Effects of Band Nonparabolicity and Band Offset on the Electron Gas Properties in *InAs/AlSb* Quantum Well

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Abstract

One-band effective mass model is used to simulation of electron gas properties in quantum well. We calculate of dispersion curves for first three subbands. Calculation results of Fermi energy, effective mass at Fermi level as function of electron concentration are presented. The obtained results are good agreement with the experimental dates.

Keywords

Quantum Well, In-Plane Dispersion, *InAs*, *AlSb*, Two Dimentional Electron Gas, Effective Mass, Cyclotron Mass

1. Introduction

In semiconductors, *InAs* and *InSb* of the conduction band are characterized by a strong nonparabolicity and recently intensively studied heterostructures based on them [1]-[3]. Nonparabolicity of the conduction band and the nature of the spin splitting of the electron in the quantum well (QW) are studied by the cyclotron resonance [4]-[7].

In [8] has been investigated *InAs/AlSb* based QW with well width L = 15 nm, where two dimensional (2D) electron concentration ranges from 2.7×10^{11} to 8×10^{12} cm^{-2}. In this work has been found increase of the effective mass of almost 2 times.

The purpose of this work—the calculation of: 1) subbands dispersion curves, 2) the density of states of 2D electron gas and 3) concentration dependence of effective mass in Fermi level for *InAs/AlAs* QW with width L = 15 nm.

It is shown that an abrupt change in the density of states leads to a peculiar change in

the concentration dependence of effective mass.

2. The In-Plane Dispersion

Consider a single QW with width L (area A—*InAs*), concluded between barriers with height V (area B—*AlAs*). The energy is measured from the bottom of the band of the bulk *InAs*.

In the one band effective mass approximation, the solution of the three-dimensional Schrödinger equation can be represented as $\psi = e^{i(k_x x + k_y y)}\phi(z)$. Then for the area A and B, respectively, we can write the following one-dimensional equations

$$\frac{\partial^2 \phi_A(z)}{\partial z^2} + q^2 \phi_A(z) = 0, \quad q = \sqrt{\frac{2m_A(E)}{\hbar^2}E - k^2} \tag{1}$$

$$\frac{\partial^2 \phi_B(z)}{\partial z^2} + \chi^2 \phi_B(z) = 0, \quad \chi = \sqrt{\frac{2m_B(E)}{\hbar^2}(V - E) + k^2} \tag{2}$$

Here $k^2 = k_x^2 + k_y^2$ and $k-$ is in plane wave vector, $m_{A,B}(E)$ —energy-dependent effective mass of the electrons in the material A or B. Solving Equations (1) and (2), using the boundary condition

$$\phi_A(0) = \phi_B(0), \quad \frac{1}{m_A(E)}\frac{d\phi_A(z)}{dz}\bigg|_{z=0} = \frac{1}{m_B(E)}\frac{d\phi_B(z)}{dz}\bigg|_{z=0} \tag{3}$$

$$\phi_A(L) = \phi_B(L), \quad \frac{1}{m_A(E)}\frac{d\phi_A(z)}{dz}\bigg|_{z=L} = \frac{1}{m_B(E)}\frac{d\phi_B(z)}{dz}\bigg|_{z=L} \tag{4}$$

we find the dispersion equation

$$E = E_\parallel + E_0 \left[\pi \cdot n - 2\,Arc\sin\left(\sqrt{\frac{\gamma^2\left(E - E_\parallel\right)}{\gamma(\gamma-1)E + \gamma\,V + \left(1 - \gamma^2\right)E_\parallel}}\right)\right]^2 \tag{5}$$

here $E_\parallel = \hbar^2 k^2 / 2m_A(E)$, $E_0 = \hbar^2 / 2m_A(E)L^2$, $\gamma = m_B(E)/m_A(E)$.

Nonparabolicity of conduction band well takes into account by formulas

$$\frac{m_0}{m_A(E)} = 1 + \frac{E_{PA}}{3}\left[\frac{2}{E + E_{gA}} + \frac{1}{E + E_{gA} + \Delta_A}\right] \tag{6}$$

$$\frac{m_0}{m_B(E)} = 1 + \frac{E_{PB}}{3}\left[\frac{2}{E - V + E_{gB}} + \frac{1}{E - V + E_{gB} + \Delta_B}\right] \tag{7}$$

where, m_0 —the free electron mass, E_P —the Kane parameter, E_g —the band gap, Δ — the spin-orbital splitting of valence band, V—conduction band offset. Band parameters of *InAs* and *AlSb* are shown in Table 1.

To describe the statistics of electrons, Equation (5) is non convenient because it is not solvable with respect to E or k. Therefore, we replace Equation (5) is by simple approximation

$$E\frac{m_A(E)}{m_A(0)} \approx \frac{\hbar^2 k^2}{2m_A(0)} + E_n \frac{m_A(E_n)}{m_A(0)} \tag{8}$$

Table 1. Band parameters of *InAs* and *AlSb*.

	InAs (*A*)	*AlSb* (*B*)
E_g, eV	0.42	2.37
Δ, eV	0.38	0.75
E_P, eV	21.2	20.85
$m(0)$, [m_0]	0.023	0.11
V, eV	0	1.35

where, E_n—is bottom of n-th subbands. Now, approximation (8) is the best solution of (5). However, values of E_n in (8) now are obtained from Equation (5) at $k = 0$ by use numeric method.

For *InAs/AlSb* QW with $L = 15$ nm, we have: $E_1 = 0.0454$ eV, $E_2 = 0.158$ eV, $E_3 = 0.304$ eV, and for case $L = 6$ nm we have: $E_1 = 0.163$ eV, $E_2 = 0.509$ eV, $E_3 = 0.903$ eV.

Calculated dispersion curves from Equation (5) and approximation (8) are compared in **Figure 1(a)**, **Figure 1(b)**.

From **Figure 1(a)**, **Figure 1(b)** follows that, the approximation (8) is sufficiently accurate and/or (8) is the best solution of (5) in a wide range of width QW. It is convenient when studying the statistics of electrons, kinetic, optical, or other characteristics of the 2D electron gas. Inconveniences approximation (8) is such that $E_n \, (n = 1, 2, 3, \cdots)$ depends on L, V and on other parameters of materials A,B. Therefore every time when changing these parameters, the value of E_n is recalculated from Equation (5) at $k = 0$.

3. The Fermi Energy and Thermodynamic DOS

The total electron concentration is

$$n_s = N_0 \sum_{n=1} \int_{E_n}^{E_F} \mathrm{d} \left(\frac{\hbar^2 k^2}{2 m_A (0)} \right) \tag{9}$$

where

$$N_0 = \frac{m_A (0)}{\pi \hbar^2} = \frac{m_A (0) \cdot 0.413 \times 10^{15}}{\text{эВ} \cdot \text{см}^2} \; .$$

According (8) we have

$$n_S = \sum_{n=1} n_S^{(n)} \; , \quad n_s^{(n)} = N_0 \left[E_F \frac{m_A (E_F)}{m_A (0)} - E_n \frac{m_A (E_n)}{m_A (0)} \right] \theta \left(E_F - E_n \right) \tag{10}$$

where $n_s^{(n)}$—is *n*-th subband concentration.

In Equation (10), the terms in the sum should be positive. The negative terms in $n_s^{(n)}$ excluded by the Heaviside function. It establishes a link between the Fermi energy E_F and full 2D electron concentration n_s. They also determine the concentration of electrons in separate subbands $n_s^{(n)}$ for a given n_s.

From (10), we can estimate the critical concentrations of n_{c1}, in which the Fermi level comes to bottom of the second subband $E_F = E_2$. In the structure of InAs/AlSb QW
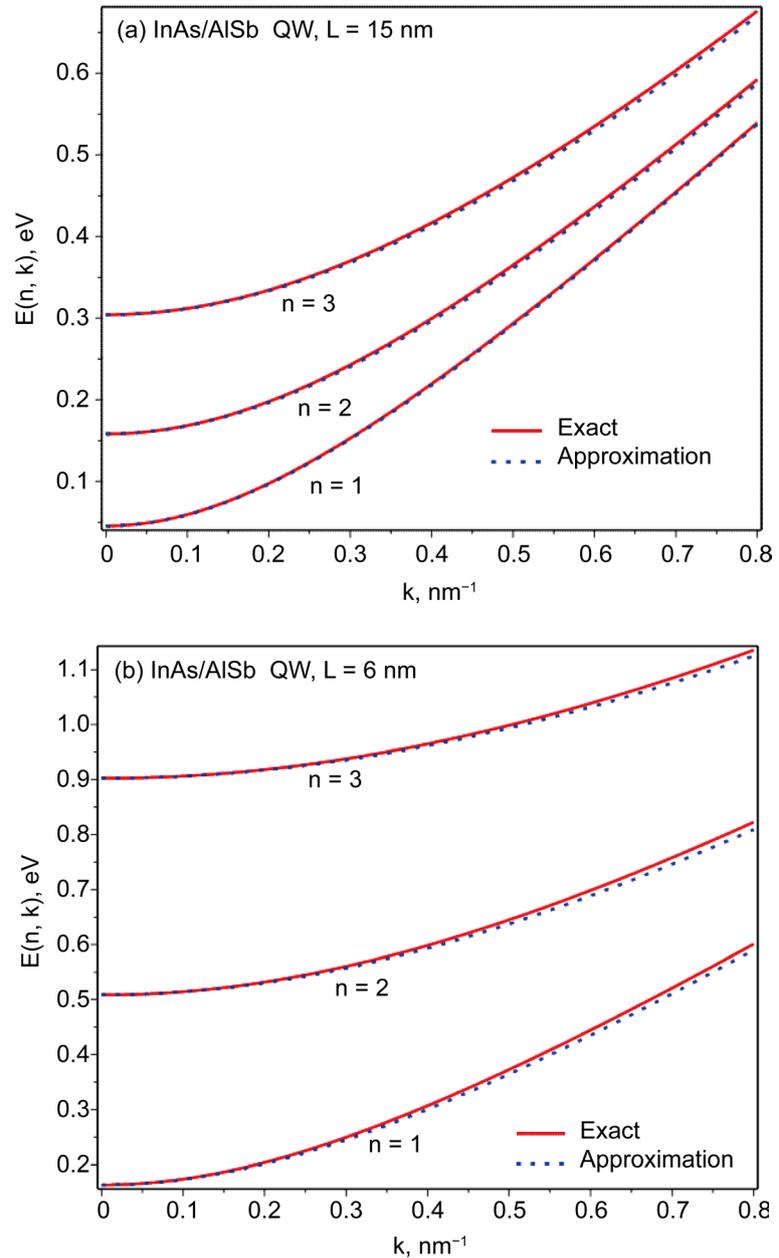
Figure 1. The dispersion curves of the first three subbands (n = 1, 2, 3) in *InAs/AlSb* QW: the full (red) line—according to Equation (5), the dotted (blue) line—approximation (8); (a) L = 15 nm, (b) L = 6 nm.

with the well width L = 15 nm can be found

$$n_{c1} = N_0 \left[E_2 \frac{m_A(E_2)}{m_A(0)} - E_1 \frac{m_A(E_1)}{m_A(0)} \right] = 1.52 \times 10^{12} \text{ cm}^{-2} \tag{11}$$

This estimation is close to experimental measured date $n_{c1,\exp} = 1.2 \times 10^{12}$ cm^{-2} [8]. Similarly, the critical concentration of n_{c2}, in which the Fermi level comes to bottom of the third subband $E_F = E_3$, is $n_{c2} = 6.87 \times 10^{12}$ cm^{-2}.

The dependence $E_F(n_s)$ is shown in **Figure 2**. It is obtained from Equations (10) by changing the Fermi energy in the range of $E_F = 0 \div 0.33\,\text{eV}$. The graph shows that, depending on $E_F(n_s)$ there exist a fractures—slowing of increase the Fermi's energy. They are caused by abrupt changes (by jumps), the density of states at the critical points: $n_s = n_{c1}$, $E_F = E_2$, $n_s = n_{c2}$, $E_F = E_3$.

These fractures occur at the critical concentrations of $n_{c1}, n_{c2} \cdots$, where E_F intersects the Fermi level of the bottom of the next subband.

The thermodynamically DOS of electron gas at Fermi level $N_T(E_F) = \mathrm{d}n_S/\mathrm{d}E_F$ is shown in **Figure 3**.

4. The Cyclotron Mass

According approximation (8), the electron effective mass at the Fermi level (cyclotron mass) $m_c = \hbar^2 k \left(\mathrm{d}E/\mathrm{d}k\right)^{-1}\Big|_{E=E_F}$ is

$$m_c = \left(m_A(E) + E\frac{\mathrm{d}m_A(E)}{\mathrm{d}E} \right)_{E=E_F} \tag{12}$$

The dependence $m_c(n_s)$ is shown in **Figure 4**.

This dependence can be obtained from Equations (10) and (12) by changing the Fermi energy in the range $E_F = 0 - 0.33\,\text{eV}$.

This figure shows also the dependence of experimentally measured value of the effective masses (cyclotron mass) m_c at the Fermi level of the total concentration of 2D n_s [8]. Fracture in the $m_c(n_s)$ occur at critical points: $n_s = n_{c1}$, $E_F = E_2$ and $n_s = n_{c2}$, $E_F = E_3$.
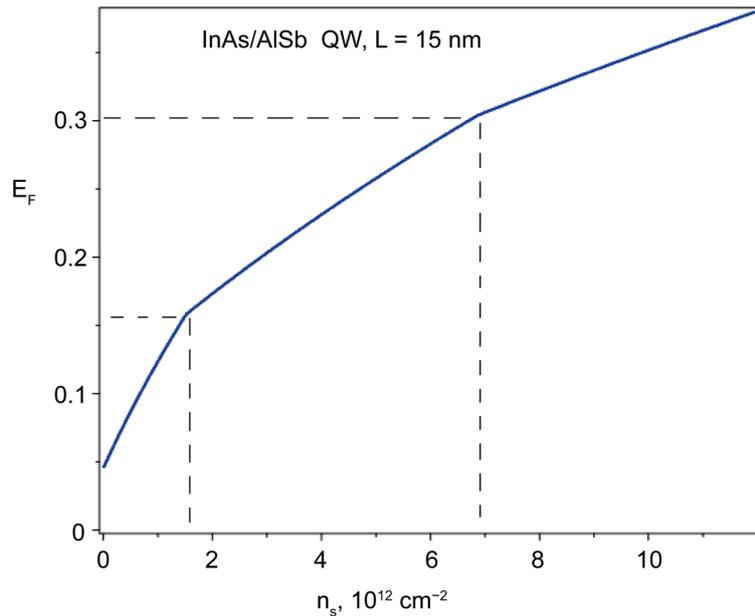
Figure 2. The dependence of the Fermi energy on the 2D concentration in *InAs/AlSb* QW with *L* = 15 nm, *V* = 1.35 eV. The critical points $n_s = n_{c1}$, $E_F = E_2$ and $n_s = n_{c2}$, $E_F = E_3$ shown by the shaded lines.
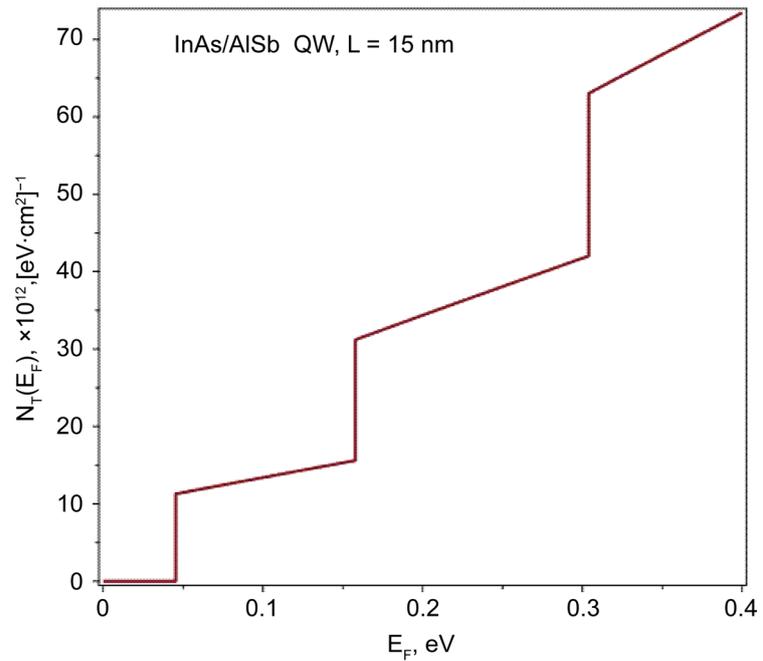
Figure 3. The thermodynamically DOS of electron gas at Fermi level in *InAs/AlSb* QW, *L* = 15 nm, *V* = 1.35 eV.
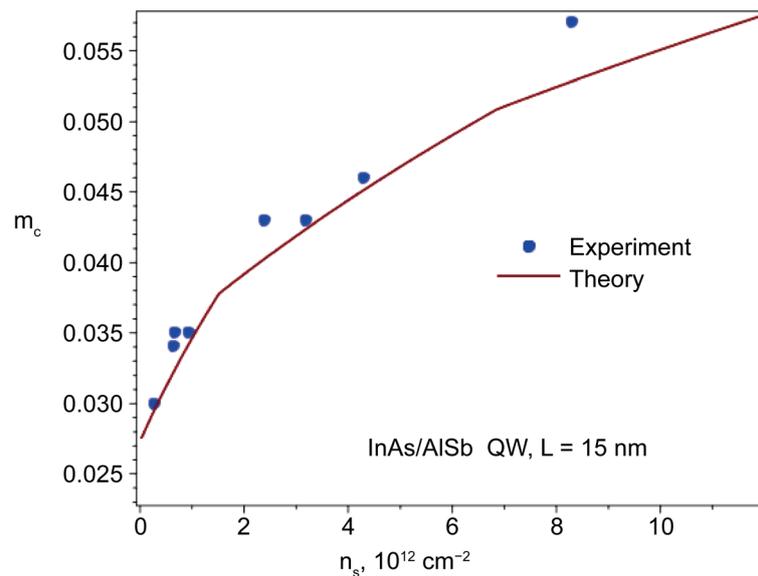
Figure 4. The dependence of the effective mass on the total concentration for InAs/AlSb QW, *L* = 15 нм, *V* = 1.35 eV.

5. Conclusion

In this study are provided useful approximation (8) of subband dispersions and simplified Equation (10) to calculate the statistics of a degenerate electron gas in heterostructured InAs/AlSb QW, which satisfactorily describes the experimental results [8]. They are also useful to study of calculation of the transport, optical and magnetic properties

of electron gas in a Kane type 2D system. The above description of the algorithms can be applied to other QW heterostructures based on semiconductor group A_3B_5.

Acknowledgements

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