Influence of dimensionality on the emission spectra of nanostructures

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(Received 1 July 2003; accepted 16 September 2003)

We report on our results of the numerical simulations of a quantum dot (quantum wire)-quantum well cascade structure. Experimental work on the quantum dot structure was recently reported in the literature. For parameters of such a structure, the calculated emission spectra has a single peak for up to four electrons in the dot. The width of the emission line is found to be due to long-range in-plane disorder, resulting mainly due to fluctuations of the height of the dots. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1625785]

It has been long established that dimensionality of electronic systems plays an important role on the electronic and optical properties, due to its influence on the density of states.[1] Since the inception of the quantum cascade laser,[2] there have been persistent efforts to reduce the dimensionality of the quantum wells in the active region.[3] The question of how the emission spectra of various nanostructures are influenced by their dimensionality has come to the fore because of recent reports on the quantum dot (QD)-quantum well (QW)[4] and quantum wire (QWR)-quantum well[5] cascade structures. The system of Ref. 4 consisted of the coupled AlInAs self-assembled quantum dots[1] and GaAs quantum wells. Electrolumenscence spectra from such a cascade system showed (i) a clear single peak at 158 meV and (ii) a finite width of the peak around 15 meV. Our numerical simulations on QD cascade structures reported earlier[6] indicated that generally the emission spectra from such a structure should have multiple peaks. Absence of these additional peaks in Ref. 4 can be understood from the estimate of the number of electrons per dot, which participate in formation of the luminescence spectra. We estimate that there are only one or at most two electrons per dot in the structure of Ref. 4.

In order to understand more clearly the structure of emission spectra we performed numerical calculations for a QD–QW cascade system with the parameters taken from Ref. 4. We have considered only the active region of the system, i.e., a quantum dot with base diameter D, and two quantum wells, as shown in Fig. 1. The base diameter of the dot is considered as a parameter of the system and is varied around the average value $D=20$ nm, as reported in Ref. 4. To study the effect of dimensionality we have also done calculations for a QWR–QW cascade structure with the same parameter of the active region as for QD–QW (see Fig. 1).

The single-electron Hamiltonian for our system is

$$\mathcal{H}' = \frac{p_x^2}{2m^*} + \frac{p_y^2}{2m^*} + V_{\text{plane}}(x,y) + \frac{p_z^2}{2m^*} + V_{\text{conf}}(z),$$

where the confinement potential in the z direction is

$$V_{\text{conf}}(z) = -eFz + \begin{cases} 0 & \text{for wells} \\ U_0 & \text{for barriers} \end{cases} \quad (1)$$

with F being the electric field in the z direction, and U_0 is the conduction band discontinuity.[6] The confinement potential in the xy plane is zero for the quantum well and for the quantum dot is taken to be of two forms: a parabolic potential $V_{\text{QD,PP}}(x,y)=\frac{1}{2}m^*\omega^2(x^2+y^2)$ where ω_x is the confinement energies, corresponding to the oscillator length of $l=(\hbar/m^*\omega)^{-1/2}$; or the hard wall confinement

$$V_{\text{QD,HW}}(x,y) = \begin{cases} 0 & \text{for } (x^2+y^2)^{1/2} < D/2 \\ U_0 & \text{for } (x^2+y^2)^{1/2} > D/2 \end{cases}.$$

For the quantum wire, the in-plane confinement exist only in one dimension. The corresponding confinement potential is also taken to be parabolic $V_{\text{QWR,PP}}(x,y)=\frac{1}{2}m^*\omega^2x^2$.

For the N-electron system, we also take into account the Coulomb interaction between the electrons $\mathcal{H}_{\text{int}}=e^2/\epsilon\cdot\Sigma_{i<j}|\mathbf{r}_i-\mathbf{r}_j|^{-1}$, where ϵ is the background dielectric constant. We restrict the single electron basis by 10 lowest states and numerically obtain the eigenstates of the N-electron system with $N=2-4$.

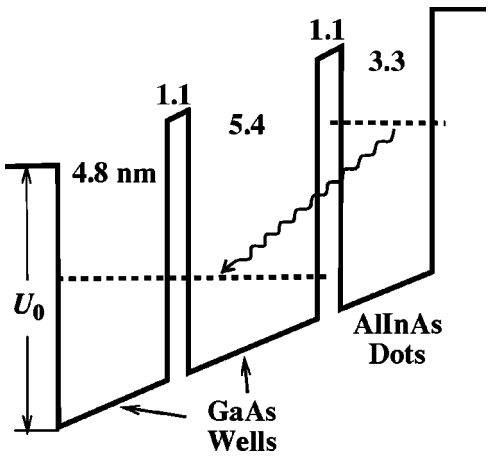

FIG. 1. Active region of a QD–QW (QWR–QW) cascade system is shown schematically. Optical transition between the initial excited electronic state, where all electrons are in the AlInAs quantum dot (quantum wire), and the final state, in which one electron is in the GaAs quantum well and all other electrons are in the dot (wire), is illustrated by an wavy arrow.

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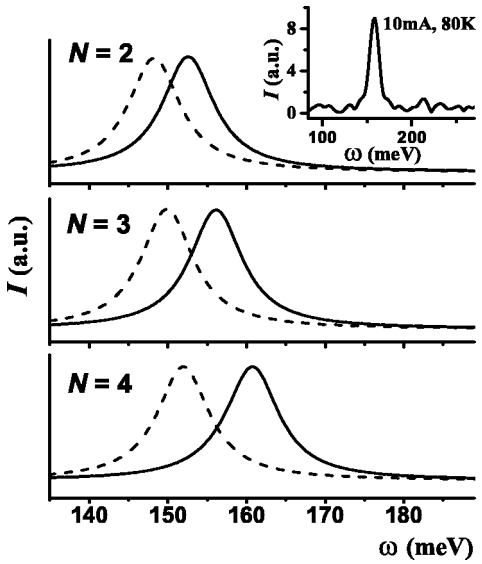

FIG. 2. Shape of the luminescence spectra for different number of electrons, $N=2,3$, and 4 for QD–QW (solid line) and QWR–QW (dashed line) structures. The diameter of quantum dot base is $D=30$ nm, and is the same as the width of the quantum wire, $d=30$ nm. The in-plane confinement potential for the dot has the parabolic form, $V_{\text{plane,PP}}(x,y)$. The intensity I is in arbitrary units. Experimental results from Ref. 4 are presented as inset.

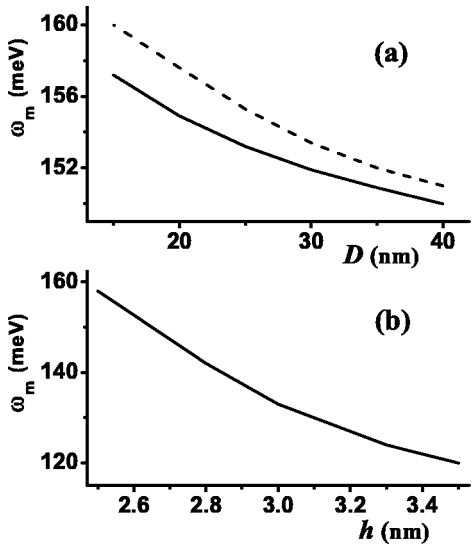

FIG. 3. Position of the maximum of emission spectra (see Fig. 2) as a function of the diameter of the base of the dot (a) and as a function of the height of the dot (b). The dashed and solid lines in figure (a) correspond to the hard wall confinement, $V_{\text{plane,HW}}$, and parabolic confinement, $V_{\text{plane,PP}}$, respectively. The number of electrons per dot is two, $N=2$.

During the optical transition in the active region of a QD/QWR–QW system, in the initial state (before optical emission) all N electrons are in the quantum dot/quantum wire (for the in-plane motion) and in the second subband (for electron motion in the z direction). In the final state (after optical emission) one electron is in the quantum well (for the in-plane motion) and in the first subband (for electron motion in the z direction), and all other $N-1$ electrons are in the quantum dot/quantum wire and in the second subband. The intensity of optical transitions is calculated from

$$\mathcal{I}_{if}(\omega)=\frac{1}{Z}\sum_{if}\ \delta(\omega-E_i+E_f)\times\left|\int\chi_1(z)z\,\chi_2(z)dz\int\Phi_i^*(x_1y_1,\cdots,x_Ny_N)\times\Phi_f(x_1y_1,\cdots,x_Ny_N)dx_1dy_1\cdots dx_Ndy_N\right|^2\times\exp(-\beta E_i),$$

where $Z=\Sigma_i e^{-\beta E_i}$ is the partition function and $\beta=1/kT$. In all our computations, we take $T=50$ K. The wave functions $\chi_1(z)$ and $\chi_2(z)$ correspond to the first and second subbands, respectively, and Φ_i, Φ_f are the initial and the final wave faction for the in-plane motion. To take into account the effect of disorder in the system we introduce the spreading of each emission line in the Lorentz form so that the final intensity is

$$\mathcal{I}(\omega)=\int d\omega_1\mathcal{I}_{if}(\omega_1)\,\frac{\Delta}{\pi[\Delta^2+(\omega-\omega_1)^2]}.$$

The parameter Δ in our calculation is taken to be $\Delta=5$ meV.[7]

We have analyzed two aspects of the emission spectra: the shape and width of the emission line. In Fig. 2, we present the emission spectra for different number of electrons in the initial state ($N=2-4$). The data for QD–QW are shown only for the parabolic confinement potential for the quantum dots. For the hard wall confinement the trend is the same. We see that in all cases the emission spectra consist of a single line. In the experiments the number of electrons per dot is not higher than two and as a result in the emission spectra there is only a single line. The present calculations demonstrate that even for a higher electron density (up to four electrons per dot) the emission spectra will not acquire any additional structure, which might result from the discrete structure of the energy spectra of the quantum dots. Insensitivity of the emission spectra on the discreteness of the energy spectra of the dot is due to a large size of the dot (diameter of the base), i.e., small gaps in the energy spectra of dot system. Another property of the luminescence spectra (also observed in Ref. 6) is the blueshift of the emission line as a function of number of electrons. This shift is partially due to interactions between the electrons. Comparing the QD–QW and QWR–QW structures, we see that the blueshift is larger for QD–QW system, which means that the interaction effects in the quantum dots are stronger than in the quantum wires. This is due to a larger spreading of electrons in the quantum wires than in the quantum dots.

The second aspect of the emission spectra, which characterizes the lasing properties of quantum cascade system is the width of the emission line. We assume that this width comes from the inhomogeneous dot distribution. The main parameters that characterize the dot geometry are the diameter, D, of the base of the dot and the height, h of the dot. Fluctuations of the dot diameter comes from fluctuations of the in-plane disorder potential with characteristic size much smaller than the size (diameter) of the dot. Conversely, fluctuations of the height of the dot is due to fluctuations of the disorder potentiual with the size much larger than the diameter of the dot. In other words, the short-range and the long-range in-plane fluctuations of the disorder potential are responsible for the fluctuations of the dot diameter and the height of the dot, respectively. To describe the effect of these

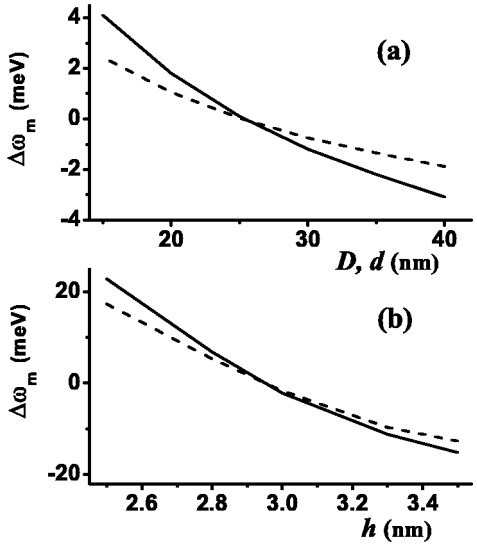

FIG. 4. The relative position of the maximum of emission spectra (see Fig. 2) is shown for $N=2$ as a function of the dot diameter, D, and the width of the wire, d, (a); and as a function of the height of the dot and the wire (b). The solid and dashed lines in figures (a) and (b) correspond to the quantum dot and quantum wire, respectively.

parameters on the spectral width, we have studied their influence on the position of emission line in the homogeneous system, where all the dots have the same values of D and h. In Fig. 3 the position of the emission line is shown as (a) a function of the diameter of the base and (b) as a function of the height of the dot. Evidently, there is only a weak sensitivity of the emission spectra on the dot diameter. For example, when the diameter increases from 10 to 40 nm the position of the line is moved only by $\approx 5\%$ (8 meV). This is true both for the parabolic potential (solid line) and for the hard wall confinement (dotted line). We therefore conclude that the fluctuation of the diameter of the dots have small contribution to the width of the luminescence line. It follows also from this conclusion that the fluctuation of the shape of the dots does not strongly affect the width of the line. On the other hand, from Fig. 3(b) we notice that the emission spectra becomes very sensitive to the height of the dots. Clearly, if the height is changed between 2.5 and 3.5 nm, the position of the line is moved by ~ 60 meV. In other words, for the width of the line equal to 15 meV the inaccuracy in the height of the dots should be less than 10%.

A similar trend concerning the effect of the geometric parameters of the quantum wire on the width of the emission line is found for the QWR–QW cascade structures. To make a more detailed comparison between the two different structures, i.e., QD–QW and QWR–QW, we present in the same figure, Fig. 4, the dependence of the position of the emission line on the width and the height of the quantum wire (for QWR–QW structure) and on the diameter and the height of the dot (for QD–QW structure). The data in Fig. 4(a) demonstrate that the width of the emission line is almost half as sensitive to the fluctuations of the width of the wire in the QWR–QW structures than to the fluctuations of the dot diameter in the QD–QW structure. Such a relation can be understood from the single-particle picture, in which the energy of in-plane motion is $\hbar\omega$ for the parabolic quantum dot and $(1/2)\hbar\omega$ for the quantum wire. At the same time, it is clearly seen in Fig. 4(b) that the sensitivity to the height is almost the same in QWR–QW and QD–QW structures. Our detailed study presented here indicate that, the main contribution to the width of the emission spectra in QD–QW (QWR–QW) structures comes from the fluctuations of the dot (wire) height, i.e., long-range in-plane fluctuations of the disorder potential.

The authors would like to thank N. Ulbrich (WSI, München) for sending them their experimental results reported in Ref. 4.

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[7] This value of Δ comes from the following estimates: $\Delta \sim 2\ \omega\ \delta h/h$, where $\omega \sim 100$ meV is the typical energy of emitted photon, $\delta h \sim 0.2$ nm is the typical inhomogeneity within a single quantum dot (of the order of a width of a single atomic layer–typical accuracy for the system grown by molecular beam epitaxy), $h \sim 10$ nm is the typical size of the dot.