Modelling of GaAs quantum dot embedded in a polymorph AlGaAs nanowire.

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***Abstract*—We present a numerical model of quasi one-dimensional and quasi zero-dimensional semiconductor heterostructures strictly based on experimental structures of polyphorm cylindrical nanocolumns.**

I. Introduction

The challenge of the quantum dot (QD) fabrication technology is to obtain highly homogeneous arrays with little dispersion in size, composition and shape in order to maximize quantum efficiency. One of the most promising solution for application in nanoelectronics [1], and nanophotonics [2] is the growth of free standing semiconductor nanowires (NW) and nanocolumns (NC). The technology of manufacturing such NWs is now intensively developing [3]- [4], and allows to control the sizes and location of NW at the nanometer scale.

However, GaAa/AlGaAs NWs also possess growth mechanisms that might have strong influences on their electronic properties, since the crystal structure of a $< 111 >$ nanowire may spontaneously switch during the growth from zinc-blende (Zb) to wurzite (Wz) phases [5], leading to a strong modification of the time resolved photoluminescence spectra [6].

Only quite recently the electronic structures and the variation of the fundamental gap of the Wz phase of these crystals have been studied, but only a relative small amount of parameters for bandstructure calculations are available in the literature. We mention quasiparticle calculations of Wz polymorphs of InAs and GaAs using the GW approximation [7], calculations of the bulk electronic band structures of non-nitride III-V semiconductors in the Wz phase using empirical pseudopotentials [8], and electronic structure of the Wz phases of GaAs and InP with using Tight Binding model [9].

We have simulated an AlGaAs NW with an embedded GaAs QD, considering two different cases, a pure Zb case and a polymorph Wz-Zb case, respectively. Dimensions, structural and geometric parameters have been strictly derived from experimental data.

II. Theory

We have implemented an 8-band $\vec{k} \cdot \vec{p}$ model [10] for bandstructure calculations including electromechanical fields

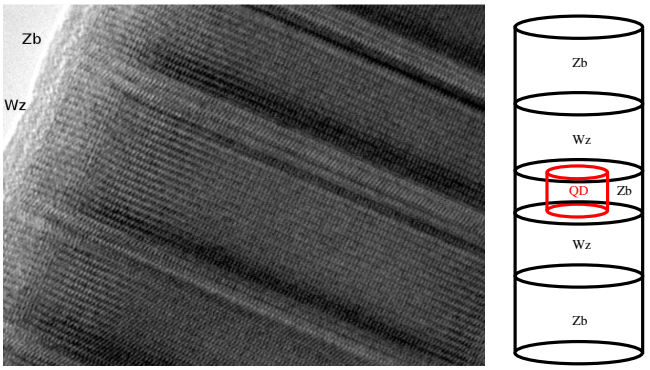

Fig. 1: Left: TEM image of an AlGaAs NW with wurtzites and zincblende phase alternations. Right: a scheme of the simulated AlGaAs nanowire with the embedded GaAs quantum dot (QD) for Mx case. The different crystal phases of the correspondent layers are also indicated. All the dimensions are given in the text.

[11]. The parameters for the Pikus-Bir Hamiltonian of the Wz materials have been derived from the correspondent Zb materials using the cubic approximation [12], while the stiffness parameters of Wz crystals have been estimated from Martin's transformations [13], [14] using the Zb parameters. Models and parameters for electromechanical fields and $\vec{k} \cdot \vec{p}$ calculations have been derived in detail in our recent paper [15].

In the left side of Figure1 a TEM image of one of our AlGaAs NW clearly shows the of phase transitions from Zb to Wz crystal structures. Here, layers parallel to the growth direction correspond to ABAB lattice repetitions of Wz, whereas the layers which appear to zigzag correspond to the ABC repetitions of the Zb phase. Darkest layers between the two crystal phases suggest the presence of a strain field given by a lattice mismatch between Zb and Wz phase of AlGaAs. In our model we have studied an $Al_cGa_{1-c}As$ nanowire ($c = 0.25$, diameter of 40 nm, height of 50 nm), with an embedded GaAs QD (diameter of 20 nm and hight of 5 nm), comparing two

different cases: a pure Zb case, and a mixed structure (Mx) (Figure 1, right side) where the GaAs QD is sandwiched by two adjacent 8 nm high Wz layers and surrounded by a Zb AlGaAs shell. The Mx structure is completed by Zb layers at the top and at the bottom.

III. Results

We plot in Figure 2 the conduction (E_c) and valence (E_v) band along the z direction for Zb and Mx structures.

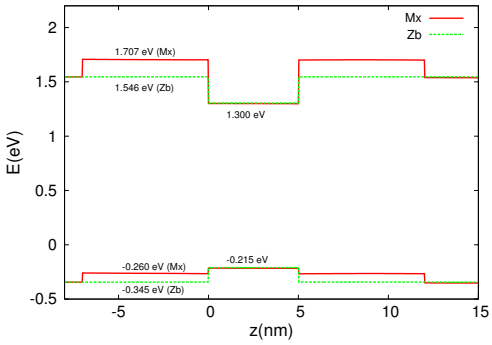

Fig. 2: Conduction (top) and valence (bottom) band along the z direction for both the Zb and the Mx cases Energy in eV, where the 0 is given by the Fermi level.

Besides the usual case of a Zb QD embedded in a Zb matrix, we notice for the Mx conduction band, the well of the QD is surrounded by the energetically higher barrier of the Wz layers. This results in an increased quantum confinement for the electron states. The hole bands of the Mx structure exhibit a sort of double well given by the potential profile of the QD and the two adjacent Wz layers, which act as a second wider well, able to contain several confined states.

In Figure 3 we plot all the confined states for the electrons and the holes for both Zb and Mx situations. The main

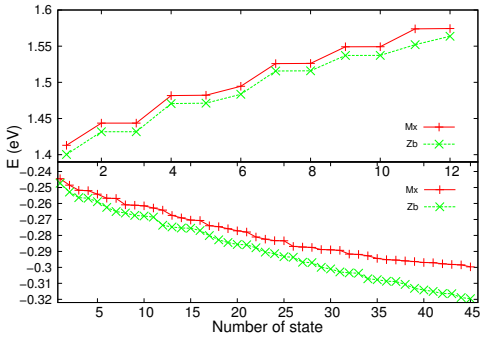

Fig. 3: The calculated states for electrons (top) and holes (bottom). The x scales enumerates the number of the correspondent state (different scale for electrons and holes). The energy in the y axis is referred to the Fermi level as in Figure 2.

difference we observe between the Zb case and the Mx case for the electron states is a higher degree of quantum confinement in the latter, which slightly increases the energy

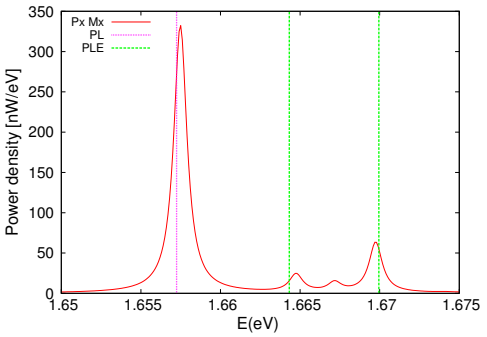

Fig. 4: Oscillator strengths in x directions for the Mx model compared with the positions of experimental transition results: time resolved photoluminescence (PL) for the first transition, photoluminescence excitation (PLE) for the second and third ones.

levels. Concerning the holes, the higher energy states (in absolute value) display different trends. The states of the Mx model are systematically lower in energy, and the onset of this change corresponds to states that start to delocalize in the Wz layers, adjacent to the QD.

In Figure 4, the lowest range of the Mx simulated spectrum is compared with the positions of three peaks given by experimental results from a specific nanowire sample with approximately the same dimensions of our model. Despite the fluctuations of measurement data from different samples, which cannot completely validated the model, the agreement for this particular sample is very good.

References

[1] T. Bryllert, L.E. Wernersson, T. Lowgren, and L. Samuelson, Nanotechnology 17, S227 (2006).
[2] S. Gradecak, F. Qian, Y. Li, H.G. Park, and C.M. Lieber, Appl. Phys. Lett. 87, 173111 (2005).
[3] V.G. Dubrovskii, G.E. Cirlin, I.P. Soshnikov, A.A. Tonkikh, N.V. Sibirev, Yu.B. Samsonenko, and V.M. Ustinov, Phys. Rev. B71, 205325 (2005).
[4] Joël Bleuse, Julien Claudon, Megan Creasey, Nitin S. Malik, Jean-Michel Gérard, Ivan Maksymov, Jean-Paul Hugonin, Philippe Lalanne, Phys.Rev.Lett. 106, 103601 (2011).
[5] D. Spirkoska,J. Arbiol, A. Gustafsson, S. Conesa-Boj, F. Glas, I. Zardo, M. Heigoldt, M. H. Gass, A. L. Bleloch, S. Estrade, M. Kaniber, J. Rossler, F. Peiro, J. R. Morante, G. Abstreiter, L. Samuelson, and A. Fontcuberta i Morrall, Phys. Rev. B 80, 245325 (2009).
[6] V.N. Kats, V.P. Kochereshko, A.V. Platonov, T.V. Chizhova, G.E. Cirlin, A.D. Bouravleuv, Yu.B. Samsonenko, I.P. Soshnikov, E.V. Ubyivovk, J. Bleuse, and H. Mariette, Semicond. Sci. Technol. 27, 015009 (2012).
[7] Z. Zanolli, F. Fuchs, J. Furthmüller, U. von Barth, and F. Bechstedt, Phys. Rev. B 75, 245121 (2007).
[8] A. De and Craig E. Pryor, Phys. Rev. B 81, 155210 (2010).
[9] J.-M. Jancu, K. Gauthron, L. Largeau, G. Patriarche, J.-C. Harmand, and P. Voisin, Appl. Phys. Lett. 97, 041910 (2010).
[10] L. C. Lew Yan Voon and M. Willatzen, *The $k \cdot p$ Method: Electronic Properties of Semiconductors*, Springer (2009).
[11] D. Barettin, S. Madsen, B. Lassen, and M. Willatzen, *Commun. Comput. Phys.*, 11, 797-830 (2012).
[12] S. L. Chuang and C. S. Chang, Phys. Rev. B, 54, 2491 (1996).
[13] R. M. Martin, Phys. Rev. B 6, 4546 (1972).
[14] A. F. Wright, J. Appl. Phys. 82, 6, (1997).
[15] D. Barettin, A. V. Platonov, A. Pecchia, V. N. Kats, G. E. Cirlin, I. P. Soshnikov, A. D. Bouravleuv, L. Besombes, H. Mariette, M. Auf der Maur, A. Di Carlo, IEEE Journal of Selected Topics in Quantum Electronics, Volume: PP, Issue: 99 Page(s): 1.