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Numerical simulation of a coupling effect on electronic states in quantum dots

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ABSTRACT

Lasers operating at 1.3 μm have attracted considerable attention owing to their potential to provide efficient light sources for next-generation high-speed communication systems. InAs/GaAs quantum dots (QDs) were pointed out as a reliable low-cost way to attain this goal. However, due to the lattice mismatch, the accumulation of strain by stacking the QDs can cause dislocations that significantly degrade the performance of the lasers. In order to reduce this strain, a promising method is the use of InAs QDs embedded in InGaAs layers. The capping of the QD layer with InGaAs is able to tune the emission toward longer and controllable wave-lengths between 1.1 and 1.5 μm. In this work, using the effective-mass envelope-function theory, we investigated theoretically the optical properties of coupled InAs/GaAs strained QDs based structures emitting around 1.33 μm. The calculation was performed by the resolution of the 3D Schrödinger equation. The energy levels of confined carriers and the optical transition energy have been investigated. The oscillator strengths of this transition have been studied with and without taking into account the strain effect in the calculations. The information derived from the present study shows that the InGaAs capping layer may have profound consequences as regards the performance of an InAs/GaAs QD based laser. Based on the present results, we hope that the present work make a contribution to experimental studies of InAs/GaAs QD based structures, namely the optoelectronic applications concerning infrared and mid-infrared spectral regions as well as the solar cells.

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1. Introduction

With the advent of semiconductor nanostructures and the discovery of their greater physical properties, extensive research has been conducted to make use of these reduced dimensionality structure properties for future applications. The study of low-dimensional semiconductor heterostructures is one of the main subjects in Solid-State Physics owing to their application to optoelectronic devices like light-emitting diodes and lasers. In particular quantum dots (QD), achieving the limit in carrier confinement, have attracted great interest due to their large potential for application in novel devices for optoelectronics and quantum information processing [1–4]. Moreover, the ability to precisely control the lateral position of self-assembled epitaxial quantum dots (QDs) [5] may open the way to the integration of single QD devices with new functionalities such as single photon emission [6,7] and qubit operations [8]. A self-assembled InAs/GaAs material system is especially interesting for device applications such as QD mid-IR emitters or detectors [9,10] and it is therefore vital to gain an insight into (de) the growth processes and optical properties of InAs QDs on GaAs surfaces. In particular, InAs/GaAs quantum dot (QD) lasers operating at 1.3 μm have attracted considerable attention owing to their potential to provide low-cost and efficient light sources for next-generation high-speed communication systems. In such structures, it is possible to extend the optical-emission range of GaAs-based devices up to 1.3 μm, the first window of the optical fibers which cannot be reached by InAs/GaAs quantum wells. Solomon et al. [11] have used the vertical coupling of stacked layers of InAs QDs separated by GaAs layers which produces an effective potential and products a red shift of electronic levels with respect to those of a single layer of QDs. However, da Silva and Quivy [12] have produced vertically coupled InAs QDs separated by thin spacer layers where part of the GaAs material was substituted by InGaAs in order to obtain samples emitting around 1.3 μm with a reduced number of interfaces and a narrower line width. In fact, stacked QD structures have been extensively employed in order to increase the modal gain of the QD lasers, nevertheless, the accumulation of strain due to the lattice mismatch of the surface material and the deposited material can cause dislocations that greatly degrade the performance of the lasers [13–16]. Therefore, it is necessary to reduce the strain in the stacked QD structures.

In this paper, we investigate theoretically the optical properties of coupled InAs/GaAs QDs based structures emitting around 1.33 μm. The energy levels of confined carriers, the optical transition energy as well as the oscillator strength of transition are investigated by the resolution of the 3D Schrödinger equation using the effective-mass envelope-function theory. The effect of strain is included in our calculations.

2. Theory and calculation

Due to the relative ease of growth and well established integration in semiconductor devices, the self assembled QDs provide a great advantage over other types of nanostructures. The numerical simulation of the electrical and optical features of semiconductor devices offer a fast and cheap means to check test device designs and processes. The system under investigation consists of rectangular InAs quantum dots embedded into a GaAs surrounding matrix. A thin $In_{0.15}Ga_{0.85}As$ capped layer has been used between InAs QD and GaAs layer. A schematic representation of the structure used in the calculation is shown in Fig. 1. This geometry is not realistic but provides a good starting point since this method should be versatile to solve for any cross-section and any potential. We start from the 3D three-dimensional constant effective mass Schrödinger equation given by [17]:

$$-\frac{\hbar^2}{2}\nabla\left(\frac{1}{m^*(x,y,z)}\nabla\right)\psi(x,y,z)+V(x,y,z)\psi(x,y,z)=E\psi(x,y,z) \quad (1)$$

where m^* is the electron or hole effective mass, and $V(x,y,z)$ is the 3D confining potential energy. Eq. (1) is expanded in terms of finite differences. So as to obtain a numerical solution for $\psi(x,y,z)$ over a three-dimensional volume (Lx, Ly, Lz), the structure is discretized into an array of N_x, N_y, N_z