ELECTRIC FIELD EFFECT ON THE INTERBAND TRANSITIONS IN NEAR-SURFACE QUANTUM WELLS

Ecaterina C. NICULESCU¹, Florin BURCEA²

Dependența de câmpul electric a tranzițiilor interbandă într-o groapă cuantică localizată în vecinătatea interfeței cu vidul este studiată utilizând aproximarea masei efective. În calcul se ține seama de efectul interacțiiei repulsive între purtătorii de sarcină și sarcina lor imagine. Pentru grapi cu strat înveliș subțire se observă o dependență accentuată a energiilor uniparticulă de prezența sarcinii imagine și o deplasare Stark asimetrică pentru energia tranziției bandă-bandă. O asemenea dependență a proprietăților optoelectronice de geometrie și de câmpul electric extern poate fi utilizată pentru proiectarea unor dispozitive.

The electric field dependence of the interband transitions in a near-surface quantum well (NSQW) under an applied electric field is investigated in the effective mass approximation and taking into account the electrostatic self-energy due to the repulsive interaction of the carriers with their image charges. For small capped layer thicknesses we observe strongly changes in the single particle spectrum and an asymmetric Stark shift of the interband transition energy. Such a dependence of the optoelectronic properties on the geometry and electric field strength in NSQWs can be very useful for several potential device applications.

Keywords: Quantum well, electronic states, electric field, image-charge.

1. Introduction

The quantum well Stark effect and intersubband optical properties have attracted a great deal of interest because of their potential applications in optical devices [1-10]. By engineering the well width and barrier height, quantum well devices with desirable properties may be fabricated. As a special type of dielectric quantum wells, the near-surface quantum wells (NSQWs) have been received increasing attention because of their potential to sustain electro-optic operations under a larger range of applied electric fields. It has been predicted [11] that the electronic levels in narrow semiconductor layers surrounded by a dielectric of a smaller dielectric constant have to be significantly enhanced. This effect originates from the modification of the carriers interaction by the images induced

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A well developed technique of growing and etching of InGaAs/GaAs QW structures allows one to fabricate such structures with well defined both InGaAs QW and GaAs cap layer thicknesses [13, 18]. For more detailed studies of the dielectric confinement in such structures, one can apply external electric or (and) magnetic fields. The energy levels are significantly modified by the applied fields leading to new possibilities to study the dielectric confinement effect in detail.

In the present study we have carried out a systematic theoretical study of the effect of image charges on the electronic properties in the InGaAs/GaAs NSQWs under a static electric field. The paper is organized as follows: in Sec. 2 the theoretical model for the image charge and electric field effects on the subband states in NSQWs is described. The eigenfunctions and eigenenergies for the conduction and valence band are obtained using the effective mass approximation and a transfer matrix method. In Sec. 3 we present the results of the numerical calculations on InGaAs NSQW with GaAs barriers under an electric field. Finally, our conclusions are summarized in Sec. 4.

2. Theory

In mass effective approximation, the NSQW electron (hole) Hamiltonian in the electric field \( E(0,0,F) \) takes the form

\[
H_{e(h)} = -\frac{\hbar^2}{2m^*_{e(h)}} \frac{\partial^2}{\partial z^2} + \tilde{V}_{e(h)}(z) + V_{self}(z) \pm eFz
\]

where \( m^*_{e(h)} \) is the electron (heavy hole) effective masses and the band-offset potentials are given by

\[
V_{e(h)}(z) = \begin{cases} 
\infty, & z < -L_e - L_w / 2 \\
0, & -L_w / 2 \leq z \leq L_w / 2 \\
V_e (V_h), & -L_e - L_w / 2 < z < -L_w / 2 \text{ and } z > L_w / 2
\end{cases}
\]

The third term in Eq. (1) is the electrostatic self-energy due to the repulsive interaction of the carriers with their image charge,

\[
V_{self}(z) = \frac{e_0^2}{2\varepsilon} \left( \varepsilon - 1 \right) \frac{1}{2|z|}
\]

where \( \varepsilon \) is the dielectric constant of the semiconductor. For simplicity, we neglect a small difference between \( \varepsilon \) values in In\textsubscript{x}Ga\textsubscript{1-x}As and GaAs.
The conduction and valence band potential profiles of the In$_{0.18}$Ga$_{0.82}$As/GaAs NSQW are plotted in Fig. 1. The dotted curves show the ground subband wave functions in the absence of the electric field.

![Fig. 1. The potential profiles for the conduction and valence band of the GaAs/In$_{0.18}$Ga$_{0.82}$As NSQW. The dotted curves show the ground subband wave functions in vanishing electric field.](image)

Our calculation proceeds in two steps. First, using the matrix transfer method, we find the electron and hole single-particle bound states in the heterostructure in the absence of the electric field. Once the electron and hole ground state wavefunctions, $\varphi_e(z)$ and $\varphi_h(z)$, and the corresponding energies $E_e^0$ and $E_h^0$ are determined, the bound states in the applied electric field can be evaluated by means of the variational principle. To account for the redistribution of the electronic charge density under electric field parallel to the growth axis, we choose the trial wave functions

$$
\Psi_{e(h)}(z, \lambda_{e(h)}) = \varphi_{e(h)}(z) \exp(-\lambda_{e(h)} z).
$$

Here $\lambda_{e(h)}$ are the variational parameters determined by minimizing the electron (hole) energy

$$
E_{e(h)}(F) = \min_{\lambda_{e(h)}} \frac{\langle \Psi(z, \lambda_{e(h)}) | H_{e(h)}(z, F) | \Psi(z, \lambda_{e(h)}) \rangle}{\langle \Psi(z, \lambda_{e(h)}) | \Psi(z, \lambda_{e(h)}) \rangle}.
$$

Neglecting the exciton effects, the interband transition energy is given by

$$
E^* = E_e + E_h + E_{\text{InGaAs}}^g.
$$

3. Results and discussion

The numerical calculations were carried out for a In$_{0.18}$Ga$_{0.82}$As/GaAs NSQW with the well width $L_W = 0.5$ nm by using the material parameters [12] listed in Table 1.
Table 1

<table>
<thead>
<tr>
<th>Material parameters used in calculations</th>
</tr>
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<tbody>
<tr>
<td>Material</td>
</tr>
<tr>
<td>$V_e$ (meV)</td>
</tr>
<tr>
<td>$V_h$ (meV)</td>
</tr>
<tr>
<td>$m_e/m_0$</td>
</tr>
<tr>
<td>$m_{ih}/m_0$</td>
</tr>
<tr>
<td>$m_{hh}/m_0$</td>
</tr>
<tr>
<td>$E_{g}^{\Gamma}$ (meV)</td>
</tr>
<tr>
<td>$\varepsilon$</td>
</tr>
</tbody>
</table>

The effective confining potential of the electron $V_{eff} = \tilde{V}_e(z) + V_{self}(z) + eFz$ in a NSQW with $L_W = L_c = 0.5$ nm in the applied electric field without (A) and with (B) the image charge effect is plotted in Fig. 2.

Fig. 2. The effective confining potential of the electron in a $L_W = L_c = 0.5$ nm NSQW in the applied electric field without (A) and with (B) the image charge effect.
We observe that if we do not consider the image charge effect, the potential profile of the NSQW is asymmetric, since the barrier height at the SV interface is infinitely high while the barrier height at the other side of the QW is finite. The image charge leads to a gradually change of the left barrier and a reduction of this asymmetry.

The single particle electron and hole energies in In$_{0.18}$Ga$_{0.82}$As/GaAs NSQW are presented in Table 2 for different capped layer thickness $L_{\text{cap}}$ with and without the image charge effect.

<table>
<thead>
<tr>
<th>$L_c$ (nm)</th>
<th>Energy (meV)</th>
<th>electron</th>
<th>hole</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(a)</td>
<td>(b)</td>
<td>(a)</td>
</tr>
<tr>
<td>1</td>
<td>81.63</td>
<td>76.35</td>
<td>28.62</td>
</tr>
<tr>
<td>2</td>
<td>71.51</td>
<td>66.65</td>
<td>25.34</td>
</tr>
<tr>
<td>3</td>
<td>65.84</td>
<td>61.59</td>
<td>23.76</td>
</tr>
<tr>
<td>4</td>
<td>62.72</td>
<td>59.03</td>
<td>22.87</td>
</tr>
<tr>
<td>5</td>
<td>60.94</td>
<td>57.74</td>
<td>22.28</td>
</tr>
<tr>
<td>6</td>
<td>59.88</td>
<td>57.06</td>
<td>21.86</td>
</tr>
<tr>
<td>7</td>
<td>59.21</td>
<td>56.72</td>
<td>21.53</td>
</tr>
<tr>
<td>8</td>
<td>58.77</td>
<td>56.54</td>
<td>21.27</td>
</tr>
<tr>
<td>9</td>
<td>58.46</td>
<td>56.44</td>
<td>21.07</td>
</tr>
<tr>
<td>10</td>
<td>58.23</td>
<td>56.39</td>
<td>20.89</td>
</tr>
</tbody>
</table>

(a) with image charge effect; (b) without the image charge effect.

It is seen that the subband energies are enhanced significantly due to the image charge effect which is more important for narrow capped layers. Also, we observe that the capped layer decreasing causes a strong blueshift of the energies. This increasing of the energy with decreasing $L_c$ is due to two reasons. The first one is the influence of the high vacuum potential barrier in a close vicinity of the well. This effect has a tunneling origin and it is called „tunneling blueshift” [15]. The second reason for the blueshift is the repulsion between charges and their self-images, described by the term $V_{\text{self}}$. This is a „dielectric blueshift” [15].
In Fig. 3 we show electric field effect on the single particle electron and hole energy levels.

![Fig. 3](image)

It should be pointed out that the Stark shifts $\Delta E = E(F) - E_0$ are asymmetric with respect to the electric field and it becomes smaller when the capped layer thickness increases. This asymmetric Stark shift arises from the competition between the electric field effect and the image charge effect. The blueshifts or redshifts of the energies are determined by the direction and strength of the electric field. When the electric field is applied along the positive $z$ axis, the electron is pushed in the opposite directions toward vacuum-semiconductor interface. Thus, the repulsive interaction with their image charges increases and leads to an enhanced energy.

Note that for the electron in NSQWs with very small capping-layer thickness only the energy blueshift occurs. In contrast, the hole is moved along the applied field and the image charge effect becomes weaker.

Consequently, when the electric field becomes strong the electron and the hole are pushed in the opposite directions: the electron becomes more and more localized inside the well, whereas the hole leaks out of the QW. This feature can be observed in Fig. 4, which shows the probabilities of finding the particles in the well as function of the electric field for several layer capped thicknesses.
Fig. 4. The probability for finding the electron (A) and the heavy-hole (B) as a function of the electric field for several values of the capped layer thickness. Notations a, b, c, d and e are the same as in Fig.3.

To show clearly the electric field effect on the absorption peak in the NSQW structure, in Figure 5 we plot the interband transition energy as a function of the electric field for different capped layer thicknesses.

As seen from figure 5, for narrow capped layers the variation of the interband transition energy as a function of electric field is different from the behavior of larger $L_c$. For $L_c = 2$ nm the interband transition energy increases for $F \leq 40$ kV/cm and the absorption spectrum presents blueshift, then this quantity decreases and the absorption spectrum shows redshift.

By increasing the capped layers thickness the dielectric enhancement induced by the image charge is weakened. Thus the transition energy presents the
well-known transition from a quadratic field to a linear field dependence, typical for a quantum well under an electric field. Such a dependence of the interband transition energy on the geometrical confinement and external field strengths in NSQWs can be very useful for potential device applications.

4. Conclusions

In this paper we have studied the electronic properties of the near-surface quantum well in the presence of an applied electric field. We used the effective mass approximation and a matrix transfer method to calculate the energy spectrum for a wide range of capped layer thicknesses and electric field strengths. We have shown that using capping layers of various thicknesses it can be control the carrier confinement in NSQW structures. The interband transition energy in these systems in different geometrical confinement regimes has been calculated. We found that the corresponding absorption peak can be easily modulated by varying the electric field strength and the capped layer thickness.

REFERENCES