

# Non-linear optical properties of InGaAs/AlGaAs nanostructures grown on (N11) surfaces

M Povolotskyi<sup>1</sup>, J Gleize<sup>1</sup>, A Di Carlo<sup>1</sup>, P Lugli<sup>1</sup>, S Birner<sup>2</sup>, P Vogl<sup>2</sup>, D Alderighi<sup>3</sup>, M Gurioli<sup>3</sup>, A Vinattieri<sup>3</sup>, M Colocci<sup>3</sup>, S Sanguinetti<sup>4</sup> and R Nötzel<sup>5</sup>

<sup>1</sup> INFN-Università di Roma 'Tor Vergata', via del Politecnico 1, 00133 Rome, Italy

<sup>2</sup> Walter Schottky Institute, Am Coulombwall 3, D-85748, Garching, Germany

<sup>3</sup> LENS-INFN-Università di Firenze, Via Sansone 1, 50019, Sesto Fiorentino, Italy

<sup>4</sup> INFN-Università Milano Bicocca, Via Cozzi 53, 20125, Milano, Italy

<sup>5</sup> eITT/COBRA Inter-University Research Institute, Eindhoven University of Technology, 5600 MB Eindhoven, The Netherlands

E-mail: dicarlo@ing.uniroma2.it

Received 28 July 2003

Published 10 March 2004

Online at [stacks.iop.org/SST/19/S351](http://stacks.iop.org/SST/19/S351) (DOI: 10.1088/0268-1242/19/4/116)

## Abstract

We report on experimental and theoretical study of GaAs/InGaAs quantum systems grown along the [N11] direction. Time-resolved photoluminescence measurements have revealed a strong non-linear optical response from a sidewall quantum wire. The experimental results were reproduced by theoretical calculations taking into account strain, piezo-charge and excitonic effect. Also we theoretically investigated the effect of strain and piezo-charge on the properties of a quantum dot.

## 1. Introduction

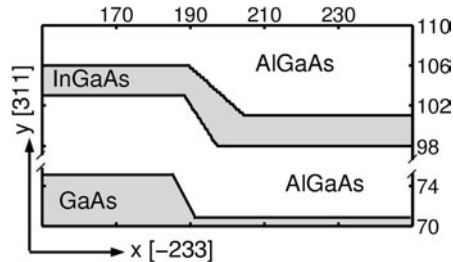
Semiconductor low-dimensional heterostructures are widely used nowadays in electronic and optoelectronic devices [1]. A number of photoluminescence (PL) studies were performed over InGaAs/GaAs quantum wells, wires and dots (QWs, QWRs and QDs) [2, 3] grown on (N11) substrates. These structures are very attractive because of the significant piezoelectric field, which is induced in such oriented systems due to the non-zero shear strain. Theoretical studies of QDs and QWRs were performed in the framework of the envelope function approximations [4], as well as in more refined approaches [5].

In this paper we focus on the influence of strain and piezo-electric fields on the optical properties of (N11) oriented QWRs and QDs. The paper is organized as follows: in section 2 we demonstrate the experimental results that show an optical non-linearity of a QWR. These results are reproduced by means of a theoretical model. In section 3 we theoretically investigate similar effects in a QD. The last section summarizes our results.

## 2. Optical non-linearity of a quantum wire

We investigated an  $\text{In}_{0.2}\text{Ga}_{0.8}\text{As}$  QWR grown on a (311)A oriented GaAs substrate. Similar QWRs were successfully grown and investigated experimentally [2]. Indeed, the growth of an  $\text{In}_{0.2}\text{Ga}_{0.8}\text{As}$  quantum well, surrounded by  $\text{Al}_{0.5}\text{Ga}_{0.5}\text{As}$  barriers, can be performed on a patterned GaAs substrate, allowing for the appearance of a QWR region near the step on the substrate, as shown in figure 1.

Time-resolved photoluminescence (TRPL) measurements were performed on the QWR sample. Details about the experimental set-up can be found elsewhere [6]. The obtained time-dependent spectrum has revealed two contributions that we attribute to the PL of a QW (higher energies) and a QWR (lower energies). For the short delays (less than 300 ps) both spectra are very broadened and overlap. Due to the band filling at such time delays the PL peak energy is higher than the fundamental transition energy. For the longer delays the two PL signals are spectrally separated and the peak energy is considered to be equal to the fundamental transition energy. Yet the transition energy continues to decrease because the photo-induced charge carriers screen the built-in electric field and reduce the Stark effect. The evolution of the transition



**Figure 1.** Schematic drawing of the QWR.

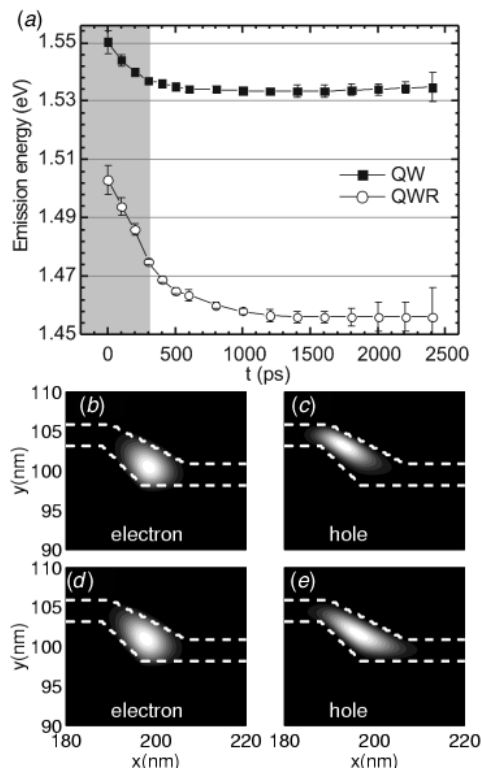
energy is shown in figure 2(a). In our QWR structure built-in electric fields originate mainly from a piezo-electric effect which occurs in strained zinc-blende materials grown on (N11) surfaces.

In order to reproduce the decrease of the transition energy in a QWR, we calculated the strain distribution and the piezo-electric field by means of the macroscopic continuous medium theory [7, 8, 10]. In order to specify the sign of the field one has to take into account the substrate termination. Namely, if the GaAs terminates with a gallium plane (A-type) then the electric field in the quantum well is collinear with the growth direction. In the other case (B-type) the field changes its direction to the opposite. In order to get the atomic equilibrium positions in a strained lattice we first consider the macroscopic deformation of the unit cells, and then take into account the internal strain to obtain equilibrium atomic positions inside the cell [5]. Here we made use of an analogy between a frozen optical phonon and the internal strain displacements [11].

We calculated the fundamental electronic transition energies within the empirical tight-binding (ETB) approach [12], using the  $sp^3s^*d^5$  ETB parametrization derived by Jancu *et al*, for interactions between the nearest neighbours in the supercell [13]. Following these authors, we included strain effects by scaling the ETB parameters with respect to the cation–anion bond length, according to Harrison’s rule. A precise description of the electronic energies of our systems also requires a relative offset between the valence bands of all the quantum regions included in the supercell. We included this in our simulation by shifting the on-site ETB parameters according to theoretical values of these offsets for bulk materials [14, 15]. We note here that these offsets are only an approximation, as they were calculated for strained layers grown on (001) GaAs. Finally, the dangling bonds on the surfaces of the supercell are saturated, in order to avoid the appearance of surface states inside the gap of heterostructure.

We also calculated the fundamental transition energy and the exciton binding energy in the effective mass approximation (EMA). We considered the heavy holes only, with an anisotropic effective mass that depends on strain. The strain-induced shift of the conduction band depends only on the hydrostatic part of the strain:  $\delta E_c = -a_c \text{Tr}(\varepsilon_{ij})$ . Band shift and effective mass tensor for the heavy hole band were obtained from the Bir–Pikus  $\mathbf{k}\cdot\mathbf{p}$  Hamiltonian [16].

In this paper, we focus on the two opposite cases, namely if the piezo-electric field is totally screened because of the high concentration of photo-induced carriers, and if the concentration is very low so that the field is not screened at all. We consider the exciton effect only for the case when the concentration of the free carriers is negligible. The obtained



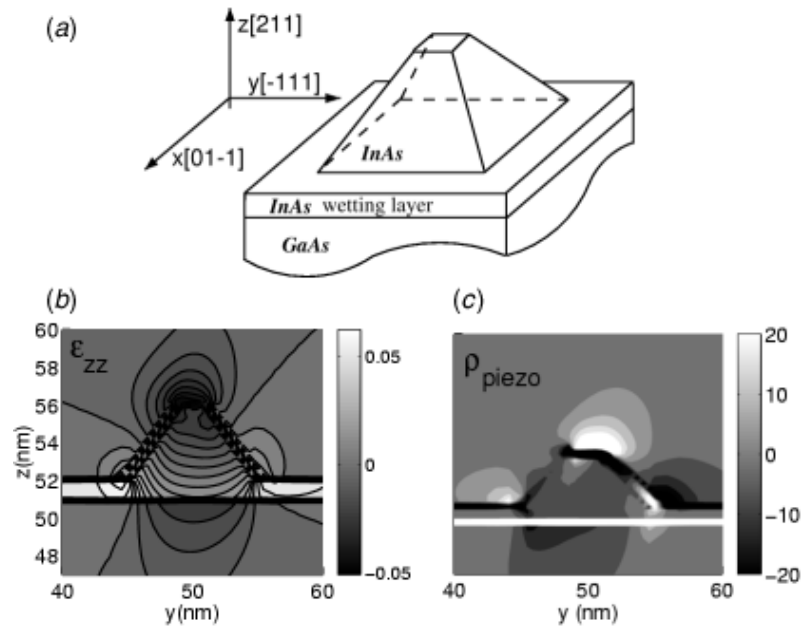
**Figure 2.** (a) PL peak energies with respect to the time delay after the excitation pulse. The time domain, where carrier concentration is very high (band filling regime) is depicted with a grey colour. (b)–(e) Squared modulus of the single-particle wavefunction for the ground state of electron and hole. (b) and (c) correspond to the case when the field is not screened. (d) and (e) correspond to the case of full field screening. In (b)–(e) the dashed lines indicate the barrier interfaces.

results show that even in the absence of the piezo-electric field the electron and hole wavefunctions are spatially separated (see figures 2(b) and (c)). A piezo-electric field in our case can enlarge the separation between electron and hole (see figures 2(d) and (e)), resulting in the lowering of the transition energy. Besides, if the concentration of the photo-induced carriers is low, the transition energy gets smaller due to the exciton effect.

The transition energy, calculated in the framework of EMA without considering the exciton effect, decreases from 1.477 eV down to 1.468 eV. If we take into account the exciton effect then it decreases down to 1.457 eV. These results agree with the QWR peak energy evolution starting from 300 ps up to 2500 ps. Microscopic ETB description without considering excitonic effects predicts higher values for the transition energy, namely from 1.596 eV down to 1.585 eV. We attribute such discrepancy to the value of the band offset between strained InGaAs and GaAs, that needs to be refined for the case of [N11] growth direction. Interestingly, if one neglects internal strain then values become even higher, namely 1.614 eV and 1.603 eV, so the information about atomic positions is very important.

### 3. Theoretical study of a quantum dot

The same optical effect as described in section 2 can occur in QDs [3]. We consider a ‘model’ shape of the QD



**Figure 3.** (a) Schematic plot of the quantum dot. (b) Contour plot of the strain tensor component  $\varepsilon_{zz}$  in the dot cross section parallel to the  $x$ -axis. (c) Piezo-charge density distribution in the same coordinates as in (b). The units of the colour bar are  $10^{18} \text{ e cm}^{-3}$ .

(see figure 3(a)): a truncated InAs pyramid a height of 4 nm and two square bases lies on the InAs wetting layer of 1 nm thickness. The pyramid bases have size  $10 \times 10 \text{ nm}^2$  and  $2 \times 2 \text{ nm}^2$ , respectively. The structure is grown on a thick (211) oriented GaAs substrate. We calculated the strain distribution and the corresponding piezo-electric polarization that occur due to the lattice mismatch. Here we consider both cases of A and B substrate type. Our calculations reveal a non-symmetric character of the strain distribution in the QD (figure 3(b)), due to the fact that the growth direction [211] does not coincide with a symmetry axis of a zinc-blende crystal. Hence, even without a piezo-electric field the electron and hole are spatially separated due to the strain. Depending on the substrate termination type, the piezo-electric field can enlarge or reduce this separation.

In order to estimate the role of the piezo-electric effect we calculated the fundamental transition energies using EMA, described in section 2. These energies for A-type and B-type substrates are equal to  $E_A = 1.244 \text{ eV}$  and  $E_B = 1.232 \text{ eV}$ , respectively. If we assume that the piezo-electric field is screened then the transition energy is equal to 1.241 eV, that is between  $E_A$  and  $E_B$ . Due to the simplified description of a dot geometry our study does not pretend to be a complete description of the QD properties, but rather shows the importance of the piezo-electric field consideration.

#### 4. Conclusions

In this paper we demonstrated experimental results that show non-linear optical properties of nanostructures grown on (N11)

oriented substrates. Theoretical simulations were performed both in ETB and in the effective mass approximation. The results show the possibility of a detailed microscopic description of the structures. Future work will include a microscopic model of elastic deformation and excitonic effect.

#### References

- [1] Alferov Z I 2001 *Rev. Mod. Phys.* **73** 767
- [2] Nötzel R, Ramsteiner M, Niu Z, Schönherr H-P, Däweritz L and Ploog K H 1997 *Appl. Phys. Lett.* **70** 1578
- [3] Sanguinetti S, Gurioli M, Grilli E, Guzzi M and Henini M 2000 *Appl. Phys. Lett.* **77** 2979
- [4] Stier O, Grundmann M and Bimberg D 1998 *Phys. Rev. B* **59** 5688
- [5] Di Carlo A 2003 *Semicond. Sci. Technol.* **18** R1
- [6] Alderighi D, Zamfirescu M, Gurioli M, Vinattieri A, Colocci M, Sanguinetti S, Di Carlo A, Povolotskiy M and Nötzel R 2003 *Phys. Status Solidi* **0** 1433
- [7] Pryor C, Pistol M-E and Samuelson L 1997 *Phys. Rev. B* **56** 10404
- [8] Jogai B 2000 *J. Appl. Phys.* **88** 302
- [9] De Caro L and Tapfer L 1993 *Phys. Rev. B* **48** 2298
- [10] Nextnano<sup>3</sup> device simulation package, see web site <http://www.nextnano.de>
- [11] Anastassakis E and Cardona M 1981 *Phys. Status Solidi B* **104** 589
- [12] Slater J C and Koster G F 1954 *Phys. Rev.* **94** 1498
- [13] Jancu J M, Scholtz R, Beltram F and Bassani F 1998 *Phys. Rev. B* **57** 6493
- [14] Vurgaftman I, Meyer J R and Ram-Mohan L R 2001 *J. Appl. Phys.* **89** 5815
- [15] Wei S H and Zunger A 2001 *Appl. Phys. Lett.* **72** 2011
- [16] Chao C Y-P and Chuang S L 1992 *Phys. Rev. B* **46** 4110