Design of columnar quantum dots for polarization-independent emission using 8–band k·p method

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Abstract. Control of the polarization of the emitted light can be highly beneficial for certain optoelectronic applications such as optical amplifiers. It has been recently demonstrated experimentally that semiconductor quantum dots with large height to base length aspect ratio are able to emit polarization–independent light from the edge of the wafer. However, analysis of the physics responsible for the observed polarization properties of such nano–objects (like columnar quantum dots or quantum rods) is still rather limited. In particular, the role of the material surrounding the columnar QD on the strain and thus on the polarization properties has not been considered previously. We report here, based on original software, the results of eight–band k·p calculations of the electronic and polarization properties of columnar InyGa1−yAs quantum dots (CQD) with high aspect ratio (up to 6) embedded in an InyGa1−yAs/GaAs quantum well. We calculate the relative intensities of transverse-magnetic (TM) and transverse-electric (TE) linear polarized light emitted from the edge of the semiconductor wafer as a function of the two main factors affecting the heavy hole – light hole valence band mixing and hence the polarization dependent selection rules for the optical transitions, namely i) the composition contrast y/x between the dot material and the surrounding well, and ii) the dot aspect ratio. Our numerical results show, in contrast to the previously reported expectations, that the former is the main driving parameter for tuning the polarization properties. This is explained analyzing the biaxial strain in the CQD, based on which it is possible to predict on the TM to TE intensity ratio.

1. Introduction

Quantum dots (QDs) have a potential for application in semiconductor optical amplifiers (SOAs), due to their high saturation power related to the low differential gain, fast gain recovery and wide gain spectrum compared to quantum wells (QWs) [1]. For in-line amplifier applications polarization-independence is a key requirement. Due to their flat shape and quasi-biaxial compressive strain, self-assembled quantum dots have a valence-band ground state of the heavy-hole (hh) type, which only couples to the in-plane light polarization (transverse-electric, TE) and not to the polarization along the...
growth axis (transverse-magnetic, TM). By varying the QD aspect ratio, both the shape of the confinement potential and the strain distribution can be changed. As a result, semiconductor quantum dots with large height to base length aspect ratio are able to emit polarization-independent light from the edge of the wafer [2], [3] and [4]. Such “columnar” quantum dots (CQDs) [5] with large aspect ratio can for example be obtained by cycled submonolayer deposition, and are thus promising candidates for amplifier applications. On the other hand, the analysis of the physics responsible for the observed polarization properties of such nano-objects is still rather limited and has considered only the influence of the dot geometry within quite a narrow aspect ratio range [6]. In particular, the role of the material surrounding the CQD on the strain and thus on the polarization properties has not been considered.

2. Computational approach

For the calculations of the electronic states and optical transitions in columnar quantum dots we have developed a three–dimensional strain–dependent eight–band \( \mathbf{k} \cdot \mathbf{p} \) model. The model is implemented and all physical equations are numerically solved using the finite difference method. The model includes strain fields, piezoelectric effects and the spin–orbit interaction. The linear strain field has been calculated using continuum mechanical elastic theory. The detailed description of such calculations is given for instance in [7]. Based on strain field, the linear piezoelectric potential [8] and the potential resulting from deformation potential have been derived. Afterwards, the energy levels were calculated by using the multi band approach developed by Bahder [9]. In order to calculate the TE and TM mode transition intensities in the columnar QDs, we first calculate the oscillator strength for the electron-hole transition between the initial and final states, according [10], where the matrix elements between these states are calculated according to the scheme in [11].

3. Results

The geometrical model of the columnar QD with 2D surrounding (immersion) layer is presented in figure 1, including an illustration of the linear polarization directions. The TE-mode polarization vector lies in the X-Y plane, while the TM-mode is polarized along the growth (Z) direction. Light is considered to be emitted from the CQD along either the [110] or [1-10] direction. The CQD is placed in the centre of the box and the height of the 2D immersion layer is assumed the same as the height of the CQD (see the TEM images in [5]). The border between CQD and the faces of the numerical box used for calculating the strain field is 45 nm with a fixed boundary condition at the base of the box and with free-standing boundary conditions at the other faces of the box. For the numerical box for calculating of energy levels the border is 15 nm with fixed boundary conditions at the all faces of the box.

![Figure 1](image-url)
All the simulations presented assume a cuboid QD with a square base of the diagonal length of 20 nm (14.14 nm base length), and with the aspect ratio (height to base length) changed from 3 to 6 (height between 42.42 and 84.84 nm). All the material parameters used in the calculations are taken from [12], assuming room temperature values for the lattice constants and energy band gaps.

In figures 2 and 3 there are presented the calculated oscillator strength of the optical transitions and the fraction of the intensity in the TM polarization for a CQD with an aspect ratio 3 and 6 respectively, and In content of 45% inside the dot. The In content in the immersion layer is changed from 15% down to 9 % in figures 2 (a) to (c) and figures 3 (a) to (c), respectively (which corresponds to the compositional contrast between the dot and the 2D surrounding changing from 3 to 5). For clarity, only those transitions which have a significant intensity are shown. In addition, we also plot on the right hand axes in figure 2 and figure 3 the light hole contribution to each valence band wave function calculated as in [6].

Several conclusions can be drawn directly from figures 2 and 3. We can see that there is a significant TM polarization contribution when the contents contrast equals 3 but this contribution is mainly found in the higher order transitions for both aspect ratios equal 3 and 6 in figure 2a and figure 3a, respectively. Increasing the contents contrast from 3 to 4 or further to 5 can dramatically enhance the TM polarization even for the lowest energy transitions. But still for high compositional contrast of 5 the TM will not dominate over TE if the aspect ratio is low (e.g. 3).

Based on these calculations, we have obtained that the strong TM polarization is directly connected with the value of the biaxial strain inside the quantum dot and that the minimum requirement is that it needs to be negative. Figure 4 presents biaxial strain calculated in the middle of the CQD for In content equal to 45% inside dot and for various In concentrations in the immersion layer. It is seen,
that negative biaxial strain (and hence high intensity in TM polarization) can be obtained for high contents contrast being then weakly dependent on the aspect ratio. On the other hand, the TM mode will never be strong for small composition contrast (like 3, i.e. the case of 15 % In in the immersion layer in figure 4) for even very high aspect ratios.

4. Conclusions
We have theoretically studied the optical properties of In$_y$Ga$_{1-y}$As/GaAs columnar QDs from the point of view of their possible application in polarization independent optical amplifiers. We have taken into consideration and shown the importance of a 2D In$_x$Ga$_{1-x}$As layer of lower composition ($x < y$) which surrounds such dots in–plane in real structures. We have shown how this immersion layer can strongly affect the TM to TE intensity ratio of the optical transitions. Eventually, we have found that if biaxial strain in the quantum dot has a negative value, then there exist conditions for strong TM intensity, which can be further enhanced by increasing the aspect ratio of the columnar dot.

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