Journal of Physics: Conference Series

PAPER • **OPEN ACCESS**

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To cite this article: I Filikhin *et al* 2021 *J. Phys.: Conf. Ser.* **2122** 012011

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Modeling electron transfer from the barrier in InAs/GaAs quantum dot-well structure

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Abstract. We study single electron tunnelling from the barrier in the binary InAs/GaAs quantum structure including quantum well (QW) and quantum dot (QD). The tunneling is described in the terms of localized/delocalized states and their spectral distribution. The modeling is performed by using the phenomenological effective potential approach for InAs/GaAs heterostructures. The results for the two and three-dimensional models are presented. We focus on the effect of QD-QW geometry variations. The relation to the PL experiments is shown.

1. Introduction

Weakly coupled binary semiconductor nanoscale systems demonstrate perspectives for nanosensor applications due to high sensitivity of electron localization and resonance tunnelling between the objects of the system on symmetry violation [1]. The single electron tunneling properties of one dimesional (1D), 2D and 3D structures as well as double quantum wells (DQWs), double quantum dots (DQDs), and quantum rings (DQR) are well known. The electron spectra of such quantum objects in two- and three dimensional (2D and 3D) were studied in previous works [2] with relation to the electron localizations and tunneling between the objects. The wave function of electron may be localized in one of the QDs or be delocalized when it is spread over the whole system. Tunneling occurs in the last case. In the condition of weak coupling objects, electron wave function can be localized in the both objects but with different probability. We explore experimental possibility for optical registration of electron localizations in binary quantum systems. In this work we focused on the resonance tunneling in 3D/1D and 2D/1D nanoscale InAs/GaAs dot-well complex. This complex has the mixed spectral structure: discrete spectrum for QD (in 3D and 2D) and continuous spectrum for QW when this QW is considering in three- or two-dimensional space [3, 4, 5]. Our modeling carrier transfer from the barrier in InAs/GaAs dot-well tunnel-injection structure is performed by using the band gap model based on the effective potential [6, 7]. It has to be stressed that the tunneling is described in the terms of localized/delocalized states and their spectral distribution [2]. We have simulated the main effect of the optical PL experiments given by Yu. I. Mazur et al. in [8].

2. Model

Presented work was motivated by the experimental results of coherent coupling between photo-excited quantum-dots and a quantum well reported in [8, 9, 10, 11, 12]. The schematic explanation the PL experiments [8] is given in Fig. 1 and Fig. 2. The coupling in the QD-QW complex was investigated in [8] by the dependence of quantum-dot photoluminescence as a function of quantum dot-well barrier thickness. It was shown that the resonant tunnelling rate is varied by changing the effective barrier thickness. This strongly affects the exciton dynamics in these hybrid structures as compared to isolated QW or QD. A specific behaviour of the communication between a quantum-dot and quantum wall was discussed in [11, 12].

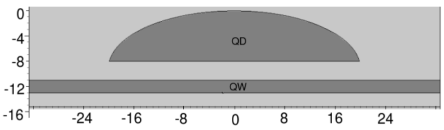

Figure 1. (Left) Geometry of the QD-QW complex (2D model). The sizes are given in nm. The profile of the fabricated QD is presented in [10].

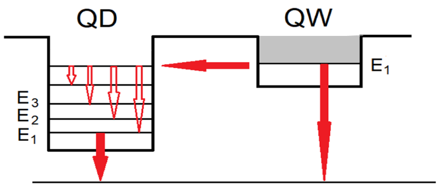

Figure 2. Schematic description of the PL experiments from [8]. Electron confinement structure and energy levels. The tunneling between QD and QW is shown by horizontal arrow.

The InAs/GaAs quantum heterostruction is modelled using the effective potential model. The effective potential simulates the strain effect in the InAs/GaAs heterostructures [6, 7]. The band gap model for description of the QDs (and QWs) is presented in Fig. 3. Here, the effective potential is given by V_s and the bang gap potential is V_c.

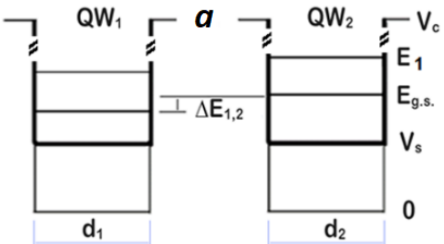

Figure 3. Band gap model for InAs/GaAs double quantum well (in 1D). The system includes two quantum wells, QW_1 and QW_2, which are differ by the sizes d_1 and d_2. Inter-well distance is a.

We consider the QD-QW complex as two-level quantum system [13] and describe the electron tunneling in the system within terminology of spectral distributions of the localized/delocalised states [1].

Double quantum dot is an example of the two-level quantum systems. The spectrum of single electron confinement states in DQDs is a set of quasi-doublet levels. The electron can be localized in one of the quantum dots or be delocalized over both the QDs. The electron tunnelling between QDs in DQD is indicated by changing of the type of electron localization. The tunneling occurs through the anti-crossing of levels and, in case identical QDs, extremely sensitive on shape symmetry violations in the systems [1, 2]. To evaluate the electron localization, one can use the electron average coordinate $\langle x \rangle$ which is calculated as: $\langle x \rangle = \langle \Psi | x | \Psi \rangle$, where Ψ is wave function of the system. In the approach of the two-level system, Ψ is represented by superposition of the wave functions ψ_1 and ψ_2 of separated left (1) and right (2) quantum dots. The x-coordinate origin is the mid-point of the two QWs. The average coordinates $\langle x \rangle_+$ and $\langle x \rangle_-$, for the electron wave functions of the quasi-doublet, Ψ_+ and Ψ_-, can be written as

$$\langle x\rangle_+ = -\cos^2\left(\frac{\Theta}{2}\right)|\langle x\rangle_1| + \sin^2\left(\frac{\Theta}{2}\right)|\langle x\rangle_2| + 2\sin\left(\frac{\Theta}{2}\right)\cos\left(\frac{\Theta}{2}\right)\langle x\rangle_{12},$$

$$\langle x\rangle_- = -\sin^2(\Theta/2)|\langle x\rangle_1| + \cos^2(\Theta/2)|\langle x\rangle_2| - 2\sin(\Theta/2)\cos(\Theta/2)\langle x\rangle_{12},$$

where, $\Theta = arctg\,(W/\Delta E_{12})$. The parameter W is a coupling coefficient of the quantum system elements. It depends on the wave function overlap for the "unperturbed states" ψ_1 and ψ_2. $\Delta E_{12} = E_1 - E_2$ is energy difference of separated QWs as is shown in Fig. 3. The matrix element W (which is also proportional to the quasi-doublet energy splitting ΔE) can be described using the following relation [14]: $W \sim S$, where S is the overlap integral, approximated by $S = \int_\Sigma \psi^2(x,y)\,dxdy$, with the integration domain Σ being the area between the QWs. It is clear, that the electron localization in DQW is extremely sensitive to small violations of DQW symmetry, when $\Delta E_{12} \approx 0$ [1].

3. Numerical modeling for carrier transfer from the barrier in InAs/GaAs–InGaAs/GaAs dot-well

The tunneling in the hybrid QD-QW complex is considered with relation to the PL experiments [8] (see Fig. 2). The QD - QW tunneling has been experimentally indicated by the existing PL peaks between lowest QD and QW peaks which were observed for separated QD and QW.

The 3D modeling is including the QD and QW having the rotation symmetry as is shown in Fig. 4(Right). Neumann boundary conditions were used for the QW. The results of numerical modeling are given in Fig. 4(Left) for the spectral distributions of the localized/delocalized states shown for several chooses of QD-QW geometry. The tunneling between QW and QD is occurred for the first energy level of QW. This situation directly comparable with the experimental picture proposed in Ref. [8]. The tunneling is possible for the close depositing of QD and QW. The

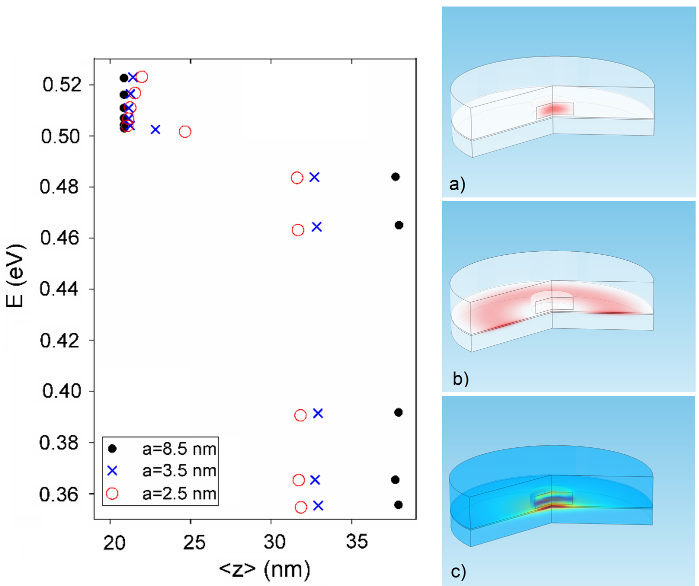

Figure 4. (Left) The spectral distribution of localized/delocalized states in 3D InAs/GaAs dot-well complex for different barrier thicknesses, a, shown by various symbols along the averaged coordinate $\langle z\rangle$. Electron tunneling occurs on the QW lowest energy level and relates to the delocalized state (noted by the arrow). (Right) The square of the wave function. The electron localized a) in QD, b) in QW and delocalized c) over the QD-QW complex.

dependence presented in Fig. 4(Left) shows that the barrier thickness a=8 nm is critical for the tunneling which is occurred when $a \ll 8$ nm and detected for $\langle z\rangle$ in diapason of [22,30] nm. When a>8 nm, the tunneling is not possible and we see the spectra of separated QD and QW. The spectrum of QD is discrete and electron localizes about $\langle z\rangle$ ≈38 nm. The QW spectrum is quasi-continuous due to numerical approximation and the electron is localized in QW with

$\langle z \rangle$ ≈21 nm. In Fig. 4(Right) we illustrate the tunneling and show the electron wave functions for the different energy levels.

In Fig. 5, we present the results of numerical modeling for tunneling taken a place in the 2D-1D QD-QW complex. One can see in Fig. 5 (Left) that the QD and QW may be described as separated for large barrier thickness. The electron spectrum relates to single QD or QW. Corresponding localization is noted as "QD" or "QW" in the figure. The tunneling occurs for the lowest QW level (or higher confinement state of QD) when a is decreased to 8 nm and electron is localized in QD and QW, with $\langle y \rangle$ ≈9 nm. This property is again directly related to the experiments [8]. Experiments given in [9] can be modeled by increasing the size of QD-QW complex. The schematic description of the PL experiments [9] is presented in Fig. 6.

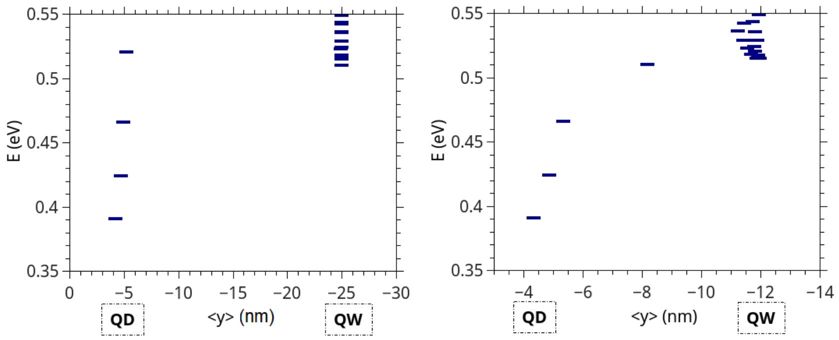

Figure 5. The spectral distribution of localized/delocalized states in 2D InAs/GaAs dot-well complex for different barrier thicknesses, a. (Left) a=20 nm and there are no delocalized (tunneling) states. (Right) a=8 nm.

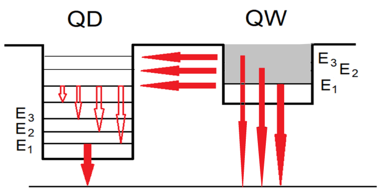

Figure 6. Schematic description of the PL experiments from [9]. Electron confinement structure and energy levels. The tunneling between QD and QW is shown by horizontal arrows.

The results of numerical modeling for tunneling taken a place in reconfigured 2D-1D QD-QW complex are presented in In Fig. 7. The calculations were performed for different value of the barrier thickness a. Once more, one can see that the tunneling is possible when the QD and QW are enough close. The tunneling is occurred through higher levels of discrete spectrum of QD and quasi-continuous spectrum of QW. Comparing this result with the QD-QW experiment one can conclude that the QW in experiment has quasi-continuous spectrum too. Our interpretation for this fact is that region of interaction between QD and QW is local and has a limitation by size of QD-QW interface B. The spectral level energy can be evaluated as L^2/B^2, where $L = 1, 2, 3, \ldots$ for each bands generated by the QW thickness.

4. Conclusion

We modeled the resonance tunneling in InAs/GaAs QD-QW complex including 2D (3D) and 1D quantum objects in terms of localized/delocalizad states of electron confinement spectrum according the formalism of two-level quantum systems. This simulations covers the main phenomenons of the optical PL experiments given by Yu. I. Mazur et al. in [8] and [9]. It was shown that the resonance tunneling spectral distribution depends on geometry factors of the QD-QW complex which can be predicted in theoretical simulations. The optical registration of electron localization in binary quantum systems can be used in new nono-sized devices.

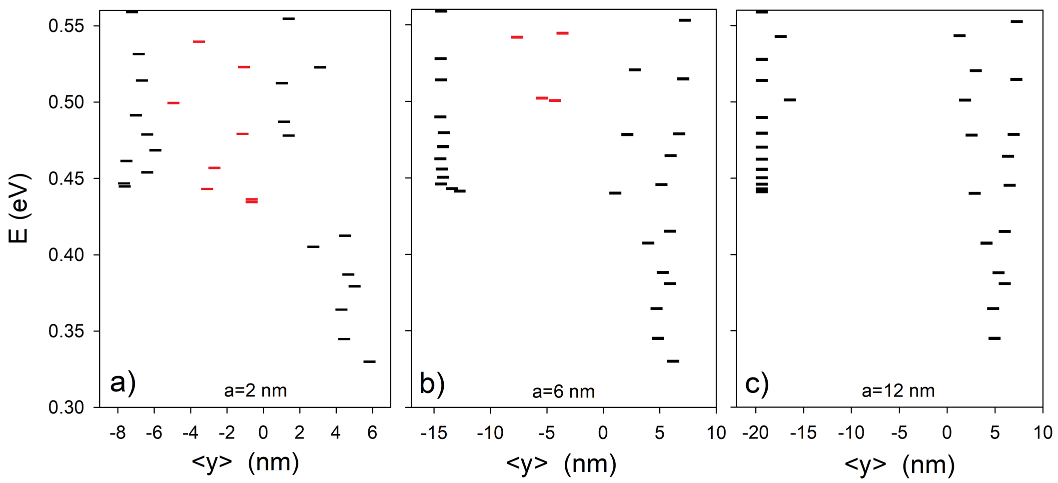

Figure 7. The spectral distribution of localized/delocalized states in 2D InAs/GaAs dot-well complex for different barrier thicknesses a) a=2 nm, b) a=6 nm and c) a=12 nm. Delocalized states are shown in red.

Acknowledgments

This work is supported by the RISE 1829245, DNS 2016-ST-062-000004 and DMR-1523617 awards.

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