Quantum confined Stark effect in $\eta$-type delta-doped quantum wells

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Electronic states in Si $\delta$-doped GaAs quantum wells with an electric field applied perpendicular to the layers have been studied. Thomas-Fermi approximation for the self-consistent external potential in the tight binding model and a spin-dependent Green-function matching method. The Stark shifts of the electronic states have been obtained for various Si $\delta$-doped concentrations. The Stark shifts are compared with the available results in the case of rectangular and graded gap quantum wells.

Keywords: Quantum confined Stark effect; Si $\delta$-doped quantum wells; tight-binding method.

1. Introduction

Investigation of electric field effects (Stark effects) in the $\delta$-doped semiconductor heterostructures has become possible due to the abilities of modern crystal growth techniques to control purity and dimensions. Quantum confined Stark effect in quantum wells (QWs) is of great interest due to the fact that most of the devices based on QWs work under application of an electric field [1,2]. The single and multiple $\delta$-doped structures are experimentally and theoretically intensively investigated in order to study their subband spectra which is important for the numerous potential applications in optoelectronic devices. In this work, we present numerical calculations of electronic energy states in Si $\delta$-doped GaAs QWs at different impurity concentrations $n_{2D}$ and under application of an external uniform electric field $F$. The calculations are conducted using the semi-empirical tight binding (TB) method, which is often used to treat field-related effects in electronic and optical properties of nanostructured materials and devices [3-5]. Theoretical works about electric field effect in single and multiple Si $\delta$-doped GaAs systems have been done mainly in the effective mass approximation [6-10]. To the best of our knowledge, there are no tight binding considerations of the Stark effect in these $\delta$-doped systems. The detailed realistic microscopic description based on the TB is nowadays a required step to understand the behavior of modern semiconductor nanostructures and in such a way to support the project of new promising nanostructures and nanostructured devices [11].

2. Model and method

We consider a Si $\delta$-doped GaAs QW with impurity concentration $n_{2D}$ from $1 \times 10^{12}$ to $10 \times 10^{12}$ cm$^{-2}$ with a step of $1 \times 10^{12}$ cm$^{-2}$. The inhomogeneous Si $\delta$-doped finite region (V-shaped $\delta$-doped QW) consists of 250 monolayers (MLs) and is matched with two semi-infinite homogeneous GaAs barriers. We use the $sp^3s^*$ spin dependent semi-empirical TB model and the surface Green function matching method, as it is described in [12]. The calculations are performed at the center of the two-dimensional Brillouin zone for the GaAs [100] growth direction. The $\delta$-potential is treated as an external potential in the Thomas-Fermi approximation [13]. The external constant electric field is applied between the two sides of the QW in the growth direction. We add it as an external potential to all diagonal elements of the Hamiltonian matrix in each atomic layer:

$$TB_{ii}(n) = TB_{ii}(0) + neF,$$

where $n$ labels the atomic layer number in the growth direction; $e$ is the electron charge; $TB_{ii}$ are the diagonal TB pa-
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3. Results and discussion

We have calculated the bound states in the $\delta$-doped QW described above. The number of bound states increases with increasing donor concentration. Our calculations give many more bound states than other calculations based on the envelope function approximation [6]. For example, for $n_{2D} = 10.10^{12}$cm$^{-2}$ and $F = 10$ kV/cm we found 9 bound states, while in Ref. 6 only three bound states appear at high doping. Figure 2 presents the calculated energies of the ground ($E_{C0}$) state and three excited states ($E_{C1}$, $E_{C2}$, and $E_{C3}$) for four different two-dimensional carrier concentrations ($n_{2D} = 3, 5, 8, and 10$) as a function of the electric field.

Figure 4. Spatial distributions of the total spectral strength for the ground C0 (dotted line) and first excited C1 state (solid line), at given values of applied F in units (kV/cm) and for (a) $n_{2D}=1.10^{12}$cm$^{-2}$, (c,d) $n_{2D}=10.10^{12}$cm$^{-2}$. We notice that the electric field
effects on energy levels are similar for all impurity concentrations. Increasing the value of the field decreases the energies. It is seen that at larger donor concentrations the energy levels are less sensitive to the electric field influence. Besides, the changes in the energies with \( n_{2D} \) are less pronounced for the ground (Fig. 2a) than for the three excited energy levels (Fig. 2b,c, and 2d). Figure 3 shows the Stark shift of the considered energy levels. When increasing the field, all energy shifts increase in absolute value. The Stark shift of the ground electron energy \( E_{C0} \) varies linearly with the applied electric field and does not depend on the impurity concentrations \( n_{2D} \). The dependence of the \( E_{C1} \) and \( E_{C2} \) Stark shifts on the electric field is almost linear, too, but it slightly increases with decreasing \( n_{2D} \). The Stark shift of \( E_{C3} \) is also almost linear with \( F \) and slightly decreases with decreasing \( n_{2D} \), contrary to that of \( E_{C1} \) and \( E_{C2} \). We have verified that the Stark shift of the considered energy levels has the same magnitude if \( F \) has an opposite direction. Figure 4 shows some of the total spectral strength spatial distributions for the ground \( C0 \) and first excited \( C1 \) electron energy states, calculated for different electric fields and impurity concentrations indicated on the figure. At zero field, all spatial distributions are symmetrically situated around the center of our QW. At electric fields different from zero, the spatial distributions are displaced from the center to the right. This is more pronounced for states with higher energy. The displacement is larger for lower \( n_{2D} \) and larger \( F \), as seen in Fig. 4. At a given \( F \) value, which depends on \( n_{2D} \), a secondary QW appears on the right side of the \( \delta \)-doped QW, as also observed in [8,10]. With increasing \( F \), the \( \delta \)-doped QW becomes narrower and shallower (from the right side), while the secondary QW gets wider and deeper. As a result, the bound states spatial distributions increasingly penetrate in the secondary well (Fig. 4a). After a given \( F \) value, the system represents an asymmetric double QW with corresponding bound states. That value of \( F \) depends on \( n_{2D} \) as follows: \( n_{2D} = 1 \), \( F = 8 \); \( n_{2D} = 2 \), \( F = 14 \); \( n_{2D} = 5 \), \( F = 25 \); \( n_{2D} = 8 \), \( F = 40 \); \( n_{2D} = 10 \), \( F = 60 \). Further, we have calculated the intersubband transition energies between the states \( C0 \) and \( C \) \( (i = 1, 2 \) and \( 3) \) for different values of the applied electric field. Figure 5 shows the Stark shifts of the intersubband transition energies for four different \( n_{2D} \) values as a function of \( F \). With increasing \( F \), the Stark shifts of these three transitions increase in absolute value, but in a different way depending on \( n_{2D} \) and the transition. For lower \( F \), the concentration \( n_{2D} \) has a weak influence on the curves. For larger \( F \), the increase is faster for lower \( n_{2D} \) values in the case of \( \Delta E(C0 - C1) \) and \( \Delta E(C0 - C2) \), while it is opposite in the case of \( \Delta E(C0 - C3) \).

The above described behavior of the bound states and intersubband transition energies with an increasing electric field is similar to the results reported by other authors [6,8,10]. The quantitative comparison of the Stark shifts shows a little bit lower values compared to the results from Ref. 8 and larger values compared to [10].

In Refs. 4 and 5 we have studied the Stark shift of the interband transitions in rectangular and graded gap QWs. The comparison with the results presented here concerning the intersubband transitions in \( \delta \)-doped QWs shows that the Stark shift has the same direction and the same order of magnitude for similar values of the electric field. However, the spatial overlap between the initial and final state wave functions is better preserved in the case of \( \delta \)-doped QWs. Therefore, \( \delta \)-doped QWs are more suitable for device applications at low field values. The Stark shift of the intersubband transition energies in Si \( \delta \)-doped GaAs QWs is large enough to be measured experimentally at electric fields above \( \sim 5 \) kV/cm. At larger fields, the secondary QW dominates the potential profile and the initial \( \delta \)-doped QW gradually vanishes.

4. Conclusions

The first TB calculations of the quantum confined Stark effect in Si \( \delta \)-doped GaAs QWs is presented. We have studied in detail the Stark shifts of the electronic states and their spatial distributions, as well as the subband spectra and intersubband transitions of electrons. The results obtained help to
better understand the properties of δ-doped QWs with different impurity densities subjected to an electric field with different magnitudes. Such investigations are very promising in looking for δ-doped structures that provide good Stark effect characteristics for potential device applications, such as FETs and infrared devices, based on the electron intersubband transitions. The results demonstrate that the TB method can be used to investigate the Stark effect in a double asymmetric QW system, which is interesting for coherent intraband radiation applications.

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