \tag{4}$$

$$J_p = -e\mu_p pE - eD_p\frac{dp}{dx} \tag{5}$$

The electronic charge modulus e is positive here, and n and p denote the electron and hole densities, respectively. The use of the Einstein relations linking the mobilities, μ_n, μ_p, and the diffusion coefficients, D_n, D_p, is common. These relations are specified by

$$D_n = (kT/e)\mu_n \tag{6}$$

$$D_p = (kT/e)\mu_p \tag{7}$$

The heterostructure drift-diffusion Eq.4 and Eq.5 may be solved analytically for the case of steady-state transport in one dimension, provided that recombination and generation may be neglected. The equations and their solutions can be incorporated into the conventional pn junction theory to obtain expressions for the $I(V)$ characteristics of a heterojunction.

2.2. Transport Carriers Mechanisms

The current across heterostructure junction is mainly due to majority carriers, by three distinct mechanisms: **diffusion** of carriers, **thermionic emission** of carriers and **quantum-mechanical tunneling**. The diffusion theory assumes that the driving force is distributed over the length of the depletion layer. The thermionic emission theory on the other hand postulates that only energetic carriers, those, which have an energy equal to or larger than the conduction band, contribute to the current flow. Quantum-mechanical tunneling through the barrier takes into account the wave-nature of the electrons, allowing them to penetrate through thin barriers. In a given junction, a combination of all three mechanisms could exist. However, typically one finds that only one current mechanism dominates. The analysis reveals that the diffusion and thermionic emission currents can be written in the following form:

$$J_n = evN_c exp(-\frac{\phi_B}{V_t})[exp(\frac{V_a}{V_t}) - 1] \qquad (8)$$

This expression states that the current is the product of the electronic charge e, a velocity v, and the density of available carriers in the semiconductor located next to the interface, where V_a is the applied voltage, ϕ_B the Schottky barrier height and N_c is the effective density of states. The velocity equals the mobility multiplied by the field at the interface for the diffusion current and the Richardson velocity for the thermionic emission current. The minus one term ensures that the current is zero if no voltage is applied as in thermal equilibrium any motion of carriers is balanced by a motion of carriers in the opposite direction.

Diffusion Current

Assuming that the depletion layer is large compared to the mean free path, so that the concepts of drift and diffusion are valid. The resulting current density equals:

$$J_n = e\mu_n E_{max} N_c exp(-\frac{\phi_B}{V_t})[exp(\frac{V_a}{V_t}) - 1] \qquad (9)$$

where E_{max} is electric field at the heterostructure interface. So that the prefactor equals the drift current at the heterostructure interface, which for zero applied voltage (V_a) exactly balances the diffusion current.

Thermionic Emission Current

The thermionic emission theory assumes that electrons, with an energy larger than the top of the barrier, will cross the barrier provided they move towards the barrier. So the current can be expressed as:

$$J_{MS} = A^* T^2 exp(-\frac{\phi_B}{V_t})[exp(\frac{V_a}{V_t}) - 1] \qquad (10)$$

where A^* is the Richardson constant and ϕ_B is the Schottky barrier height. The expression for the current due to thermionic emission can also be written as a function of the average velocity with which the electrons at the interface approach the barrier. This velocity is referred to as the Richardson velocity $v_R = \sqrt{\frac{kT}{2\pi m}}$, so that the current density becomes:

$$J_n = ev_R N_c exp(-\frac{\phi_B}{V_t})[exp(\frac{V_a}{V_t}) - 1] \qquad (11)$$

Tunneling Current

The tunneling current is obtained from the product of the carrier charge, velocity and density. The velocity equals the Richardson velocity, the velocity with which on average the carriers approach the barrier. The carrier density equals the density of available electrons, n, multiplied with the tunneling probability, Θ, yielding

$$J_n = env_R\Theta \qquad (12)$$

The tunneling probability term Θ, is added since the total current depends on the carrier flux arriving at the tunnel barrier multiplied with the probability Θ, that they tunnel through the barrier. The tunneling probability is obtained from:

$$\Theta = exp(-\frac{4}{3}\frac{\sqrt{2em^*}}{\hbar}\frac{\phi_B^{3/2}}{E}) \qquad (13)$$

3. OPTICAL PROPERTIES

The interaction of light with a semiconductor, allows us to observe the phenomena of **absorption**, **reflection** and **transmission**. From these optical effects, we obtain much of the information we have concerning the energy band structure and electronic precesses in semiconductors.

3.1. Complex Refractive Index and Absorption Coefficient

By means of classical electromagnetic theory we may relate complex refractive index (n^*) through the complex dielectric function (ε^*) as defined by means of the equation,

$\varepsilon^*(\omega) = \varepsilon(\omega) - i\sigma/2\pi v = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$, where ε is the ordinaty permittivity and σ the conductivity. The complex refractive index and dielectric function are related by means of the equation:

$$n^*(\omega) = n(\omega) + ik(\omega) = [\varepsilon_1(\omega) + i\varepsilon_2(\omega)]^{\frac{1}{2}} \quad (14)$$

From Eq.14 it follows that, $\varepsilon_1 = n^2 - k^2$ and $\varepsilon_2 = 2nk$, these quantities are most frequently plotted in order to describe the optical proprieties of a material.

The real part of the refractive index $n(\omega)$ determines the propagation velocity. The imaginary part $k(\omega)$ called the extinction coefficient, also called the attenuation index, determines the absorption coefficient:

$$\alpha = \frac{4\pi}{\lambda}k \quad (15)$$

In semiconductors, the absorption coefficient is a strong function of the wavelenght or photon energy. Near the absorption edge, the absorption coefficient can be expressed as

$$\alpha \propto (hv - E_g)^\gamma \quad (16)$$

where hv is the photon energy and γ is a constant. There exist two types of band-to-band transitions: allowed and forbidden (forbidden transitions take into accont the small but finite momentum of photons and are much less probable). For direct bandgap materials, transitions mostly occur between two bands of the same k value, as transitions (a) and (b) in Fig.2. While allowed direct transitions can occour in all k values, forbidden direct transitions can only occur at $k \neq 0$. In the one electron approximation, $\gamma = 1/2$ for allowed and $\gamma = 3/2$ for forbidden direct transitions. For $k = 0$ at which the bandgap is defined, only allowed transition occurs and thus it is used in determining the bandgap experimentally. For indirect transitions ((c) in Fig.2), phonons are involved in order to conserve momentum. In these transitions, phonons (with energy E_p) are either absorbed or emitted, and the absorption coefficient is midified to $\alpha \propto (hv - E_g \pm E_p)^\gamma$ where γ equals 2 and 3 for allowed and forbidden indirect transitions, respectively.

3.2. Reflectivity and Transmissivity

The reflectivity at the surface of a semi-infinite crystal can be calculated by considering incident and reflected waves in the vacuum and a trasmitted wave in the crystal. By applying electromagnetic boundary conditions at the crystal surface one can obtain an expression for the reflectivity. This expression is somewhat complicated for an arbitrary angle of incidence, so let consider a case of normal incidence. The amplitude of the electric field in the reflected wave, $E_{ref} = r(\omega)E_{inc}$, where $r(\omega)$ is give by

$$r(\omega) = \rho(\omega)exp[i\theta(\omega)] = \frac{n + ik - 1}{n + ik + 1} \quad (17)$$
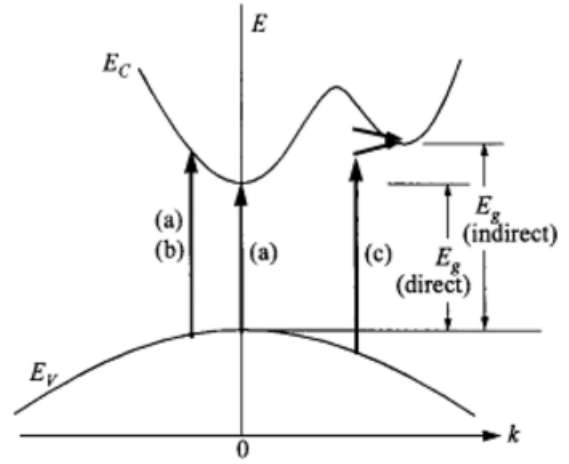

FIG. 2. Optical Transitions: (a) allowed and (b) forbidden direct transitions; (c) indirect transition involving phonon emission (upper arrow) and phonon absorption (lower arrow)[5].

where $\rho(\omega)$ is the modulus of $r(\omega)$, and $\theta(\omega)$ is the phase difference between the electric filds of the reflected and incident waves. The experimentally measurable reflectivity, $R(\omega)$, relates the incident and reflected intensities, I_{inc} and I_{ref}, $I_{ref} = R(\omega)I_{inc}$ where

$$R(\omega) = |r(\omega)| = \rho(\omega)^2 = \frac{(n-1)^2 + k^2}{(n+1)^2 + k^2} \quad (18)$$

and the transmission coefficient for the normal incidence is given by

$$T(\omega) = \frac{(1 - R^2)exp(-4\pi x/\lambda)}{1 - R^2 exp(-8\pi x/\lambda)} \quad (19)$$

where x is the thickness of the sample.

When light passes through a semiconductor, absorption of light and generation of electron-hole pairs occur, and the light intensity P_{op} diminishes with distance, $dP_{op}(r)/dr = -\alpha P_{op}(r)$, the solution of this expression gives an exponential decay of intensity, $P_{op}(r) = P_0(1 - R)exp(-\alpha r)$, where P_0 is the external incident light intensity and R is the reflection (Eq.20).

In a semiconductor sample of thickness x where the product αx is not large, multiple reflections will occur between the two interfaces. Summing up all the light components in the backward direction, the total reflection coefficient is calculed to be:

$$R_t = R[1 + \frac{(1 - R^2)exp(-2\alpha x)}{1 - R^2 exp(-2\alpha x)}] \quad (20)$$

and the transmission coefficient for the normal incidence is given by

$$T_t = \frac{(1 - R^2)exp(-2\alpha x)}{1 - R^2 exp(-2\alpha x)} \quad (21)$$

where x is the thickness of the sample.

By analyzing the $R_t - \lambda$ or $T_t - \lambda$ data at normal incidence, or by making observations of R_t or T_t for different angles of incidence, both n^* and k can be obtained and related to transitions energy between bands.

3.3. Optical Absorption

A typical relationship between the absorption coefficient and the photon energy observed in a crystalline semiconductor is shown in Fig.3, where various possible absorption processes are illustrated. Some of this processes will be discussed in the next topics.
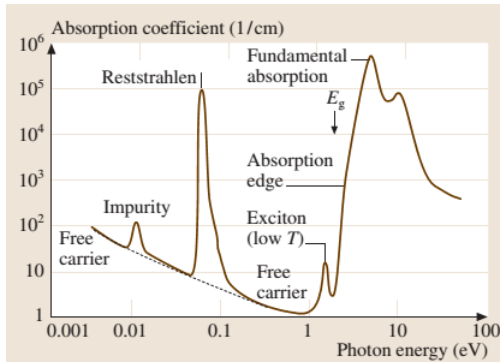

FIG. 3. Absorption coefficient plotted as a function of the photon energy in a typical semiconductor, illustrating various possible absorption processes [8].

Exciton Absorption

As indicated in Fig.3, some structure in the absorption spectra of semiconductors is often observed just below the fundamental absorption edge. This structure is due to exciton absorption. The energy band approximation for one electron, where the rest of the crystal was treated as a periodic potential, in this case there are no allowed energy states between the minima of the conduction bands and the maxima of the valence bands. When a electron-hole pair is created by absorption of a photon inside a semiconductor, the pair experiences an attractive Coulomb force. The latter is responsible for the creation of a bound state called an exciton. The appropriate modification of Eq.16 for exciton absorption (allowed direct transition) is $\alpha \propto (h\nu - E_g - E_{xn})^{1/2}$ where E_{xn} is the exciton energy.

Free Carrier Absorption

When the energy of the incident radiation is too small to create electron-hole pairs or excitons, other absorption processes can occur. The absorption of radiation by electrons in the conduction bands or by holes in the valence bands produces an absorption background below the fundamental absorption edge which increases with wavelength as indicated in Fig.3. In this process the electric fild of the incident radiation accelerates the free carries, which, in turn are decelerated by collisions with the lattice. Thus the energy is converted to heat.

Lattice Absorption

Fig.3 shows an absorption band due to optical phonons which is almost as strong as absorption due to electron transitions from the valence to conduction bands. This absorption is due to electric dipole coupling between photons and phonons which arises from the motion of charged atoms in the crystal (the structure on the high-energy side is due to multiple phonon absorption). Thus this absorption is strong for semiconductors with an ionic component of bonding and weak for those with ourely covalent bonding. If the radiation from a hot body is reflected several times from an ionic crystal, the dominant remaining frequencies will be those in this band of energy. For this reason this absorption is called the "restrahlen" or "residual ray" band.

Impurity Absorption

This absorption process is that due to direct band-to-impurity transition. The transition probability has the same form as for direct band-to-band transitions.

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